FACSS Presents

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National Meeting of: Society for Applied Spectroscopy (SAS)

15

North American Society for Laser-Induced Breakdown Spectroscopy (NASLIBS)

FINAL PROGRAM

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SEPTEMBER 27 - OCTOBER 2 PROVIDENCE, RI

scixconference.org / facss.org

Providence,

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MEMBERSHIP

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 - Collection of tutorial and plenary lectures





www.asms.org

Attention Presenters: Check this final program to verify the schedule of your talk or poster. Changes may have occurred since the preliminary program.

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SciX Conference and FACSS International Office

2019 Galisteo Street, Building I-1, Santa Fe, NM 87505 (505) 820-1653 O (505) 820-1648 O facss@facss.org O www.scixconference.org O www.facss.org On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) it is our pleasure to welcome you to Providence for SciX 2015. If you had the pleasure of attending SciX last year in Reno, you know that FACSS has launched into its fourth decade of sponsoring a conference dedicated to promoting analytical chemistry and spectroscopy. This marks the fourth year of the conference presented as SciX - the great **Sci**entific e**X**change, which was launched in Reno in 2011. We now have 12 member organizations of FACSS, and they strive to bring the highest quality science together in one meeting. From the beginning, the Federation understood that best science evolves and develops from networking and stimulating conversations with colleagues. As a result, not only is the most relevant and cutting edge research presented year after year, but the scientific community has blossomed due to the cultivation of relationships, collaborations and friendships at the conference.

The central focus of the meeting is the technical program, which is spearheaded by the Program Chair, Glen Jackson. The New England area provided significant inspiration for the program, including the Sunday Keynote speaker Mr. Rob Munier, Vice President for Marine Facilities and Operations at Woods Hole Oceanographic Institute (WHOI). The program also features additional mass spectrometry and forensic sessions, including the Monday morning Plenary lecture by Dr. Chris Palenik, Vice President and Senior Microscopist at Microtrace LLC. A dominant feature of every SciX program is the celebration of awards and top-quality award sessions presented by FACSS member organizations during the week. Award sessions include the FACSS Charles Mann Award (Sanford Asher), the ANACHEM Award (Jonathan Sweedler), the Lester W. Strock Award (Kenneth Marcus), the Applied Spectroscopy William F. Meggers Award (Eric Brauns), the Coblentz Society Craver Award (Ji-Xin Cheng), the ACS Spectrochemical Award Winner (Frank Bright), the AES Mid-Career Award (Adam Woolley) and the Bruce Kowalski Award in Chemometrics (Thomas Bocklitz).

Throughout the meeting you will find quality presentations by aspiring students, hardworking young professionals and seasoned scientists. Poster presentations at SciX provide a casual venue to discuss cutting edge scientific results, while student presenters are also vying for daily poster awards. The section chairs and session chairs provide valuable scientific contributions , which involve the thoughtful construction of a coherent and balanced program with a blend of experienced luminaries and up-and-coming scientists in each session. The chairs also work hard to secure financial support from our supporting industrial partners, whom are essential to the success of the program. We are pleased to celebrate a lifetime of atomic-spectroscopy-contributions of Prof. Ed. Steers on Wednesday afternoon, and to honor the finalists in the competitive FACSS Innovation Award session on Thursday afternoon. We close out the diverse technical program with a trans-spectral celebration of spectroscopy and the United Nations Year of Light with world-renown experts in their respective areas: Prof. Christoph Rose-Petruck of Brown University (X-rays), Prof. Igor Lednev, SUNY Albany (Raman), Prof. Peter Griffiths, U. Idaho (IR/Near IR) and Prof. Richard Temkin, MIT (THz).

SciX 2015 is the National Meeting for the Society for Applied Spectroscopy and the North American Society for Laser-Induced Breakdown Spectroscopy. SciX 2015 boasts a large number of networking opportunities including, but not limited to: The SAS Student Poster session and opening mixer on Sunday evening, the Exhibit Hall opening on Monday, the SAS members-only Wine and Cheese Awards reception, and the Wednesday night all-inclusive event in the theme of the Great Gatsby. As you settle into your accommodations, if you have a smart phone or tablet device, please take advantage of the free SciX app to map out your week's schedule. It is our hope that you leave SciX 2015 brimming with new research ideas, collaborative networks and knowledge of the most cutting edge science going on internationally.

On a final note, it is important to remember that SciX and FACSS are run by the consensus of the 12 non-profit member societies – by scientists, for scientists. Planning for each conference starts years in advance, takes thousands of emails and hours of conversations, and an immeasurable number of volunteered hours by section and session chairs. Each year, we rely on dozens of experienced colleagues to help judge posters and select award winners. We count on people like you to get involved. So think about what you can do to contribute to future meetings. The volunteer SciX 2015 team and the FACSS Executive Committee are grateful for the unwavering support at the FACSS / SciX International Office – Cindi Lilly and Marin Walker. Both of these women contribute to the success of the SciX meeting and the Federation by accomplishing much of the behind the scenes labor to make everything run without a hiccup.

We hope you enjoy SciX 2015. With an exceptional program, world-class plenary lectures, awards symposia, poster sessions, networking events, an extensive exhibition, all in a beautiful New-England city of Rhode Island, we're confident that this conference will leave a lasting impression on attendees!

Edita Botonjic-Sehic, Morpho Detection - SciX General Chair 2015 Glen P. Jackson, West Virginia University – SciX Program Chair 2015 Mike Carrabba, Hach – SciX Exhibits Chair 2006 - 2017 Mark Henson, Shire Pharmaceutical – SciX Workshop Chair Heather Brooke, CAMO Software, Inc. – SciX Workshops Chair John Wasylyk, Bristol-Myers Squibb – SciX / FACSS Marketing Chair 2014-2016 Greg Klunder, Lawrence Livermore National Laboratory, Governing Board Chair, 2014-2015 GENERAL INFORMATION

LOCATION. All plenaries, symposia, and the exhibits are located at the Rhode Island Convention Center. Workshops will be held at the Omni Hotel adjacent to the convention center.

SPEAKERS. There will be an LCD projector for each symposium. Speakers must supply their own computer with their presentation. Please arrive 30 minutes before your session begins. Each speaker should adhere to the time allotted for the talk.

POSTER SESSIONS.

Sunday SAS Sponsored Student Poster Session, Ballroom A 7:15 – 9:15 pm SAS Poster Session and SciX Welcome Mixer

Monday Poster Session – Ballroom A

Set up posters between 7:00 - 8:00 am and remove by 5:00 pm 9:00 - 10:20 am - Poster Session

3:00 - 3:50 pm - Poster viewing and break

Tuesday and Wednesday Poster Sessions – *Exhibit Hall C/D* Posters remain up all day on their designated day. Set up posters between 7:30 - 8:00 am and remove Tuesday posters by 4:30 pm and Wednesday posters by 3:50 pm.

9:00 - 10:20 am - Poster Session

3:00 - 3:50 pm - Poster viewing and dessert break

Thursday Poster Session – Ballroom A

Posters remain up all day. Set up posters between 7:00 - 8:00 am and remove at 3:50 pm

9:00 - 10:20 am - Poster Session

3:00 - 3:50 pm - Poster viewing and break

WORKSHOPS. A list of workshop, descriptions, and the locations begins on page 42. You must register for a SciX workshop at the conference registration desk

EMPLOYMENT BUREAU/ INTERNET CAFE. Available in the west pre-function conference registration area. See page 4 for additional information.

EXHIBITS. The exhibition is located in Exhibit Hall C/D and will be open as follows. See page 31 for details.

WHAT'S HOT VENDOR PRE	SENTATIONS.
Wednesday	9:00 am – 4:00 pm
Tuesday	9:00 am – 4:30 pm
Monday (Opening Reception	n) 5:30 pm – 7:30 pm

Sunday, 4:10 – 6:00 pm, *Ballroom B/C* Tuesday, 11:40 am – 1:10 pm, *Exhibit Hall C/D* Wednesday, 11:40 am – 1:10 pm, *Exhibit Hall C/D*

BREAKS. A complimentary lunch will be served at noon in the exhibit hall on Tuesday and Wednesday for all registered conferees.

Monday and Thursday morning and afternoon break.

11:00 am – 12:00 pm & 3:00 – 3:50 pm – *Ballroom A*

Tuesday and Wednesday morning and afternoon break.

11:00 am – 12:00 pm & 3:00 – 3:50 pm – *Exhibit Hall C/D* INTERNET ACCESS. Complimentary wireless internet access will

be available.

REGULATIONS AND CODE OF CONDUCT. The following regulations are in the best interest of the conference.

1. There is no smoking in any conference areas.

2. An official name badge is required at all times.

3. No advertising may be placed in the conference area.

4. Only official exhibitors may display in the Exhibit Hall.

5. No distribution of product/meeting literature in sessions.

6. No Photography of PowerPoint Lectures or Posters

7. Be respectful and considerate of others and the facilities.

8. Harassment, intimidation or discrimination in any form will not be tolerated.

COMPANION REGISTRATION. Does not include access to symposia. Cost is \$75 and includes the following: **Sunday** - Evening Welcome Mixer. **Monday** - coffee/pastries 9:00 am and Exhibit Hall Opening Reception. **Wednesday** – Conference Evening Event *Future Meeting: September 18 – 23, 2016, Minneapolis, MN*

 SPECIAL EVENTS. Events below will be held in convention center

 SUNDAY

 6:15 pm

 SciX 2015 Welcome. Edita Botonjic-Sehic

 Keynote Lecture. Pre-adaptation: How Basic

 Research Helps Oceanographers Meet Global

 Challenges; Robert S. C. Munier, Woods Hole

 Oceanographic Institute. Ballroom B/C

7:15 – 9:15 pm Welcome Mixer and SAS Sponsored Student Poster Session. SAS, Coblentz, and FACSS Student Award Presentations, *Ballroom A*

MONDAY

7:50 am **Opening Address.** *Ballroom B/C*

- 8:00 am Keynote Lecture. Forensic Microscopy and the Lost Art of Observation; Chris Palenik, Microtrace LLC, *Ballroom B/C*
 - Noon Coblentz and SAS Speed Mentoring Session, Rotunda

Noon Coblentz Challenge, 558B

- 5:30 7:30 pm **Reception for Exhibit Opening** (wine, beer, light hors d'ouvres) *Exhibit Hall C/D*
 - 7:30 pm NASLIBS and SAS Sponsored Reception, *Room Rotunda*. All conferees are invited.

TUESDAY

- 8:00 am Coblentz Society Craver Award. Vibrational Spectroscopic Imaging of Living Systems: Emerging Platform for Biology and Medicine; Ji-Xin Cheng, Purdue University, *Ballroom B/C*
- 8:30 am FACSS Charles Mann Award for Applied Raman Spectroscopy. UV Resonance Raman Spectroscopic Studies of Protein Structure and Dynamics; Sanford Asher, University of Pittsburgh, Ballroom B/C
- 12:00 pm Complimentary lunch in the Exhibit Hall.
- 6:00 pm Raman Reception. Ballroom B/C
- 7:30 pm Society for Applied Spectroscopy Wine and Cheese Awards Reception. *Ballroom A*

WEDNESDAY

- 8:00 am SAS's Lester W. Strock Award. Sampling Atmospheric Pressure Glow Discharge Microplasmas: Evolving towards Versatility, Practicality, and Transportability; R. Kenneth Marcus, Clemson University, *Ballroom B/C*
- 8:30 am Applied Spectroscopy William F. Meggers Award. Mid-Infrared Diffuse Reflection on Ultrafast Time Scales; Eric Brauns, University of Idaho, *Ballroom B/C*

12:00 pm Complimentary lunch in the Exhibit Hall.

6:00 pm Wednesday Evening All Inclusive Event

THURSDAY

- 8:00 am ANACHEM Award. Mass Spectrometry Tools for Probing Cell to Cell Chemical Heterogeneity; Jonathan Sweedler, University of Illinois, Ballroom B/C
- 8:30 am AES Mid Career Award. Microchip Electrophoresis: A Mid-Career Method?; Adam Woolley, Brigham Young University, Ballroom B/C

3:50 pm Plenary Session, Ballroom B/C FACSS Distinguished Service Awards FACSS Innovation Award Session

FRIDAY

8:00 am Special Plenary Session. Room 555-556 Announcement of Innovation Award A Trans-Spectral Celebration of the International Year of Light Preview of 2016 Conference

EVENTS OF SPECIAL INTEREST TO STUDENTS

SUNDAY EVENING, Ballroom A

- Welcome Mixer: 7:15 9:15 pm
- SAS Sponsored Poster Session: 7:15 9:15 pm
 - SAS and Coblentz Student Award presentations
 - FACSS Student Award and Tomas Hirschfeld Scholar Award presentations

MONDAY through THURSDAY

• FACSS Student Poster Awards will be presented daily

MONDAY through THURSDAY

• Employment Bureau (Monday through Thursday), Registration Area

WEDNESDAY WORKSHOP

• 9:00 am - 3:00 pm. Professional Analytical Chemists in Industry: What Does an Analytical Chemist Do?

This seminar begins with a discussion of the education requirements and salaries that an analytical chemist may expect in industry. The different roles (including scientific consultant, methods development and problem solver) of the industrial analytical chemists are explained. A majority of time is spent on problem solving, both the process and solving real-world problems. Students will learn a "framework" for approaching problems. Time will be available to ask questions on these topics and other related subject. The course text includes supplementary material on finding a job, summer employment, etc. The entire course, especially the problem solving, is participation structured for extensive and interaction. Additional information available is at http://www.pg.com/science/prof chemists.jhtml. The course is intended primarily for undergraduate students to educate them about careers as analytical chemists in industry. However, graduate students, high school teachers, and college faculty have indicated it was worth their time to attend. Instructor: Diane Parry, Procter and Gamble.

EMPLOYMENT BUREAU

The Employment Bureau is located in the Registration Area in conjunction with the internet café Monday through Thursday

EMPLOYERS: Bring either hard copy or electronic copy of job opportunities and display on poster board in the employment area. There will be copies of resumes for you to review or to take with you.

JOB SEEKERS: Bring copies of your resume to be made available for prospected employers to review.

A message board will be available for employers and job seekers to communicate.

FACSS and SciX CONFERENCE ORGANIZATION

MEMBER ORGANIZATIONS OF FACSS

American Chemical Society, Division of Analytical Chemistry AES Electrophoresis Society American Society for Mass Spectrometry ANACHEM The Coblentz Society Council for Near Infrared Spectroscopy The Infrared and Raman Discussion Group International Society of Automation-Analysis Division North American Society for Laser-Induced Breakdown Spectroscopy Royal Society of Chemistry Analytical Division Society for Applied Spectroscopy The Spectroscopical Society of Japan

SciX is the Annual North American Meeting of FACSS National Meeting of: Society for Applied Spectroscopy North American Society for Laser-Induced Breakdown Spectroscopy

2015 SciX Conference Chair Persons

General Chair	Edita Botonjic-Sehic, Morpho Detection
	Email: ebontonji@morphodetection.com
Program Chair	Glen P. Jackson, West Virginia University
	Email: glen.jackson@mail.wvu.edu
Exhibit Chair	Mike Carrabba, Hach Company
	Email: mcarrabba@hach.com
Workshop Chair	Heather Brooke, CAMO Software, Inc. and Mark Henson, Shire
Marketing Chair	John Wasylyk, Bristol-Myers Squibb
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2015 Program Section Chairs

2013 11051	In Section Chan's
Atomic Spectroscopy	Jorge Pisonero, Universidad de Oviedo
Awards	Alexandra Ros, Arizona State University
Biomedical and Bioanalytical	Karen Esmonde-White, University of Michigan
Chemometrics	Peter Harrington, Ohio University
Electrophoresis	Edgar Goluch, Northeastern University and Ryan Kelly, PNNL
Laser-Induced Breakdown Spectroscopy	Mattheiu Baudelett, University of Central Florida and Amy Bauer, TSI
Mass Spectrometry	Glen P. Jackson, West Virginia University and Rebecca Jockush, University of Toronto
Molecular Spectroscopy	Curt Marcott, Light Light Solutions and University of Delaware
Pharmaceutical Analysis	Rina Dukor, BioTools, Inc. and John Wasylyk, Bristol-Myers Squibb
Process Analytical Technology	James Rydzak, GlaxoSmithKline
Raman Spectroscopy	Duncan Graham , University of Strathclyde; Ian R. Lewis , Kaiser Optical Systems; and Pavel Matousek , Rutherford Appleton Laboratory
Security and Forensics	Greg Klunder , <i>Lawrence Livermore National Laboratory</i> and Guido Verbeck , <i>University of North Texas</i>
Surface Plasmon Resonance	Jean-Francois Masson, Université de Montreal
Surface Science	Kateryna Artyushkova, University of New Mexico

2015 FACSS Executive Committee

Greg Klunder, <i>LLNL – Forensic Science Center</i>
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Steven Ray, Indiana University
Ian R. Lewis, Kaiser Optical Systems, Inc.
S. Douglass Gilman, Louisiana State University
Christopher Palmer, University of Montana
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GENERAL CHAIR, SciX



Edita Botonjic-Sehic Morpho Dtection LLC

Dr. Edita Botonjic-Sehic has completed her Bachelor in chemistry and mathematics from Assumption College in Worcester MA. She continued on to receive her PhD in analytical chemistry/spectroscopy from the University of Rhode Island under supervision of Dr. Christopher W. Brown. During her study at the URI she worked at Digilab, LLC as an application intern. Upon completion of her studies Edita worked as an application scientist at Axsun Technologies (Billerica, MA) in development of miniature NIR spectrometers. Then she went on to work for GlaxoSmithKline (King of Prussia, PA) as a principal scientist to work in research and development and in the implementation of process analytical technology (PAT). Her experience at GSK gave her an opportunity to be a lead principal scientist for the implementation of PAT in manufacturing at Barr Pharmaceuticals/TEVA Phamraceuticals (Pomona, NY) on commercial products. Edita has now returned to the Boston area where she is at Morpho Detection LLC, Safran Group as Sr. Engneering Program Manger R&D leading the development of different technologies (Andover, MA).

Dr. Botonjic-Schic has authored and coauthored number of publications and more than 50 presentations. She belongs to several professions organizations, including Coblenz, and SAS. She is currently the general chair for SciX 2015 in Providence, RI. She has served as a section chair for PAT at SciX for over 5 years.

PROGRAM CHAIR, SciX



Glen P. Jackson *West Virginia University*

Dr. Jackson joined the faculty of WVU in the fall of 2012 as a Ming Hsieh Distinguished Professor of Forensic and Investigative Science. He also holds appointments in Biology and the C. Eugene Bennett Department of Chemistry. Before moving to WVU, he was an Associate Professor of Chemistry and Director of the Forensic Chemistry Program at Ohio University. His PhD research involved the development of pulsed glow discharges through a variety of fundamental spectroscopic studies. His current research in mass spectrometry instrumentation development and forensic applications has been funded through DOE, NIJ, NSF, and NIH, in addition to an NSF CAREER Award in 2007.

Dr. Jackson is the author or coauthor on two patents, more than 50 publications and more than 100 presentations. He belongs to several professional organizations, including the ACS, RSC, ASMS, AAFS, FIRMS and SAS. He is currently the program chair for SciX 2015 in Providence, RI, and chair of the Forensic and Security Interest Group at ASMS 2015. He was program chair for the 2015 ASMS Sanibel conference on Forensic and Security Applications of Mass Spectrometry. He has served as a grant reviewer for NSF, NIH, DOE and NASA and has reviewed manuscripts for more than a dozen different analytical journals. He is a member of the NIST OSAC subcommittee on Seized Drugs, has taught several forensic related mass spectrometry workshops, and is an active forensic chemistry consultant.

SciX / FACSS CHAIRS

EXHIBITS CHAIR, SciX



Mike Carrabba Hach Company

Dr. Mike Carrabba joined the Hach Company in 2004 as the Director of Hach Homeland Security Air Systems and he is currently the Global Director of Open Innovation where he has the responsibility of finding and developing relationships for new and emerging technologies.

He received his B.S. in Chemistry (magna cum laude) from Salem State College in 1981 and his Ph.D. in Physical Chemistry from Tufts University in 1985. Dr. Carrabba's graduate work was conducted under the tutelage of Dr. Jonathan Kenny and focused on the utilization of laser-induced fluorescence to examine ultracooled gas phase molecules in a supersonic jet molecular beam. After graduate school, Dr. Carrabba joined EIC Laboratories where he eventually became Vice-President for the Spectroscopy Division. He conducted a variety of research programs, including photoelectrochemical etching of semiconductors, fiber optic chemical sensors and state-of-the-art Raman spectroscopy. During this time, he introduced the use of holographic filters for Raman spectroscopy and developed numerous types of field Raman instrumentation and techniques, several of which resulted in U.S. After leaving EIC, he joined Chromex, Inc, a patents. manufacturer of Raman spectroscopy systems, as Marketing Manager and was previously the OEM Division Manager at Jobin Yvon, Inc.

Dr. Carrabba has been very active in the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) over the years. He has served as Governing Board Chair (2002), Program Chair (2000), Program Section Chair for Raman (1992-1999, 2001), Chairperson of the Long Range Planning Committee (1999-2008) and as a member of the Governing Board. Since 2006 he has been serving as the FACSS/SciX Exhibits Chair.

In 2003 Dr. Carrabba received the Award of Merit and became a Fellow of ASTM for his 12 years of service as the Chairman of the ASTM Subcommittee on Raman Spectroscopy. In 2004 he received the FACSS Charles Mann Award for Applied Raman Spectroscopy and in 2007 he received the Williams-Wright Award for Industrial Vibrational Spectroscopy. He has also been honored with the Distinguished Service Awards from FACSS in 2009 and from the Society for Applied Spectroscopy (SAS) in 2011. In 2012, Dr. Carrabba was named a Fellow of the Society for Applied Spectroscopy (SAS). Dr. Carrabba is also member of the Coblentz Society.

GOVERNING BOARD CHAIR, FACSS



Greg Klunder Lawrence Livermore National Laboratory

Greg Klunder is a staff scientist at Lawrence Livermore National Laboratory (LLNL) where he is an active member of the Forensic Science Center involved with a variety of different analytical projects in support of national security. He received a B.S. in Chemistry from Virginia Tech and a Ph.D. from North Carolina State University studying flame spectroscopy under the direction of Dr. Charles Boss. In 1990, he took a post doctoral position at Lawrence Berkeley Laboratory with Dr, Richard Russo and then moved to LLNL where he has been since.

Greg has been a regular attendee at FACSS and SciX since graduate school which has been helpful in providing him with a broad background and understanding of many different analytical techniques. The exposure to the various analytical methods has been directly applied to his career at LLNL where he has been involved in a wide range of projects with diverse applications. Project applications have covered areas including fundamentals, environmental analysis, forensics, national security, and remote The different applications require chemical detection. implementing a variety of analytical methods. To that end, Greg has been involved in a number of different of areas in his research including spectroscopy (fluorescence, photothermal, infrared, near infrared, and terahertz), fiber optic chemical sensors, separations (capillary electrophoresis, TLC, and SPME GC-MS), laser ablation mass spectrometry, thermal analysis, and NMR. His current projects include near-infrared spectroscopic identification of uranium ore concentrates, thermal analysis coupled with IR and MS for explosives characterization and femtosecond laser ablation coupled with ICP-MS.

Outside the lab, Greg enjoys a many activities including, cycling, running, guitar, hiking, camping, skiing and snowshoeing. Greg has 2 very active sons (Will, 11, and David, 10) who keep him busy and he has thoroughly enjoyed being their Little League baseball coach for several years.

PROGRAM and CONFERENCE SPONSORS SciX 2015 and FACSS greatly appreciate the support it receives from its sponsors.

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FACSS AWARDS

DISTINGUISHED SERVICE AWARDS

Awarded to an individual(s) for recognition of exceptional, long-term service to the FACSS organization.

The 2015 recipients have served with excellence in many different capacities and contributed to the continuing success of FACSS through consistent dedication and sacrifice.

Awards will be presented Thursday, 3:50 pm, *Ballroom B/C*

Michael Blades

The University of British Columbia



Michael Blades received his BSc at St. Mary's University (Halifax, Nova Scotia) and a PhD at the University of Alberta in 1980 (under the supervision of Dr. Gary Horlick) working in the area of plasma spectrochemistry. He subsequently went to Indiana University to work as a postdoctoral fellow in the laboratory of Dr. Gary

Hieftje (1980-81). He has been in the Department of Chemistry at The University of British Columbia (UBC) in Vancouver since 1981.

He has published over 140 papers in refereed journals and is a regular invited speaker at international symposia. He has received a number of honours and awards including the 1987 Canadian Society for Chemistry McBryde Medal awarded annually to a young scientist "in recognition of a significant achievement in pure or applied analytical chemistry", a University of British Columbia Killam Research Prize (1988-89), and a Senior Killam Fellowship (1991-92), the Canadian Society for Chemistry 1994 Fisher Lecture Award, the 1995 Royal Society of Chemistry Analytical Spectroscopy Award, and was named a Fellow of the Society for Applied Spectroscopy in 2009. In 1999 he was the General Chair for the annual Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Meeting and in 2004 he served as the Governing Board Chair for FACSS. In addition he is currently the Editor-in-Chief for Applied Spectroscopy.

In his spare time Mike enjoys playing ice hockey and snowboarding in the winter and windsurfing and cycling in the summer.

Gary Brewer

Retired from ABB Process Analytics



Gary Brewer recently retired as a Product Manager from ABB Process Analytics in Lewisburg, WV. Gary spent most of his career working in the area of process analytics. He was with ABB for 26 years starting out as an Application Engineer for their Multiwave Photometer and them later moving to Product Manager Position for the Multiwave Photometer

and Reid Vapor Pressure Analyzer. Gary helped develop many applications for the products in the petrochemical and refinery industries. Prior to joining ABB, he worked for Menardi-Southern in Los Angeles, CA for 6 years as a coatings chemist and manufacturing manager after spending two years as an environmental chemist for General Electric in Lebanon, PA. He got started in process analytics immediately after college working for the Department of Energy near Morgantown, WV on a demonstration project of the first fluidized bed boiler in the power utility industry. Gary has authored or co-authored over 25 papers

- 1993 Edward Brame and Syd Fleming
- 1994 L. Felix Schneider
- 2001 David Coleman
- 2003 Jeanette Grasselli Brown
- 2009 Paul Bourassa and Mike Carrabba

that have been presented at various scientific conferences such as ISA, ISA AD, FACSS, and PittCon.

Gary got his B.S. in Chemistry from Fairmont State College in Fairmont, WV in 1978. He has been active in the ISA Analysis Division for over 30 years and has been the ISA AD delegate to FACSS since 2000. He has been active in FACSS/SciX and has organized several process analytics sessions. He served as the FACSS Governing Chair in 2008 and is currently serving as the Site Selection Committee chairman.

He is married to his wonderful wife Jeannie and has two children – a son Christopher who teaches math at Blacksburg High School in Virginia and a daughter who teaches dance at Bartlett Yancey High School in North Carolina. Christopher and his wife Abbie (also a math teacher) last year blessed us with a wonderful granddaughter Sophia Grace.

Gary plans on enjoying retirement in the Lewisburg, WV area by doing the things he enjoys – fishing, hiking, camping, reading and wood working. He is an avid West Virginia University fan – GO MOUNTAINEERS!!



Keith L. Olson Retired from General Motors Research Laboratories

Keith Olson attended his first FACSS / SciX conference in 1982 when he served as the assistant chair for the Continuing Education Committee. He continued as the FACSS Continuing Education Chair for three years,

from 1983 to 1985. He then served as the FACSS Governing Board Secretary for six years, from 1987 to 1993. During those years the FACSS conference left Philadelphia and resumed a rotation policy that now takes the SciX Conference to locations across North America. During those years the FACSS organization also transitioned from an all-volunteer federation to a management structure that co-operates with and relies on professionals in the FACSS National Office. Keith served on the committee that revised the FACSS bylaws to facilitate the changes.

Over the past decade (2004 - 2015) Keith has been a delegate to the FACSS Governing Board from ANACHEM (The Association of Analytical Chemists). He is currently the president of that regional, Detroit-based society. ANACHEM is proud to present its annual award at the SciX conference. Since 2004 Keith has been actively involved in arranging for the award and the award symposium.

Keith received a Ph.D. in Analytical Chemistry from the University of Illinois, Champaign-Urbana, in 1978. He spent his career as a researcher at the General Motors Research Laboratories in Warren, MI, and retired in 2013. His research focused on the development of chemical analysis methods for vehicle exhaust emissions, fuels, engine oils, coolants, brake fluids, polymer additives, and battery electrolytes. He has been a member of ANACHEM since 1978.

PREVIOUS AWARDEES

- 2010 Scott McGeorge and Alexander Scheeline
- 2011 Jon W. Carnahan and Patricia B. Coleman
- 2012 Bruce Chase and O. Karmie Galle
- 2013 Mark A. Hayes and Cynthia M. Lilly
- 2014 Ron Williams and Edward J. Havlena

FACSS AWARDS

The FACSS Student and the Tomas Hirschfeld Scholar Awards recognize outstanding contributions by individual who are Ph.D and M.Sc candidates.

FACSS STUDENT AWARDS



Marie Richard-Lacroix University of Montreal

Oral Presentation: Tuesday, 10:15 am, Room 555B

Marie Richard-Lacroix received her B.Sc. in chemistry in 2011 and is currently a Ph.D. candidate under the supervision of Prof. Christian Pellerin at the Department of Chemistry of the University of Montreal. Her research focusses on the characterization of molecular orientation and structural aspects of electrospun nanofibers by confocal Raman spectroscopy. She was the first to demonstrate that quantitative information can be obtained on individual nanofibers and to establish a quantitative correlation between the diameter dependence of molecular orientation, chain disentanglement and mechanical properties in these materials. She also developed a new, experimentally simplified method to quantify orientation by Raman spectroscopy with improved accuracy. She further works on several side projects involving the characterization of ultrathin films by attenuated total reflection infrared spectroscopy. Up to now, she has published 9 peer-reviewed papers, including 8 as first author and a review article, and coauthored more than 35 presentations in scientific conferences. She received several national scholarships from NSERC-Canada and FRQNT-Québec. She was the recipient of multiple awards, including the SAS Barbara Stull Award in 2013 and two poster awards at SciX in 2014.



Lynn X. Zhang Clemson University

Oral Presentation: Wednesday, 4:50 pm, Room 552B

Lynn X. Zhang earned her B.S. degree in Chemical Engineering at the Shenvang University of Chemical Technology in China. The seemingly magical role of the analytical instruments in the industry amazed and attracted her to the field of spectroscopy. After graduating from college, Lynn decided to continue her educational experience in chemistry. In 2011, she obtained a Master's degree in chemistry focusing on plasma temperature study at Murray State University in KY. Starting the same fall, Lynn joined the graduate program to pursue an analytical chemistry PhD in the Chemistry department at Clemson University in SC. She is currently a PhD candidate under Dr. R. Kenneth Marcus, focusing on the development and evaluation of the liquid sampling-atmospheric glow discharge (LS-APGD) and its application in analytical chemistry to solve current challenging analytical problems. Lynn's engineering background has provided a different point of view for her years of research in spectroscopy. Since 2011, she authored/co-authored 7 peer-reviewed articles and presented 7 poster/oral presentations at various conferences including SciX and Pittcon. Lynn has been awarded the Technical Division on Reference Materials (TDRM) student award in 2015 from the Association of Official Agricultural Chemists (AOAC) International for her research accomplishments. In addition to study and research, Lynn is a huge fan of homebrewing, she has brewed various styles of beers, and applied her researcher's spirit into homebrewing: creativity and reproducibility. Lynn also loves to play badminton and is currently a member of the Clemson badminton club and won the 2014 Clemson University Badminton Intramural competition for mix-doubles. Lynn is currently serving as the president of the Clemson University Student Chapter of Society for Applied Spectroscopy, and a member of the SAS website committee to show her support of the field of spectroscopy.

FACSS AWARDS

The FACSS Student and the Tomas Hirschfeld Scholar Awards recognize outstanding contributions by individual who are Ph.D and M.Sc candidates.

TOMAS HIRSCHFELD SCHOLAR AWARDS



Stephanie DeJong University of South Carolina

Oral Presentation: Thursday, 1:20 pm, Room 553A

Stephanie A. DeJong earned her B.A. degree in Chemistry from Trinity Christian College in Illinois in 2011. While an undergraduate, she spent summers participating in undergraduate research programs focused on atmospheric chemistry at Washington State University and Brookhaven National Laboratory. Currently, Stephanie is a Ph. D. candidate in analytical chemistry at the University of South Carolina, working with Dr. Michael L. Myrick. Her research has focused on the application of chemometric techniques to vibrational spectroscopy. Particularly, she has investigated the application of gap derivative transformations to spectral data in the context of multivariate calibration, demonstrating how the selection of gap sizes can dramatically influence calibration results and provide unique information about the spectra. These calibrations have been used to estimate detection limits for blood on fabric using diffuse reflection infrared spectroscopy as part of a larger project to develop a fieldready instrument to detect blood in forensic investigations. Stephanie has also recently facilitated the establishment of a student chapter of the Society of Applied Spectroscopy at the University of South Carolina, and is the founding vice-president. She has also received a 1st place FACSS student Poster award at SciX 2014, the International travel Grant Award to attend the 2013 International Council for Near Infrared Spectroscopy Conference, and the Presidential Fellowship from the University of South Carolina.



Patrik K. Johansson University of Washington

Oral Presentation: Thursday, 10:35 am, Room 551A

Patrik Johansson performed his undergraduate studies at Linköping University (LiU), Sweden, where he also earned his M.S. degree in Engineering Biology in 2013. He did his diploma work as a visiting student intern in the NESAC/BIO group at the University of Washington (UW), where he used SFG, ToF-SIMS, XPS and AFM to characterize protein surface interactions. During the fall 2013, Patrik worked at LiU as a research assistant in the lab for biomolecular and organic electronics (Biorgel) under Professor Olle Inganäs. His research was to introduce the conductive polymer PEDOT-S within lipid membranes, and the work was recently reported in a publication. During the spring 2014, Patrik received a scholarship for returning to the UW as a visiting scientist, where he applied vibrational sum-frequency scattering (SFS) for analysis of collagen fibers in aqueous environments. This was a first demonstration of this technique on protein fibers and it opens up new possibilities to better understand their structure and physico-chemical properties. Since the fall 2014, he is a graduate student in the department of bioengineering at the UW, supervised by Professor Patrick Koelsch. His research focus is to develop and demonstrate nonlinear optical techniques - such as SFS, SFG, and SHG - for detailed characterization of biomaterials.

FACSS AWARDS

FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS - Call for Applications for 2016

The Tomas Hirschfeld Scholar and the FACSS Student Awards recognize the most outstanding papers submitted to FACSS by a graduate student. Recipients will receive financial support to help them attend the SciX 2016 conference in Minneapolis, MN (September 18 - 23). In 2015 two FACSS Student Awards and two Tomas Hirschfeld Scholars are being presented. In order to have your presentation considered for a Tomas Hirschfeld Scholar Award or FACSS Student Award, students should submit their abstract using the SciX website submission form and indicate on the dropdown menu on the form their interest in these awards.

The submission process involves submitting an abstract, completing the website submission form, and submitting the following electronically to facss@facss.org

- a) the form, available on the SciX website
- b) a 250 word abstract of the work to be reported
- c) two letters of nomination, one by the student's mentor. An explanation of the inventive contributions by the student to the work should be given. Creativity was a primary characteristic of Tomas's work, and thus should be a characteristic of the awardee
- d) a copy of the candidates resumé
- e) a copy of the candidate's graduate transcript
- f) Copies of reprints and/or preprints of research accomplished.

The recipients will be included in either a session highlighting young scientists and their work or in an appropriate topic area. The SciX website will begin accepting abstracts and applications for FACSS student awards in January 2015. Go to www.scixconference.org to submit an application.

FACSS INNOVATION AWARD

The FACSS Innovation Award will be given for the most innovative and outstanding new research advancements debuted orally at the SciX Conference. All program areas are included. Only research findings presented for the first time in the public domain qualify for entry (work based on submitted papers not yet published electronically or in print at the time of abstract submission also qualify). Papers submitted for SciX will be considered for these awards – authors can check the appropriate box for their papers to be entered. Finalists will be selected for presentations at the SciX conference in special award sessions. Award winners will be selected after the award sessions are concluded. Each award includes: A cash prize of \$1,500; a plaque; and publicity.

2014 INNOVATION AWARD WINNER:

Sub-PPM Detection Limits in Powder X-Ray Diffraction Guided by Second Harmonic Generation Imaging; Garth Simpson, Purdue University

Thursday Afternoon, Ballroom B/C FACSS INNOVATION AWARD SESSION Organizer and Presider: Alexandra Ros

3:50 (800) Extended Proteomics-Bioinformatics to Characterize Metalloproteins; Joseph Caruso¹, Anna Daigle Donnell¹, Aleksey Porollo², Julio Landero-Figueroa¹, Kavitha Subramanian¹, George Deepe¹; ¹University of Cincinnati; ²Cincinnati 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; <u>Steven Soper</u>¹; ¹University of North Carolina, Chapel Hill

4:50 (803) Five-dimensional Single Particle Tracking in Live Cells; <u>Ning Fang</u>^{1,2,3}; ¹Georgia State University; ²Iowa State University; ³Ames Laboratory, USDOE

^{4:30 (802)} SERS in Live 3D Cell Cultures as a New Tool for Drug Discovery; <u>Colin Campbell¹</u>, Lauren Jamieson¹, Pierre Bagnaninchi¹, David Harrison²; ¹University of Edinburgh; ²University of St Andrews

FACSS CHARLES MANN AWARD

For Achievements in the Field of Applied Raman Spectroscopy

Sanford A. Asher

University of Pittsburgh

Presentation: Tuesday, 8:30 am, Ballroom B/C



Sanford A. Asher, Distinguished Professor of Chemistry at the University of Pittsburgh received his B.A. in chemistry at the University of Missouri, St. Louis in 1971 and completed his Ph.D. in chemistry at the University of California, Berkeley in 1977. Dr. Asher was a Research Fellow in Applied Physics at Harvard University between 1977 and 1980. In 1980 he became Assistant Professor of Chemistry at the University of Pittsburgh. Dr. Asher's research program at Pitt involves development of new materials and the development of new spectroscopic techniques. His group developed UV resonance Raman spectroscopy as a new technique for fundamental and applied structural and trace studies of molecules in complex matrices. His group is using UV resonance Raman to examine the first stages in protein folding. In addition, they are investigating the use of UV resonance Raman for the detection of explosive

molecules, especially for stand-off detection. They are working with others in developing a deep UV Raman instrument for NASA's 2020 Mars lander. In addition, Dr. Asher's research group develops new photonic crystal optical devices and chemical sensing devices from self-assembling colloidal particles. He pioneered the development of smart hydrogel materials for chemical sensing.

Dr. Asher received numerous awards. He is the recipient of the 2015 FACCS Charles Mann Award in Applied Raman Spectroscopy, the 2011 Charles E. Kaufman Award and the 2008 Pittsburgh Spectroscopy Award. He became a Fellow of the Society of Applied Spectroscopy in 2007, and received the Sigi Ziering Award from the American Society of Clinical Chemistry in 2005. The University of Missouri awarded him the 2004 St. Louis Distinguished Alumni Award. He won the 2002 ACS Pittsburgh Award, and the 2002 Ellis R. Lippincott Award from the Optical Society of America. He won the Pittsburgh Technology Council EnterPrize Award in 2000, the Coblentz Society's Bomem-Michelson Award in 1999, and the Society for Applied Spectroscopy's Lester W. Strock Award in 1998, the University of Pittsburgh's Chancellor's Distinguished Research Award in 1996, the American Chemical Society Award in Spectrochemical Analysis in 1994, the American Heart Association Established Investigator Award in 1984 and a NIH Career Development Award in 1984.

Professor Asher served as the Co-Director of the Materials Research Center of the University of Pittsburgh. He was the Chairman of the XV International Conference on Raman Spectroscopy held in Pittsburgh in 1996. He is Scientific Founder and Chairman of the Scientific Advisory Board of the startup company Vytrace Corp. (previously Glucose Sensing Technologies, LLC.), and is on the Scientific Advisory Boards of BioTools Inc. and Crystalplex Co. He consults for companies such as PPG Industries, ChemImage Corporation, Glucose Sensing Technologies, LLC, and ThermoFisher Co.

He is the author of greater than 280 publications and is the inventor in over twenty-nine patents in the area of photonic crystals.

WILEY RAMAN STUDENT AWARD

The Wiley Raman Student Award is given at the annual SciX conference presented by FACSS. The awardee is selected from research submissions for the annual SciX meeting by a panel of Raman subject matter experts and is awarded to an outstanding graduate student and is open to students in any area of Raman spectroscopy research. The student will present their research during the SciX Raman Symposium and will be presented with the award comprising a presentation piece, a certificate, and a book voucher at the annual Raman reception held on Tuesday evening.

The Award this year is being presented to Nirmal Lamsal

Standoff UV Raman Spectroscopy: Spatial Heterodyne Raman Spectrometer for Planetary Applications; <u>Nirmal Lamsal</u>¹, S. Michael Angel¹, Shiv K. Sharma², Tayro Acosta-Maeda²; ¹University of South Carolina; ²University of Hawaii. *Presentation Monday 10:35, Room 556A*



Nirmal Lamsal is a PhD candidate in analytical chemistry at The University of South Carolina and is expected to graduate in the Fall 2015. Mr. Lamsal received a Masters degree in physical chemistry in 2008 from Central Department of Chemistry, Tribhuvan University, Nepal under the supervision of Dr. Raja Ram Pradhananga. As a part of his Masters' degree research, he investigated the effectiveness of activated charcoal derived from carbonized Choerospondias axillaries' seeds (a locally cultivated fruit) for adsorptive removal of toxic metal ions, such as Cd(II) from aqueous solution, at concentrations similar to industrial waste water. After spending two years teaching chemistry at a private college in Kathamndu, Nepal, Nirmal joined The University of South Carolina in 2010, where he currently works in Dr. S. Michael Angel's research group. His PhD research focuses on designing and constructing novel Raman

spectrometers. Nirmal's recent work includes the development of a new type of deep-UV FT Raman spectrometer, known as the Spatial Heterodyne Raman Spectrometer (SHRS) for planetary applications. During his time at USC, Nirmal has written three papers and has presented his results at several meetings and conferences, including SCIX, Pittcon and the Lunar and Planetary Science Conference. Mr. Lamsal is currently seeking a position in a research laboratory.



DISTINGUISHED SERVICE AWARD

Recognizing members for their long-time service to the Society.



Gloria Story Procter & Gamble Company

Gloria Story received her A.S. in Science Technology from the University of Cincinnati - Blue Ash (1981) and worked towards a B.S. in Chemistry from UC and the University of Utah. She is a Senior Scientist with the Corporate Analytical Organization of the Procter & Gamble Company with over 31 years of service in vibrational spectroscopy.

As an over 20-year member of the Society for Applied Spectroscopy, Gloria is currently serving as secretary, as president of the Cincinnati section, and as a volunteer on the membership committee. She's been an active member of the Coblentz Society for over 25 years, currently serving as a liaison for PittCon.

Gloria has been an ACS member since 1994, currently serving as coordinator for membership, Education Grants, and museum NCW programming.

Gloria Story has authored 28 research publications (16 peer-reviewed). She has received numerous awards including Research Associate of the Year and Outstanding Service Awards from the ACS Cincinnati Section, the Global Analytical Community of Practice Recognition and Pete Rodriquez Analytical Excellence Awards from the Procter & Gamble Company, and the America Service to Youth Award from the Dan Beard Council of the Boy Scouts of America.

In her spare time, Gloria sings alto in her church choir, serves as secretary and sunscreen queen of summer camp for her local Boy Scouts of America troop, teaches infrared spectroscopy skills at P&G and Cincinnati State Technical College, plays with chemistry demos at museums, libraries, and schools, watches a little too much TV, and naps whenever possible. Her son Michael is an extruded film process engineer for Clopay Plastics.

HONORARY MEMBERSHIP AWARD

Recognizing those individuals who have made exceptional contributions to spectroscopy.



Alexander Scheeline University of Illinois and SpectroClick, Inc.

Alexander Scheeline is Professor of Chemistry Emeritus in the Department of Chemistry, University of Illinois at Urbana-Champaign, President of SpectroClick Inc., a firm developing handheld instrumentation, and Vice President of Anchor Science LLC, a materials development partnership.

Scheeline comes from Hollidaysburg, PA. He received his Bachelor of Science in Chemistry from Michigan State University in 1974, doing research in chemical kinetics under the direction of S. R. Crouch. His 1978 Ph.D. in chemistry was awarded by the University of Wisconsin-Madison for research on spark discharges under the direction of J. P. Walters. He was then a National Research Council post-doctoral fellow at the National Institute for Standards and Technology, working with J. R. DeVoe and J. C. Travis on laser diagnostics of sparks.

He was on the chemistry faculty at the University of Iowa before moving to Illinois in 1981, continuing research in atomic emission spectroscopy and optical instrumentation, as well as working extensively on oscillatory chemical reactions, sensors for reactive oxygen species, chemical pedagogy, and ultrasonically levitated drops as microreactors. His group trained 15 Ph.D. students, 6 postdoctoral fellows, 7 masters students, and 61 undergraduates. He served briefly as a Program Officer at the National Science Foundation, and was active in operations and governance of FACSS and SAS. With the Analytical Sciences Digital Library, he was founding editor of JASDL, the Library's open access journal. Cowinner of two W. F. Meggers awards, he is a Fellow of the Society for Applied Spectroscopy. He currently focuses his work at SpectroClick.



Richard A. Palmer

Richard A. Palmer was born November 13, 1935 in Austin, Texas, where he lived until 1957, when he received the BS in Chemistry from the University of Texas, Austin. After serving three years as a US Navy Destroyer deck officer, he began graduate studies in Chemistry at the University of Illinois, Urbana-Champaign in 1960. He received his PhD in 1965 (dissertation research under the direction of T. S. Piper), and then spent a year as a NIH Fellow working with C. J. Ballhausen at the University of Copenhagen. In 1966 he joined the Chemistry faculty at Duke University, where he taught classes and directed the research of both graduate and undergraduate students until his retirement in 2008. During Sabbatical leaves he held visiting appointments at the University of Texas, Austin, the University of Virginia, Ecole Superieur de Physique et Chemi Paris, Analytische Techniche Universitat Wein, Universitat Freiburg and Forschungzentrum Karlsruhe. He was director of Duke's Chemistry for Executives Program from 1992 to 2007 and of the Duke Focus Program of freshman seminars from 2008 to 2010.

He is a member of *Phi Lambda Upsilon*, *Phi Beta Kappa*, *Alpha Chi Sigma*, *The American Chemical Society* (ACS) (NC Section Chair, 1978, and National Councilor, 1992 to present), *The Society for Applied Spectroscopy* and *The Coblentz Society*. He received the 2001 Marcus E. Hobbs Service Award from the NCACS Section and was elected a Fellow of the ACS in 2012. He was also a year 2000 recipient of the Alexander von Humboldt Foundation Senior Research Award.

Richard is also recipient of the 2015 SAS Fellows Award.

EMERITUS MEMBERSHIP AWARD

Recognizing those individuals who have who have contributed to spectroscopy and have been members of the Society for Applied Spectroscopy for 15 years, and now have retired from active scientific endeavor.



Ira W. Levin

Dr. Levin received his B.S. from the University of Virginia and his Ph.D. from Brown University, as well as having postdoctoral experience at the University of Washington, serving as a Research Instructor. He retired from the National Institutes of Health after a forty eight year research career which included service as the Chief, of the Section on Molecular Biophysics and Scientific Director of the Division of Intramural Research in the National Institute of Diabetes and Digestive and Kidney Diseases.

His early research interests lay primarily in the applications of vibrational infrared and Raman spectroscopic techniques toward the elucidation of the conformational, dynamical, thermodynamic, and functional properties of both intact and model membrane assemblies and related systems. Later research was at the forefront of developing imaging analogues of molecular spectroscopic instrumentation, specifically, technologies and studies in spectroscopic FTIR and Raman microimaging. Imaging efforts also involved the translation of basic, bench laboratory research into a variety of clinical venues.

Dr. Levin has been honored with many awards including, for example, the Bomem-Michelson Award, the Lippincott Award, the Meggers Award (three separate occasions) and various invited lecture series. He is a Fellow of the American Physical Society's Biophysical Division and, separately, a Fellow in its Division of Chemical Physics and is a Fellow of the Society for Applied Spectroscopy. He has served on numerous boards and committees, in various leadership capacities in the spectroscopy community and at NIH, as well as having published extensively over the course of his career.

LESTER W. STROCK AWARD

Established by the SAS New England section to recognize an author(s) of an outstanding paper or series of papers.



R. Kenneth Marcus *Clemson University*

Presentation: Wednesday, 8:00 am, Ballroom B/C

R. Kenneth (Ken) Marcus, Ph.D., is Professor of Analytical Chemistry at Clemson University. His undergraduate education included BS degrees in Chemistry and Physics from Longwood College (now University) in Farmville, VA in 1982. He received his Ph.D. in Analytical Chemistry in 1986 from the University of Virginia, where he worked for Prof. W. W. Harrison. Professor Marcus' research program currently covers two very distinct lines of study: 1) use of capillary-channeled polymer (C-CP) fibers and films as platforms for protein separations, and) the development of liquid sampling-atmospheric pressure glow discharge (LS-APGD) microplasmas for spectrochemical analysis. The latter efforts are the subject of his awarding of the 2015 Society for Applied Spectroscopy's Lester Strock Award. His research program is currently funded by the National Science Foundation, DTRA, and the Pacific Northwest and Savannah River National Laboratories. His research group has published over 180 refereed journal articles, made over 550 conference presentations (>130 invited), and yielded over 10 US patents. He serves on the editorial advisory boards of Spectrochimica Acta B, the Journal of Analytical Atomic Spectrometry, and Analytical and Bioanalytical Chemistry. Marcus takes great pride in the fact that over one-half of his 33 Ph.D. graduates are now employed in federal laboratories including NIST, the CDC, and the Savannah River, Oak Ridge, Sandia, Los Alamos, and Pacific Northwest National Laboratories. He has been honored as a Fellow of the Royal Society of Chemistry and the American Association for the Advancement of Science.

BARBARA STULL GRADUATE STUDENT AWARD

Recognizing a graduate student for outstanding research in spectroscopy and presented in honor of our longtime colleague Barbara L. Stull



Jay Kitt University of Utah

Jay Kitt graduated with a Bachelor of Science from the University of Utah in 2011. As an undergraduate he began pursuing research with Joel Harris and working on the use of confocal Raman microscopy in porous chromatographic silica particles. For progress in this research, Jay was awarded the 2011 Department of Chemistry Undergraduate Research Award. After graduating, Jay has continued research in the Harris lab, pursuing a Ph.D. in Analytical Chemistry. As a graduate student, Jay's research and teaching have both been recognized. In 2012, he was awarded a research fellowship in the National Science Foundation's Nanobiosensors, Nanomaterials, and Microfluidics IGERT program. That same year, his excellence as a teaching assistant in the undergraduate analytical chemistry courses was honored with the 2012 W.W. Epstein Outstanding Educator award. In the fall of 2014, the Coblentz Society recognized Jay's research in Raman spectroscopy with a Coblentz Student Award. Currently, Jay is continuing his Ph.D. research focused on using confocal Raman microscopy to probe interfacial environments within nanoporous materials and optical-trapping confocal Raman microscopy to investigate phospholipid vesicle phase-transitions.



SAS Student Poster Showcase and Awards

Please join us in celebrating the future of spectroscopy as SAS students showcase their research and compete for the annual SAS Student Poster Awards.

Sunday, September 27, 2015, 7-9 p.m. (during the SciX opening mixer)

Sponsored by The Society for Applied Spectroscopy and FACSS

WILLIAM F. MEGGERS AWARD

Recognizing the author(s) of an outstanding paper appearing in Applied Spectroscopy Presented for "Mid-Infrared Diffuse Reflection on Ultrafast Time Scales" Volume 68, Issue 1 (January 2014), pp. 1-4.



Eric B. Brauns University of Idaho Presentation: Wednesday, 8:30 am, Room Ballroom B/C

Eric B. Brauns earned his PhD in physical chemistry from the University of South Carolina in 2001 where he studied DNA dynamics using ultrafast fluorescence spectroscopy. He spent the next four years at Los Alamos National Laboratory (LANL) as a postdoctoral fellow and technical staff member. While at LANL, he began using time-resolved IR spectroscopy to study RNA folding kinetics and also developed an FT-visible hyperspectral imaging instrument. Since 2005, he has been at the University of Idaho as a faculty member in the Department of Chemistry and an affiliate faculty member in the Department of Physics. In addition to continuing his work in RNA folding, he has added ultrafast 2D-IR spectroscopy and ultrafast IR diffuse reflection to his research interests. His work has been featured on the cover of Applied Spectroscopy twice and he has received funding from the National Science Foundation. He is a dedicated teacher and has taught courses in physical chemistry and statistical mechanics. At present, he is writing a physical chemistry textbook that will be published in 2016.

BRUCE R. KOWALSKI AWARD IN CHEMOMETRICS

administered by the Society for Applied Spectroscopy Presented in honor of the legacy of Professor Kowalski by recognizing outstanding young researchers in the field of chemometrics and by extension, for advanced mathematical and/or statistical methods in chemistry



Thomas Bocklitz University of Jena Award Session: Tuesday 3:50, 554A/B

Dr. Thomas Bocklitz finished his PhD thesis entitled "Investigations on Analysis Strategies of Experiments based on the Raman Effect" in 2011. His main research focus lies on the development and application of Raman spectroscopic approaches for biomedical diagnosis. One highlight of his PhD work was the systematic comparison of different pre-processing methods and the suggestion of a genetic algorithm, which can select automatically a good preprocessing-analytical-task-combination. Overall the data pretreatment procedures and chemometric strategies developed by Thomas during his PhD work significantly advanced our understanding of the potential of Raman spectroscopy for biomedical diagnosis. In 2013 he was offered a position at the Institute of Physical Chemistry, Helmholtzweg as junior group leader with the denomination "Statistical Modeling and Image analysis". Besides the development of custom-made chemometric Raman analysis strategies, Thomas's efforts are particularly focusing on the comparability of Raman spectrometer from a theoretical point of view. Thomas and his group are involved in the Raman experiments starting from the idea, via the experimental design and realization towards the analysis of the data. The scientific results of his work were published in 29 scientific articles in premier peer-reviewed. Thomas is also involved in several interdisciplinary collaborative research projects. Dr. Bocklitz is presenting a paper on Tuesday, 10:35 in Room 551B



Jhe Society for Applied Spectroscopy Cordially Invites All SAS Members to Join Vs at Our Annual Wine and Cheese Awards Reception Juesday, September 29, 2015 7:30 p.m. Ballroom A Rhode Island Convention Center

SAS FELLOWS AWARD

Recognizes individual members for their outstanding service to the field of spectroscopy.



Colin Bain was educated at Cambridge, England and Harvard, USA, where he completed a PhD under the guidance of Prof. George Whitesides on self-assembled monolayers (SAMs). During his PhD, he developed XPS as a quantitative tool for characterising the composition, structure and reactivity of SAMs. In 1988 he returned to the UK and established the UK's first sum-frequency spectrometer, working with Paul Davies at

Cambridge University. His particular interest was in the structure and phase behaviour of surfactant films at interfaces. In 1991 he moved to a University Lectureship at Oxford University and in 2005 to a Chair at Durham University. His research is characterised by the application a suite of surface-sensitive techniques to the structure and dynamics of organic molecules at fluid interfaces, which often involves applying techniques in new ways. For example, he was the first to apply neutron reflectivity to flowing liquid surfaces and ellipsometry to high-speed jets. Recently, he has focussed on the development of total internal reflection Raman scattering for surface characterisation, including an imaging version for measurement of composition and phase separation in real time. He collaborates widely with industry in areas such as inkjet printing, lubrication, display technology, surfactant-enhanced oil recovery, agrochemicals and personal care products. Awards for his work include the Corday-Morgan and Tilden Medals of the Royal Society of Chemistry, the Craig Lectureship at Australian National University, the Founder's Lecture at the National Chemical Laboratory in Pune, the Lectureship Award of the Japanese Chemical Society and the Thomas Graham Lectureship (jointly awarded by the SCI and RSC).



Katherine A. Bakeev is the Director of Analytical Services and Support for B&W Tek in Delaware. She has many years of industrial experience in the electronics, chemical and pharmaceutical industries, with companies including GlaxoSmithKline, CAMO Software and Foss NIRSystems. Katherine earned her PhD in Polymer Science and Engineering from the University of Massachusetts in Amherst has

a Masters in Technology Management from Stevens Institute of Technology, and a BS in Macromolecular Science from Case Western Reserve University.

She is the author of numerous articles and edited a book on Process Analytical Technology, now in its second edition. She is the recipient of the 2007 Craver Award in Applied Vibrational Spectroscopy.

She has been a member of the Society of Applied Spectroscopy (SAS) since 1993, serving on the Executive Committee from 2010-2014, and continues to serves on various SAS committees. She serves on the Editorial Board of the journal Applied Spectroscopy and for NIRNews. She is the past president of SAS and the Council for Near Infrared Spectroscopy (CNIRS), and a member of the Coblentz Society, ACS, and the International Council for Near Infrared Spectroscopy (ICNIRS).



Rohit Bhargava received dual B.Tech. degrees (in Chemical Engineering and Polymer Science and Engineering) from the Indian Institute of Technology, New Delhi in 1996. Subsequently, his doctoral thesis work at Case Western Reserve University was in the area of polymer spectroscopy and infrared imaging. As a Research Fellow at the NIH (2000-2005), he developed infrared imaging technology and its

applications in cancer pathology. Rohit has been at Illinois since as Assistant Professor (2005-2011), Associate Professor (2011-2012) and Professor (2012-). Research in the Bhargava laboratories focuses on theory and simulation for spectroscopic imaging, developing new instrumentation and making chemical imaging practical for digital molecular pathology in cancer. Using 3D printing and engineered tumor models, his recent research seeks to elucidate the biology and physical aspects of hetero-cellular interactions in cancer progression. Among recent national honors for spectroscopy research are the Meggers Award (Society for Applied Spectroscopy, 2014), Craver Award (Coblentz Society, 2013) and the FACSS Innovation Award (2012). Earlier in his career, Rohit was the first assistant professor hired into the new Bioengineering department at Illinois and played a key role in the development of its curriculum and activities. His dedication to education on campus is recognized (Rose and Everitt awards) and he is routinely nominated to the list of teachers ranked excellent. Among his recent educational innovations is the development of a challenge-inspired model for undergraduate education and its use in the Cancer Scholars Program.



David Cremers received his Ph.D. (physics) from Washington State University. His dissertation work involved picosecond laser-based flash photolysis. He joined Los Alamos National Laboratory in 1980 as a Postdoctoral Fellow to develop ultra-sensitive optical methods of chemical detection. In 1981 he became a staff member at the Laboratory and began

developing laser-induced breakdown spectroscopy (LIBS) for a variety of defense and industrial applications. These applications included chemical agent detection, the detection of toxic airborne metals, and industrial process control such as real-time molten steel monitoring. Dr. Cremers also worked on other methods of chemical detection based on Raman and fluorescence spectroscopy. In the early 1990's, he along with other LIBS team members, demonstrated open path stand-off LIBS for elemental analysis, the basis of the technique deployed on the Mars Science Laboratory for laser-based stand-off interrogation of geological samples. In 2005, Dr. Cremers joined Applied Research Associates, Inc. (Albuquerque, NM) to continue research and development of laser plasma based technologies with emphasis on LIBS instrumentation for nuclear, radiological, and bio-detection.

Dr. Cremers has extensive expertise in developing LIBS instrumentation. He has received five R&D-100 Awards for instrument development, four of these relating to LIBS technology. He holds seven patents for optical based technologies including LIBS. Dr. Cremers has over 50 publications in referred scientific journals dealing with laser plasmas and the LIBS method. He has also co-authored the second edition of the "Handbook of LIBS" for John Wiley (2013).

SAS FELLOWS AWARD - continued

Recognizes individual members for their outstanding service to the field of spectroscopy.



Richard A. Dluhy received his Ph.D. degree in physical chemistry from Rutgers University in 1983. He was a research associate at the National Research Council of Canada, Ottawa, and a senior research scientist at Battelle Memorial Institute, Columbus, OH, before joining the University of Georgia, where he was an Associate and Full Professor of Chemistry.

He has been a visiting professor at the University of Bordeaux, a Alexander von Humbolt award scholar at the Max Planck Institute and a DAAD award recipient at the Robert Koch Institut. At UGA, he has been the Associate Head of the Department of Chemistry, and the Director of the Nanoscale Science and Engineering Center. His research interests are in biophysical and biomedical vibrational spectroscopy using physically and chemically self-assembled nanomaterials with applications to opto-electronics, sensors and biomaterials. He is a co-founder and President of Argent Diagnostics, Inc., a new start-up company in Athens, GA, dedicated to commercialization of nano photonics in biomedical diagnostics. As of July 2015, he was named Professor and Chairman of the Department of Chemistry at the University of Alabama at Birmingham.



Roy Goodacre is Professor of Biological Chemistry at the University of Manchester, UK. His group's main areas of research are broadly within analytical biotechnology and systems biology, specifically involving Raman spectroscopy, FT-IR and mass spectrometry. He also develops advanced data analyses (chemometrics) which are needed for the interpretation of these

spectroscopic, mass spectrometric and metabolomics data.

Over the last decade or so his group has developed a variety of Raman spectroscopy methods. These include surface enhanced Raman scattering (SERS) and UV resonance Raman spectroscopy for the identification of bacteria and their metabolic products, and more recently live cell Raman for single cell analysis, as well as SERS for multiplexed detection and quantification of a variety of analytes.

Roy is the Editor-in-chief of the journal *Metabolomics* and on the editorial advisory boards of *Analyst* and *Journal of Analytical and Applied Pyrolysis*. Finally, he is a founding director of the Metabolomics Society, and a director of the Metabolic Profiling Forum.



Detlef Günther was born in Köthen, Germany in 1963. He obtained his Diploma degree in Chemistry in 1987 and a Ph.D. degree in Analytical Chemistry from the Martin-Luther-University Halle-Wittenberg under supervision of L. Moenke - Blankenburg in 1990. After carrying out postdoctoral work in the Institute of Plant Biochemistry Halle where he worked on the development of analytical methods to

characterize heavy metal-binding proteins using HPLC-ICP-MS, he joined the group of H.P. Longerich at the Memorial University of Newfoundland, Canada. From 1995 until 1998 he was in the group of C.A. Heinrich at the Institute of Isotope Geology and Mineral Resources at ETH Zürich. In 1998 he was appointed Assistant Professor in the Laboratory of Inorganic Chemistry at the ETH Zürich. He was promoted to Associate Professor for Trace Element 20

and Micro Analysis in 2003 and became Full Professor in 2008. From 2010 until 2012 he was Chair of the Department of Chemistry and Applied Biosciences at ETH Zurich and since 2015 he is Vice President for Research and Corporate Relations at ETH Zurich. He is recipient of the Ruzicka Award (2002), the European Award for Plasma Spectrochemistry (2003), the Fresenius Award (2007), and the Lester Strock Award (2007), and he received in 2013 the "Einstein Visiting Fellowship" to Humboldt University Berlin (Germany) and the "Thousand Talent Fellowship" (Wuhan University, China). In 2014 he became a member of the German National Academy of Science Leopoldina. His research program focuses on fundamental and applied studies in inductively coupled plasma-mass spectrometry (ICP-MS) and laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS), including studies on laser- sample interaction, aerosol transport, and plasma-related excitation processes. As well particle plasma interaction and particle vaporization for single nanoparticle analysis have been studied. Fundamental processes of UV-ns and UV-fs laser ablation used with Q-ICP-MS, SF-ICP-MS, TOF-ICP-MS, and MC-ICP-MS as well as alternative excitation sources, such as glow discharge are currently under investigation. The improvements in trace element and microanalysis and isotope ratio determinations have been demonstrated on a wide variety of applications (e.g., quantification of fluid inclusions, gemstones, metals, minerals, ceramic, and various nano materials).



David Hahn received his BSME (1986) and PhD (1992) degrees from Louisiana State University in Baton Rouge. Following graduation, he was a National Research Council Research Associate at the US Food and Drug Administration (1992-1994) where he worked on laser-tissue interactions, and then a member of the technical staff at Sandia National Laboratories (1994-1998), in the

Combustion Research Facility and in the Exploratory Systems Group, where he first worked on LIBS. David joined the University of Florida (Gainesville, FL) in 1998, was promoted to Professor in 2007, and since June 2011 has served as Department Chair of the Department of Mechanical and Aerospace Engineering. His research and teaching interests are in the general area of transport, opticalbased sensing and diagnostics, with applications to laser-material interactions. He has published over 100 journal papers and book chapters and has 9 US patents. He currently serves on the Editorial Board of Spectrochimica Acta Part B, the Publication Committee for SAS, and on the Board of Directors of the Doolittle Institute, a US Air Forced funded non-profit institute chartered to foster innovation and collaboration between industry, academia and government. While at UF, he has won the College of Engineering 2007-2008 Teacher/Scholar of the Year Award, and the 2009-2010 Doctoral Dissertation Advisor/Mentoring Award. He was recipient of the SAS 2011 Lester W. Strock Award for his work on laser-induced plasma spectroscopy, and received the 2013-2014 Distinguished Alumnus Award from LSU's Department of Mechanical and Industrial Engineering. He is a Fellow of ASME.

SAS FELLOWS AWARD - continued

Recognizes individual members for their outstanding service to the field of spectroscopy.



Takeshi Hasegawa started his research carrier from the analysis of Langmuir-Blodgett films by infrared external-reflection (IR ER) spectroscopy on an electrodynamics framework under the direction of Professor Tohru Takenaka and Professor Junzo Umemura, pioneers in this field. In this series of studies, he deduced new convenient equations, in which the optical anisotropy is taken into account in a

uniquely simple way. Due to the theory, the molecular orientation analysis in an ultrathin film was made a familiar task for surface chemists, which contributed to vibrational spectroscopy greatly.

He made further outstanding achievements after he obtained a position: the experimental and theoretical establishments of Principal Component Analysis (PCA) and Multiple-Angle Incidence Resolution Spectrometry (MAIRS). PCA is a most well-known chemometric technique, but he first pointed out that a very minute signal can be extracted from very strong background signals. He demonstrated an impressive work that non-resonance Raman spectra were separated from strong backgrounds of fluorescence. The theory is established, and it enhances the potentials of vibrational spectroscopy.

MAIRS is his original outstanding achievement, which is a powerful and unique spectroscopic tool for analyzing thin films on solid substrates. The uniqueness of this technique exists in the use of "virtual light" that oscillates electric field along the traveling direction. By incorporating the virtual light in his optical theory, the spectra arising from dipole transitions parallel and perpendicular to the substrate surface can be obtained separately from a set of (reflection or transmission) spectra collected at different incident angles, which enables accurate determination of molecular orientation in thin films without any assumptions. One can understand the advantage of this technique as follows. For observing dipole transitions parallel and perpendicular to the surface, a set of spectra must be measured in both transmission and reflection modes in the conventional surface spectroscopy. That is, two different substrates, highly reflective one (metal) and transparent one, are required. This strategy cannot be used in bioanalysis because biomolecules are often denaturated on metallic surfaces due to strong interactions. Professor Hasegawa experimentally and theoretically demonstrated that orientations of biomolecules on transparent substrate can be determined only from transmission spectra. No requirement of assumption is another advantage. In conventional optical theories based on the Fresnel's equations, the refractive indices of the molecules at a frequency far from the absorption must be assumed. The removal of the assumption enables accurate determination of molecular orientation.

In this manner, the spectroscopic techniques that Professor Hasegawa developed are unique and useful. Due to these outstanding achievements, he received not only the Craver Award, but also Yamazaki-Teiichi prize, Dr. Masao Horiba Award, Awards from The Japan Society for Analytical Chemistry, etc.). His research in the area of vibrational spectroscopy has thus already garnered an international reputation.



Paul Pudney has a BSc in chemistry from Liverpool University and obtained a PhD in Physical Chemistry from the University of East Anglia 'Spectroscopic studies of adsorbates on metal single crystal surfaces' under supervision of Prof Michael Chesters . After post doctoral studies at the Leverhulme Centre for Innovative Catalysis and the Interdisciplinary Research centre in Surface Science at Liverpool University he worked at the synchrotron at

Daresbury before joining Unilever in 1994.

Paul is now a science leader in vibrational spectroscopy in Unilever Discover's, strategic science group. He has applied spectroscopy in a number of innovative ways to gain further understanding of both consumer products and their behaviour when they interact with our consumers. Examples include quantifying the complex microstructures of soft solid materials by confocal Raman spectroscopy such as foods and behaviour of molecules in ice using IR. He developed a novel in-situ Triboligical Raman instrument to help understand lubrication in a Soft Elasto-Hydrodynamic Contact to understand 'feel'. He has developed *in-vivo* Raman spectroscopic capability to measure and understand the delivery of actives to and their effect on the body, such as to the skin, scalp, axilla and oral mucosa as well as hair.

He has ~60 peer reviewed publications. He was nominated as one of the 'Prominent Young Vibrational Spectroscopists' in special addition of Vibrational Spectroscopy journal in 2004. He won the Meggers award in 2013, as well being runner up in 2012.

SOCIETY FOR APPLIED SPECTROSCOPY WILLIAM J. POEHLMAN AWARD

Recognizing an outstanding SAS Regional Section that has met the goals and ideals of the Society over the past year.

SAS New York Regional Section

The SAS New York Regional Section is being recognized for continuing to be busy in many areas and serving as an example of what a strong regional section can accomplish. Of particular note, given the challenges facing SAS at large, are their efforts towards improving section sustainability. These include active member recruitment throughout the year, whether through interactions at the workplace, hosting an exhibition booth at conferences, or supporting students through awards and at meetings. The section also keeps its web site updated regularly, demonstrating the activity in the section and keeping an active forum for updating members. Additionally, NYSAS continued its long-standing administration of the Gold Medal Award to recognize contributions to the field of Applied Spectroscopy, with a luncheon and symposium at EAS.

COBLENTZ SOCIETY'S CLARA CRAVER AWARD

The Craver Award honoring **Clara Craver** is presented annually to an outstanding young molecular spectroscopist whose efforts are in the area of applied analytical vibrational spectroscopy. Clara Craver was the editor of the Coblentz Desk reference and other subsequent libraries that later became databases of infrared spectra that is the foundation for the application of modern vibrational spectroscopy. Her efforts resulted in the creation of the endowment that supports the Coblentz Society and many of the awards that it gives out annually. The candidate must be under the age of 45 on January 1st of the year of the award. The work may include any aspect of infrared (NIR, MIR, or Far), and/or THz, and/or Raman spectroscopy in applied analytical vibrational spectroscopy. The nominees may come from an academic, government lab, or industrial backgrounds. Click here for information on the Coblentz Society Craver Award.



Ji-Xin Cheng

Purdue University

Presentation, Tuesday, 8:00 am, Ballroom B/C



Ji-Xin Cheng was born in Jixi, Anhui Province, P. R. China in 1971. He attended University of Science and Technology of China (USTC) from 1989 to 1994. From 1994 to 1998, he carried out his PhD study on bond-selective chemistry under the supervision of Qingshi Zhu at USTC. As a graduate student, he worked as a research assistant at Universite Paris-sud (France) on vibrational spectroscopy and the Hong Kong University of Science and Technology (HKUST) on quantum dynamics theory. After postdoctoral training on ultrafast spectroscopy in Yijing Yan's group at HKUST, he joined Sunney Xie's group at Harvard University as a postdoc, where he and others developed CARS microscopy that allows high-speed vibrational imaging of cells and tissues. Cheng joined Purdue University in 2003 as Assistant Professor in Weldon School of Biomedical Engineering and Department of Chemistry, promoted to Associate Professor in 2009 and to Full Professor inted as Scientific Director of Label free Imaging at Purdue's Directory Park in Oct 2014

in 2013. He was appointed as Scientific Director of Label-free Imaging at Purdue's Discovery Park in Oct 2014.

Professor Cheng's research aims to transform molecular spectroscopy from an *in vitro* analytical tool to an *in vivo* imaging platform for biological and medical applications. His pioneering work includes CARS imaging of myelin sheath in its nature state, multimodal nonlinear optical microscopy, chemical imaging of deep tissue through acoustic detection of harmonic vibration, transient absorption microscopy of nanomaterials, and lock-in free stimulated Raman spectroscopic imaging. He is authored in over 170 peer-reviewed articles that have been cited more than 10,000 times, with an h-index of 50 (Google Scholar). His leadership is demonstrated as the organizer of 23 national/international symposia, over 170 invited talks, and as co-editor of the first book on Coherent Raman Scattering Microscopy, published by CRC Press in 2012. His is a co-inventor of CARS microscope which is now available through Olympus and Leica. In 2013 He co-founded Vibronix Inc which has the mission of saving lives through vibrational imaging technology. He is the Purdue site director of NSF-funded I/UCRC Center for Biophotonics Sensors and Systems.

Professor Cheng's achievements have been recently recognized by Chang-Jiang Scholar from Chinese Minister of Education (2014), Fellow of American Institute of Medicine and Biological Engineering (2014), Purdue University Faculty Scholar (2012-17), College of Engineering Early Career Research Award (2011), Research Excellence Award from Purdue Center for Cancer Research (2011), Outstanding Young Scientist Award from Chinese National Academy of Sciences (2009).

The Coblentz Society call for Award Nominations. Visit <u>www.coblentz.org</u> For more information

- Coblentz Award
- Williams-Wright Award
- The ABB Sponsored Bomem-Michelson Award
- Ellis R. Lippincott Award
- Craver Award

The Coblentz Award is presented annually to an outstanding young molecular spectroscopist under the age of 40. The candidate must be under the age of 40 on January 1 of the year of the award. Files of candidates will be kept active until the date of age eligibility is exceeded, and annual updates of files of nominated candidates are encouraged. Nominations should include a detailed description of the nominee's accomplishments, a curriculum vitae and a minimum of 3 supporting letters. Nominations will be accepted from Jan 3^{rd} - July 15^{th} .

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SOCIET

The Williams-Wright Award is presented annually to an industrial spectroscopist who has made significant contributions to vibrational spectroscopy while working in industry. Government labs are not considered industry in this definition. No restrictions are placed on the selection of the Awardee because of age, sex, or nationality, but the Awardee must still be working at the time the award is presented. Nominations will be accepted until **May 1**st.

The ABB Sponsored Bomem-Michelson Award is dedicated to the memory of Professor A. A. Michelson, developer of the Michelson interferometer. ABB sponsors the award to honor scientists who have advanced the technique(s) of vibrational, molecular, Raman, or electronic spectroscopy. The recipient must be actively working and must be at least 37 years of age. Nominations will be accepted from **Feb 1**st - **May 1**st.

The Lippincott Award is to honor Dr. Ellis R. Lippincott's memory by the recognition of significant contributions and notable achievements in the field of vibrational spectroscopy. The medal is sponsored jointly by the Coblentz Society, the Optical Society of America and the Society for Applied Spectroscopy. The Awardee will have the opportunity to present an address related to the contributions for which he/she is being honored. Nominations will be accepted until **Oct 1st**.

Craver Award - The Craver Award is presented annually to recognize young spectroscopists for efforts in applied analytical vibrational spectroscopy. Candidates must be under the age of 45 on January 1 of the year of the award. The candidate's work may include any aspect of infrared (NIR, MIR, Far), and/or THz, and/or Raman spectroscopy in applied analytical vibrational spectroscopy. The nominees may come from an academic, government lab, or industrial backgrounds. Nominations will be accepted until **Aug 30th**.

Honorary Membership - The Coblentz Society awards honorary memberships in the Society to people who have made outstanding technical contributions to the field of vibrational spectroscopy and/or whose careers have been marked by outstanding service in the promotion of vibrational spectroscopy. Nominations close on February 1 each year, with awards announced at the Annual Members Meeting at Pittcon and presented at FACSS. Send your nominations to Mark Druy, Coblentz Society President at mark.druy@coblentz.org.

Additional information regarding eligibility, nomination requirements, and nominations procedures can be found at http://www.coblentz.org/awards.

COBLENTZ SOCIETY'S WILLIAM G. FATELEY STUDENT AWARD

The William G. Fateley Student Award is given by the Coblentz Society annually to recognize outstanding contributions to vibrational spectroscopy during a current Ph.D. program. William G. (Bill) Fateley was among the first winners (1965) of the Coblentz award, and worked tirelessly to promote the Pittsburgh Conference and FACSS. Author of more than 350 publications and recipient of numerous other awards, he returned to his alma mater, Kansas State University, as chairman of his department in 1972 and served there until his retirement 1997 and beyond. He served as the Editor of *Applied Spectroscopy* for 20 years, and served as mentor to a generation of spectroscopists



2015 Coblentz Society's William G. Fately Student Awardee and Student Award – Marie Richard-Lacroix



Marie Richard-Lacroix received her B.Sc. in chemistry in 2011 and is currently a Ph.D. candidate under the supervision of Prof. Christian Pellerin at the Department of Chemistry of the University of Montreal. Her research focusses on the characterization of molecular orientation and structural aspects of electrospun nanofibers by confocal Raman spectroscopy. She was the first to demonstrate that quantitative information can be obtained on individual nanofibers and to establish a quantitative correlation between the diameter dependence of molecular orientation, chain disentanglement and mechanical properties in these materials. She also developed a new, experimentally simplified method to quantify orientation by Raman spectroscopy with improved accuracy. She further works on several side projects involving the characterization of ultrathin films by attenuated total reflection infrared spectroscopy. Up to now, she has published 9 peer-reviewed papers, including 8

as first author and a review article, and coauthored more than 35 presentations in scientific conferences. She received several national scholarships from NSERC-Canada and FRQNT-Québec. She was the recipient of multiple awards, including the SAS Barbara Stull Award in 2013, two poster awards at SciX in 2014, and a FACSS Student Award in 2015.



In addition to Awards for professionals in industry, academia, and government laboratories, the Coblentz Society encourage young scientists to pursue studies in all areas of vibrational spectroscopy through the presentation of Student Awards. The Coblentz Student Award recognizes excellence in research involving vibrational spectroscopy and/or coursework in vibrational spectroscopy. The three leading graduate students selected by the Coblentz Award Committee will also qualify for consideration for the William G. Fateley Student Award that includes a presentation by the winner at the SciX conference (20 minute oral presentation), a plaque, and a prize of \$1000. No separate nomination for the Fateley award is required.

Coblentz Student Awards and the William G. Fateley Student Award

The Coblentz Society seeks nominations of outstanding students for the Coblentz Student Awards. Nominations by e-mail are preferred and may be sent to the Chair of the Coblentz Student Affairs Committee, Professor Rohit Bhargava, at <u>rxb@illinois.edu</u>. Graduate or undergraduate students who have shown excellence in vibrational spectroscopy research and/or coursework including vibrational spectroscopy can be nominated. The nominations window for Coblentz Student Awards is open November 1 – February 15. Winners will be announced in March.

Additional information regarding eligibility, nomination requirements, and nominations procedures can be found at http://www.coblentz.org/awards.

COBLENTZ SOCIETY'S STUDENT AWARDS

For many years, the Coblentz Society has encouraged young scientists to pursue studies on spectroscopy by seeking nominations of outstanding students for the Coblentz Student Awards. The awardees receive a copy of the Society's Deskbook, a certificate, and a year's membership in the Society. Their names, the names of their faculty advisors, their institute, and their anticipated graduation date appear in the Society's Fall Newsletter published in an issue of the journal, Applied Spectroscopy.



Stephanie A. DeJong earned her B.A. degree in Chemistry from Trinity Christian College in Illinois in 2011. While an undergraduate, she spent summers participating in undergraduate research programs focused on atmospheric chemistry at Washington State University and Brookhaven National Laboratory. Currently, Stephanie is a Ph. D. candidate in analytical chemistry at the

University of South Carolina, working with Dr. Michael L. Myrick. Her research has focused on the application of chemometric techniques to vibrational spectroscopy. Particularly, she has investigated the application of gap derivative transformations to spectral data in the context of multivariate calibration, demonstrating how the selection of gap sizes can dramatically influence calibration results and provide unique information about the spectra. These calibrations have been used to estimate detection limits for blood on fabric using diffuse reflection infrared spectroscopy as part of a larger project to develop a field-ready instrument to detect blood in forensic investigations. Stephanie has also recently facilitated the establishment of a student chapter of the Society of Applied Spectroscopy at the University of South Carolina, and is the founding vice-president. She has also received a 1st place FACSS student Poster award at SciX 2014, the International Travel Grant Award to attend the 2013 International Council for Near Infrared Spectroscopy Conference, and the Presidential Fellowship from the University of South Carolina.



Shalaka Dewan graduated with a Bachelor of Science (Chemistry) from the University of Mumbai in 2006, and went on to earn her Master of Science in Physical Chemistry in 2008, from the University of Mumbai. After a brief stint as a scientific editor from 2008-2009 at Cactus Communications Pvt. Ltd, in Mumbai India, she moved to the USA to join Professor Eric Borguet's group at Temple

University in 2009 to pursue research in the non-linear optics field. She recently defended her Ph.D. thesis titled "Ions and the structure and dynamics of interfacial water at charged surfaces." The focus of her PhD research was to understand how the presence of ions affects the structure and the vibrational dynamics of water at the mineral/water interface using vibrational sum-frequency generation (SFG) spectroscopy methods and molecular dynamics simulations. Her first experiments in SFG of silica/water interface showed a correlation between the effect of ions on the structure of water at the silica surface and the rate of silica dissolution. In her more recent experiments, she used time-resolved SFG to measure the ultrafast vibrational dynamics of interfacial water and showed that the effect of ions on the vibrational lifetime of the O-H stretch of water has a strong dependence on the surface charge density and the identity of the cation at the negatively charged silica surface. Starting in August 2015, she will be a postdoctoral fellow in the group of Professor David Gracias and Chao Wang at John Hopkins University, where she will perform spectroscopic studies of nanocatalytic surfaces used in renewable energy sources.

ACS DIVISION OF ANALYTICAL CHEMISTRY AWARD IN SPECTROCHEMICAL ANALYSIS

Advancing the fields of spectrochemical analysis and optical spectrometry in one or more of the following:

- Conceptualization and development of unique instrumentation that has made a significant impact on the field.
- Development of novel and important instrumentation.
- Elucidation of fundamental events or processes important to the field.
- Authorship of important research papers and/or books that have had an influential role in the development of the field.

Frank V. Bright

Pacific Northwest National Laboratory

Award Session Honoring 2015 ACS Spectrochemical Award Winner Frank Bright

Monday, 1:20 pm; Room 554A/B



Frank V. Bright earned his B.S. degree from the University of Redlands in 1982. His Ph.D., supervised by Professor Linda B. McGown, is from Oklahoma State University (1985). He completed his postdoctoral studies at Indiana University with Professor Gary M. Hieftje (1985-'87). In 1987 he joined the SUNY-Buffalo Department of Chemistry as a tenure-track Assistant Professor and he is currently the Henry M. Woodburn Chair and a SUNY Distinguished Professor. Frank's research program focuses on chemical sensors, materials, antifouling coatings, wound restitution and ocular surface the chemistry. He and his associates have published over 300 articles and hold 16 U.S. patents. Frank's scholarship has been recognized by several awards including the 3M, Inc. Non-tenured Faculty Award (1988-'91), the Buck-Whitney Medal of the Eastern New York American Chemical Society (1999), the Gold Medal Award of the New York Section of the Society for Applied Spectroscopy (2003), the New York Section of the Society for Applied Spectroscopy Gold Medal (2003), the

Akron Section of the American Chemical Society Award (2003), the A.A. Benedetti-Pichler Award in Microchemistry from the American Microchemical Society (2005), and the Jacob F. Schoellkopf Medal of the Western New York American Chemical Society (2006). He has been elected a member of the International Society for Contact Lens Research (2011) and named a Fellow of the Society for Applied Spectroscopy (2010) and the Royal Society of Chemistry (2014). Frank has also earned several awards for teaching including the Faculty of Natural Sciences and Mathematics Dean's Award for Excellence in Teaching (1998) and SUNY Chancellor's Award for Excellence in Teaching (2000). Frank has been an *Applied Spectroscopy* Associate Editor since 2009.



Call for Nominations ACS Division of Analytical Chemistry Awards 2016 Deadline: November 1, 2015

ELIGIBILITY

Eligibility is open to members and non-members of the Division of Analytical Chemistry. Nominees for the J. Calvin Giddings Award for Excellence in Education, however, must have demonstrated excellence in teaching through at least five years at the time the award is presented. Nominating and seconding letters may be submitted by persons who are not members of the Division.

DEADLINES

All nominations must be sent to the immediate past chairperson of the Division and must be received by November 1 of each year. The immediate past chairperson of the Division shall in turn transmit the nominations to the chairpersons of the appropriate juries. Nominations that are unsuccessful will be retained for jury consideration for the following three years.

For the 2016 Awards, nominations shall be sent by email or postal mail no later than November 1, 2015 to:

ACS Division of Analytical Chemistry Award Nominations 2019 Galisteo St., Bldg I-1 Santa Fe, NM 87505 Phone: 505-820-0443; office@analyticalsciences.org

NOMINATIONS

Nominations shall consist of:

- 1. A letter of nomination.
- 2. Two seconding letters.
- 3. A biographical statement emphasizing the accomplishments of the nominee which pertain to the award.
- 4. The nominating documents shall be submitted in one package and shall not exceed 8 pages of text, including the nominating and seconding letters, biographical statement, and attachments to the nomination. If the total pages for a nomination exceeds 8, then only the first 8 pages will be submitted to the jury for the award.
- 5. Nominating and seconding letters may be submitted by persons who are not members of the Division.

Contributions by a candidate which have been recognized by a prior Divisional or ACS national award generally will not be considered by the jury for a Divisional award, especially if an award has been received within the past three years and within a similar area. The jury shall receive from its chairperson a list for each nominee of any such prior awards, their dates, and their citations. Any candidate previously nominated for an award who was not chosen as the awardee will be considered for up to three additional years without further action by the nominator being required. More information is available at www.analyticalsciences.org.

ANACHEM AWARD

The ANACHEM Award is presented annually to an outstanding analytical chemist based on activities in teaching, research, administration or other activity, which has advanced the art and science of the field.



Jonathan Sweedler

University of Illinois

Presentation: Thursday, 8:00 am; Ballroom B/C



Jonathan Sweedler received his Ph.D. in Chemistry from the University of Arizona in 1988, spent several years at Stanford before moving to the University of Illinois at Urbana-Champaign in 1991 where he has been ever since. At Illinois, he is currently the James R. Eiszner Family Endowed Chair in Chemistry, Director of the School of Chemical Science, and affiliated with the Institute of Genomic Biology and the Beckman Institute for Advanced Science and Technology. His research interests focus on developing new approaches for assaying small volume samples, and in

applying these methods to study novel interactions between cells. These analytical approaches include micro and nanofluidics, miniaturized separations, mass spectrometry and NMR. He has used these tools to characterize small molecules and peptides in a range of animal models across metazoan life and in samples as small as individual cells and cellular domains. Sweedler, with large international teams of biologists and technologists, has performed comprehensive interrogation of the genome, transcriptome and peptidome in *Aplysia californica, Schmidtea mediterranea, Apis mellifera, Taeniopygia guttata, Strongylocentrotus purpuratus*, and other models to uncover signaling peptides and pathways involved in wide range of functions and behaviors.

Sweedler has published more than 350 manuscripts and presented 400 invited lectures. He has received numerous awards including the American Chemical Society (ACS) Analytical Division Arthur Findeis Award, the Benedetti-Pichler Award in Microanalysis, the Gill Prize in Neuroscience, the Instrumentation Award from the Analytical Division of the ACS, the Pittsburgh Analytical Chemistry Award, and the 2014 ACS Award in Analytical Chemistry. He is a fellow of both the American Association for the Advancement of Science and the American Chemical Society. He is currently the Editor-in-Chief for *Analytical Chemistry*.

AES MID-CAREER AWARD

This award is given for exceptional contributions to the field of electrophoresis, microfluidics, and related areas by an individual who is currently in the middle of their career.



Adam T. Woolley Brigham Young University

Presentation: Thursday, 8:30 am; Ballroom B/C



Adam T. Woolley graduated summa cum laude with a B.S. in Chemistry from BYU in 1992. He received his Ph.D. in Chemistry in 1997 from the University of California–Berkeley under the direction of Professor Richard Mathies. His doctoral research involved the development of micromachined electrophoretic systems for rapid DNA analysis, and his work was recognized with the 1998 Fannie and John Hertz Foundation Thesis Prize. Woolley was a Cancer Research

Fund Runyon-Winchell Foundation Postdoctoral Fellow in the group of Professor Charles Lieber at Harvard University from 1998-2000. His postdoctoral work focused on implementing carbon nanotube probes for high-resolution biological scanning probe microscopy. After postdoctoral studies, Woolley joined the Department of Chemistry and Biochemistry at BYU. He was promoted to Associate Professor in 2006 and to Professor in 2010. Prof. Woolley has also served as an Associate Department Chair since 2010.

Professor Woolley is author or co-author of more than 100 peer-reviewed papers, has given over 130 scientific presentations and has received 10 patents related to his work. Since coming to BYU he has received several recognitions, including the American Chemical Society Division of Analytical Chemistry Award for Young Investigators in Separation Science (2007), Presidential Early Career Award for Scientists and Engineers (2007), BYU Young Scholar Award (2008), BYU Reed M. Izatt and James J. Christensen Faculty Excellence in Research Award (2012), and BYU Karl G. Maeser Research and Creative Arts Award (2014).

The overarching theme of Professor Woolley's research is the interrelationship between biological molecules and miniaturization: he uses microfabrication techniques to create microfluidic systems to quantify clinically relevant biomolecules, and also utilizes biological molecules (in particular DNA) in designing and preparing nanoscale materials. He has trained over 30 undergraduate students, more than 20 graduate students, and 6 postdoctoral scholars in his group.

Woolley's current research is concentrated in three general areas: biotemplated nanofabrication, the creation of novel and sophisticated integrated microfluidic systems for enhanced biomarker quantitation, and the design of simple, miniaturized biomolecular assays. His group is developing ways to fold DNA into controlled nanoscale designs and convert these structures into functional nanomaterial systems through self-assembly and selective metallization. He is also combining affinity purification and solid-phase enrichment with electrophoretic separation in miniaturized devices to enable biomarker quantitation. Finally, his group is working to develop easy-to-use micro- and nano-fluidic chips for molecular analysis. These projects are pushing new frontiers in chemistry, medicine and engineering.

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1983 - Philadelphia Mary Kaiser Matthew O'Brien John Lephardt D. Bruce Chase Peter Keliher 28 Governing Board Chair General Program Exhibit

Governing Board Chair

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1996 - Kansas City Rachael Barbour O. Karmie Galle William Fateley Scott McGeorge

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1998 - Austin John Graham David Laude Isiah Warner and Linda McGown Scott McGeorge

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2000 - Nashville John Koropchak Arlene Garrison Michael Carrabba Scott McGeorge

2001 - Detroit David A. Laude David Coleman and L. Felix Schneider David J. Butcher Scott McGeorge

2002 - Providence Michael Carrabba Robert G. Michel Mark A. Hayes Scott McGeorge

2003 - Fort Lauderdale Ronald Williams Rina Dukor James Rydzak Scott McGeorge

2004 - Portland Michael Blades David Trimble George Agnes Scott McGeorge Governing Board Chair General Program Exhibit

Governing Board Chair General Co-Chairs Program Exhibit

Governing Board Chair General Chair Program Chair Exhibit

Governing Board Chair General Program Exhibit

Governing Board Chair General Program Exhibit 2005- Quebec City, Canada Mark Hayes Denis Boudreau Paul Farnsworth Scott McGeorge

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2007 - Memphis James Rydzak Paul Bourassa Ian R Lewis Mike Carrabba

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2009 - Louisville Becky Dittmar Jessica Jarman Curtis Marcott Mike Carrabba

2010 - Raleigh S. Douglass Gilman David J. Butcher André J. Sommer Mike Carrabba

2011 - Reno S. Douglass Gilman Greg Klunder Pavel Matousek Mike Carrabba

2012 - Kansas City Ian R. Lewis Brandye Smith-Goettler Steven Ray Mike Carrabba

2013 - Milwaukee, WI Ian R. Lewis Fred LaPlant Mike George Mike Carrabba

2014 - Reno, NV Greg Klunder Luisa T. M. Profeta José R. Almirall Mike Carrabba

Governing Board Chair General Program Exhibit

Governing Board Chair SciX General SciX Program SciX Exhibits

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SOCIETY AND COMMITTEE MEETINGS AND EVENTS

FACSS/SciX ORGANIZATION

Sunday, September 27, Ro	om 550B, convention center
8:30 - 10:30 am 4:00 - 6:00 pm	SciX Long Range Planning Meeting (Conference) FACSS Long Range Planning Meeting (Federation)
7:15 – 7:45 pm	Program Committee
Monday, September 28, Re	oom 553B, convention center
12:15 – 1:15 pm	SciX 2016 Minneapolis Meetings: Budget, and Planning Budget and Eingneg Committee
5.20 - 5.50 pm	sour 553R convention center
12:15 – 1:15 pm	SciX 2016 Minneapolis Meeting: Program
3:20 – 3:50 pm	Site Selection Meeting
Wednesday, September 30	, Room 553B, convention center
12:15 - 1:15 pm	SciX 2017 Reno Meetings: Budget, Program and Planning
Thursday, October 1 Noon	Executive Committee Meeting (for the Executive Committee only) Room 557 convention center
6:00 pm	Governing Board Meeting (light dinner will be provided), <i>Bristol/Kent, Omni Hotel</i>
9:30 pm	Governing Board Chair Reception (delegates and invitees), Newport, Omni Hotel
	COBLENTZ SOCIETY
Monday, September 28	
Noon – 1:00 pm	Coblentz and SAS Speed Mentoring Session, Rotunda, convention center. The Coblentz and SAS Societies are
	hosting a Speed Mentoring Event. Prospective mentors and mentees will interact in a fun, fast-paced one-on-one
	Registration is free and lunch will be provided.
Noon – 1:00 pm	Coblentz Challenge, <i>Room 558B, convention center</i> . The Coblentz Challenge has been established to find expert
	technical spectroscopic mentors for the Society. The Challenge will have a number of questions or tasks from
	understandings of spectroscopy techniques or methods. The mentors will be ideal scientists to impart their
	knowledge to others who wish to learn more about vibrational spectroscopy.
1:00 - 3:00 pm	Coblentz Board Meeting, Executive Boardroom in Omni Hotel
	SOCIETY FOR APPLIED SPECTROSCOPY
Saturday, September 26, <i>P</i>	Room 550B, convention center
3:00 – 9:00 pm	SAS Executive Committee
Sunday, September 27 Time TBD	SAS Members Only Event Lunch and Boat Tour
	Union Station Brewery (across from the Omni)
	36 Exchange Terrace
	Providence, RI
Monday, September 28, R_{0} 12:00 – 2:00 pm	SAS Publications Committee
Tuesday, September 29, R	oom 557. convention center
8:00 – 10:00 am	SAS Membership/Publicity Committee
12:00 - 2:00 pm	SAS Editorial Board Meeting
4:00 – 7:00 pm 7:30 pm	SAS Governing Board Meeting SAS Wine and Cheese Awards Reception, <i>Ballroom A convention center</i>
1	
SAS FAT TECHNICAL SESSION Tuesday, September 29, Room 5534	
3:30 pm SAS PAT Technical Section Business Meeting	
NASLIBS	
Monday, September 28	

12:00 pm

7:30 pm

NASLIBS Board Meeting, *Show Suite C/D* NASLIBS and SAS Sponsored Reception, *Room Rotunda*. All conferees are invited.

SciX EXHIBITORS

The exhibit is one of the focal points of the SciX Conference. Exhibits are the realization of the research presented during the scientific symposia and include innovation instrumentation, software, and supplies. New technologies and products will be shown and you will find an interesting mix of sales, scientific, and engineering expertise among their representatives.

Sunday, 4:00 pm, What's Hot Exhibitor Presentations in Ballroom B/C (raffling two Samsung Tab 4s during the session) Tuesday and Wednesday, 11:40 am, What's Hot Exhibitor Presentations in Exhibit Hall C/D Tuesday and Wednesday, 11:00 am - noon, Poster Session and Coffee Break in Exhibit Hall C/D Tuesday and Wednesday, Noon, complimentary lunch for all attendees in Exhibit Hall C/D Tuesday and Wednesday, 3:00 – 3:50 pm – Poster Viewing and Break

Refer back inside cover for exhibit hall layout

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ACS Division of Analytical Chemistry

2019 Galisteo St., Bldg I-1 Santa Fe, NM 87505

www.analyticalsciences.org

With 8,000 members, the Analytical Division is the third largest division of the American Chemical Society. It organizes programming at the spring and fall ACS meetings, Pittcon and the SciX Conference. The division website provides a variety of information and member services, including the Analytical Sciences Digital Library. The division has a wide range of outreach programs including student travel grants and regional meeting support. Its award program includes undergraduate, graduate and professional awards. This member oriented and directed group works for you! Please join or volunteer to help. Visit our website at www.analyticalsciences.org for more information.

Advanced Chemistry Development Inc. (ACD/Labs) Booth #89 8 King Street East

Ste 107

Toronto, ON, M5C 1B5 Canada www.acdlabs.com

Advanced Chemistry Development, Inc., (ACD/Labs) is an informatics company that provides solutions in support of R&D. Our software platforms unify analytical and chemical information in a collaborative environment; and provide tools that enable scientists to extract, capture, and apply knowledge from analytical experiments and predicted molecular property data

AES Electrophoresis Society

Booth #5

Booth #77

1202 Ann St Madison, WI 53713

www.aesociety.org

AES Electrophoresis Society is a unique, non-profit, international organization founded to advance and promote electric field-mediated separations, manipulations, and related phenomena. The field of electrokinetics intersects microfluidics and microdevices. biotechnology, theoretical modeling, material synthesis, nanotechnology and many others. Electrophoretic technologies play a central role in scientific investigations in clinical, basic, and applied disciplines from life sciences through chemistry and physics, to engineering. Our goal is to promote excellence in electrokinetic technologies, thus improving the overall quality and sophistication of scientific research.

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Booth #35

Booth #34

Booth #30

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Booth #100

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of its members, the society sponsors scientific conferences, creates

Coblentz Society

symposia for research presentations, provides social activities to stimulate informal discussion, and recognizes excellence in vibrational spectroscopy through four sponsored awards (the Coblentz, Craver, Williams-Wright, and Lippincott Awards). The society also administers the ABB Bomem-Michelson Award. The Coblentz website can be found at http://www.coblentz.org.

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Booth #10

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Future Meeting: September 18 – 23, 2016 Minneapolis, MN
Booth TBD

Booth #11A

FACSS/SciX 2019 Galisteo St., Bldg I-1 Santa Fe, NM 87505

www.facss.org; www.scixconference.org

SciX 2016 presented by FACSS will be held September 18 - 23 in Minneapolis, MN at the Hyatt Regency Hotel. The conference attracts top scientists from academia and industry for a powerhouse collection of lectures, posters, exhibits, and more. Symposia includes groundbreaking research and prestigious internationally recognized awards. SciX offers daily networking opportunities through its exhibits and social events.

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Fiveash Data Management (FDM) 211 Vista Road

Madison, WI 53726

Booth #18

Booth #99

www.fdmspectra.com FDM provides FTIR and Raman libraries to scientists worldwide. The FDM ALL ATR Bundle has 8 Diamond ATR libraries (polymers, adhesives and sealants, organics, inorganics, essential oils, dyes, drugs) and 3 Germanium ATR libraries, 6380 spectra in total. The FDM Raman Bundle (polymers, adhesives and sealants, organics, inorganics, minerals) has 3350 spectra. The FDM Raman Minerals has 14300 spectra run with 514, 532, 780 and 785 nm lasers from more than 2000 minerals species. The FDM ATR Drugs Mixtures has nearly 845,000 spectra and the FDM ATR Drug Kit has more than 200 2- and 3-component mixtures of drugs with adulterants or diluents.

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Bridgewater, NJ 08807

www.hamamatsu.com

Hamamatsu Corporation is a leading manufacturer of devices for the generation and measurement of electromagnetic radiation including the x-ray, ultraviolet, visible, infrared, and terahertz regions of the spectrum. These devices include photodiodes, photomultiplier tubes, light sources, image sensors, and photoconductive detectors. Capitalizing on our experience in image sensors and MOEMS, we also have a line of spectrometers for applications from the ultraviolet through the near infrared. We also provide systems ranging from cameras which include the image sensor, electronics and software for scientific imaging, to full instruments used in areas such as semiconductor inspection. Our dedication to the advancement of photonics through extensive research results in state-of-the-art products used throughout the world in scientific, industrial, and commercial applications.

Future Meeting: September 18 – 23, 2016, Minneapolis, MN

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HORIBA Scientific

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Ibsen Photonics

Ryttermarken 15-21 Farum, Other, Denmark DK-3520

www.ibsenphotonics.com

Ibsen Photonics is the global leader in transmission gratings and OEM spectrometer modules for UV, VIS, and NIR spectral ranges. The overall key benefits of our products and technologies are:

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Ibsen Photonics is a privately held company with headquarter in Farum, Denmark. For more information please visit www.ibsenphotonics.com

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ICP Information Newsletter, Inc. is a nonprofit corporation established in 1997 to foster science education, research, and study in spectroanalytical chemistry. The corporation includes three division: the ICP Information Newsletter, a monthly publication with international distribution that gathers all conference and published information related to plasma spectrochemistry; the Winter Conference on Plasma Spectrochemistry, a biennial meeting with international participation featuring state-of-the-art research developments in plasma spectrochemistry, and the University Research Institute for Analytical Chemistry, the research and development branch that provides specialty plasma spectrochemical analysis, consulting, method development, training, and applied research with ICP atomic emission and mass spectrometry. The 2016 Winter Conference is planned for January 10 - 16, 2016 in Tucson, Arizona. The ICP Information Newsletter now in its 41th year of publication is distributed to subscribers in computer - readable format on CD-ROM. Visit http://icpinformation.org for subscription and conference details.

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www.innovativephotonics.com

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www.kosi.com

Kaiser Optical Systems, an Endress+Hauser Company, is recognized as a world leader in the design and production of Raman analyzers and components for spectroscopy. Our RamanRxn Systems[™] suite of Raman analyzer includes ATEX certified process analyzers for classified installations, reaction analysis analyzers, bulk solids analyzers, gas-phase analyzers, Raman microscopes, and the Raman WorkStation[™] featuring Kaiser's revolutionary fast, quantitative PhAT technology and transmission Raman capability. Our components product lines include performance filters, high F/# spectrographs, and OEM systems. Raman analyzer installation locations include R&D, Pilot plant, manufacturing, and QA/QC. Pharmaceutical PAT applications include reaction monitoring, API production, polymorphic form quantitation, drug product unit operations (including blending, granulation, and tableting), and end product testing. Other Applications areas for RamanRxn SystemsTM analyzers include biotech, semiconductors, nanotechnology, petrochemical, polymers, and specialty chemical. We invite you to visit our booth, learn about our products, and discuss your applications needs.

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100 Marshland Road Hilton Head, SC 29926

www.kigre.com

Kigre manufactures 1.54 um "eye-safe" diode pumped erbium glass laser transmitters. These transmitters can be used in applications including Laser Induced Breakdown Spectroscopy (LIBS), laser range finding and range gated imaging. Kigre's lasers range from 1 to 10 mJ and 1 to 10 Hz with a 6 ns pulse widths.

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Laserand, Inc. 2725 Rue Notre-Dam, Ste 302 Lachine, QC H8S2H3 Canada

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Lasertel, Inc.

7775 N Casa Grande Hwy Tucson, AZ 85743

www.lasertel.com

Lasertel is a vertically integrated manufacturer of high power semiconductor laser diodes, optics and developer of custom laser solutions. For scientific applications, Lasertel offers volume contract manufacturing of diode pumped solid state (DPSS) laser systems and sub-assemblies.

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Goetzix, VA 6840, Austria www.montfortlaser.com

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NeaSNOM, an ultra-stable, easy-to-use and highly modular optical near-field microscope system utilizing a ground-breaking and patented optical background-filtering technique (PH-detection) for simultaneous acquisition of optical amplitude (reflectance) and phase (absorbance) near-field images and spectra. The NeaSNOM microscopy and spectroscopy system combines the best of two worlds - the nanoscale spatial resolution of atomic force microscopy (AFM) with the analytical power of visible, infrared and even THz imaging and spectroscopy. At a spatial resolution of only 10nm the method only requires standard AFM sample preparation. This opens a new era for modern nano-analytical applications such as chemical nano-identification in the IR fingerprint region (nano-FTIR), nano-plasmonic field mapping (VIS & IR) or free charge carrier nano-mapping and spectroscopy (THz/THz-TDS).

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830 Douglas Avenue

Dunedin, FL 34698

www.oceanoptics.com

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850 E. Duarte Rd. Monrovia, CA 91016

www.ondax.com

Ondax Inc. is a world leading manufacturer of low frequency/THz-Raman® systems and wavelength stabilized lasers to enable best-inclass Raman systems in a compact, portable footprint. Ondax's patented THz-Raman® Spectroscopy Systems and filter components extend the range of traditional Raman spectroscopy into the terahertz/low-frequency regime without limiting the ability to measure the chemical fingerprint region. THz-Raman spectra show clear differentiation of structural differences that are ideal for identification and analysis of polymorphs, phase/process monitoring and synthesis methods. Ondax's SureLock[™] wavelength-stabilized Raman lasers deliver either single-frequency or line-narrowed performance with very low power consumption. Wavelengths from 405nm to 808nm with powers up to 800mW are available in compact TO cans, pigtailed butterfly, free-space and fiber-coupled module configurations.

OPOTEK, Inc.

Booth #104

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Optigrate Corp 562 S Econ Cir. Oviedo, FL 32765

Oviedo, FL 32765 www.optigrate.com OptiGrate Corp is a pioneer and world leader in commercial volume Bragg gratings (VBGs) and VBG-based ultra-narrow hand optical

Bragg gratings (VBGs) and VBG-based ultra-narrow band optical filters. For over a decade OptiGrate has designed and manufactured a full range of VBGs in inorganic photo-thermo-refractive silicate glass and supplied VBG-based filters to more than 300 customers on 5 continents. OptiGrate's product line of Raman optical filters includes ultra-narrow band Notch filters (BragGrateTM Notch Filter) and laserline cleaning filters (BragGrateTM Bandpass Filter) with a linewidth narrower than 5 cm-1 at FWHM. Such filters are fully environmentally stable, do not degrade in high intensity light irradiation, and enable simultaneous measurements of Stokes and Anti-Stokes frequencies down to 5 cm-1 with a single-stage monochromator Raman systems. Standard filters are available at 488, 514, 532, 633, 785, and 1064 nm, while any custom wavelength in a range from 400 to 2000 nm can be ordered.

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www.pd-ld.com

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Booth #76

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Trenton, NJ 08619

www.princetoninstruments.com

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www.quantel-laser.com

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Rigaku Analytical Devices

Booth #24

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www.RigakuAnalytical.com

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www.rpmclasers.com

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Booth #7

7102 Riverwood Dr.

Columbia, MD 21046 www.ssi.shimadzu.com

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www.s-a-s.org

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Booth #32

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Campaign, IL 61821

www.spectroclick.com

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Spectroscopy Magazine / Advanstar

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Thermo Scientific

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Thorlabs

56 Sparta Ave Newton, NJ 07860

www.thorlabs.com

Thorlabs, a vertically integrated photonics products manufacturer, was founded in 1989 to serve the laser and electro-optics research market. As that market has spawned a multitude of technical innovations, Thorlabs has extended its core competencies in an effort to consistently serve its industry at the research end, as well as the

industrial, life science, medical, and defense segments. The organization's highly integrated and diverse manufacturing assets include semiconductor fabrication of Fabry-Perot, DFB, QCL, ICL, and VCSEL lasers, fiber towers for drawing glass optical fibers (silica, fluoride, tellurite, and hollow core), MBE crystal growth machines, brushless DC motor technology for advanced microscopy positioning stages, extensive glass and metal fabrication facilities, advanced thin film deposition capabilities, and optomechanical and optoelectronic shops. Headquartered in Newton, NJ, the company has over 1100 employees at 13 manufacturing and sales offices throughout the United States, United Kingdom, Germany, France, Sweden, Japan, China, Canada, and Brazil.

Tofwerk AG

Booth #19

Uttigenstrasse 22 Thun, 3600 Switzerland www.tofwerk.com

Tofwerk designs, develops and manufactures specialized and customized state of the art time-of-flight mass spectrometers (TOFMS). Tofwerk's personnel together have many decades experience in TOFMS hardware, fast data acquisition and mass spectrometry software. Tofwerk technology is being coupled to e.g. high-pressure interfaces and ion mobility drift cells. It is the core of several mass spectrometers for aerosol analysis and other atmospheric applications widely used around the world. Tofwerk's icpTOF equips the iCAP Qc from Thermoscientific with TOF detection power. The iCAP Qc provides versatile sample introduction, robust ICP, simple access to cones and lenses and the Qcell technology. The TOFMS adds simultaneous multi-element detection, QMS-like sensitivity, linear response and mass resolving power >3000. More information on: www.tofwerk.com/icp

Tornado Spectral Systems

555 Richmond Street West, Ste 705

Booth #51

Toronto, ON M5V 3B1 Canada www.tornado-spectral.com Tornado Spectral Systems Inc. is an emerging tech company developing radically superior tools for measuring the chemical composition and structure of materials in real-time for a variety of demanding industrial processes. TSS's new class of instruments – the HyperFlux PRO Raman series - can acquire chemical signatures of interrogated samples with the speed and accuracy required to perform many quality and safety measurements directly on the production line instead of using time-consuming laboratory or off-line measurements. Tornado has also developed OCTANE, a line of nanophotonic spectrometers for OCT applications. These optical instruments meet industry specifications for commercial OCT spectrometers and use integrated optics instead of free-space components as their optical

TSI Inc

core.

Box 218

500 Cardigan Road Shoreview, MN 55126 www.tsi.com

TSI's new ChemLogix[™] family of instruments simplifies complex chemical analysis. Its complete line of solutions, including Laser-

Induced Breakdown Spectrometers and Raman Spectrometers, provides rapid and reliable identification of materials and chemical composition of solids in both the laboratory and in the field.Backed by TSI's global sales and support, ChemLogix instruments truly are the smarter – and more logical – choice for chemical analysis.

Viavi Solutions

430 N. McCarthy Blvd Milpitas, CA 95035 osp.viavisolutions.com

Viavi Solutions Optical Security and Performance Products (OSP) develops and delivers high value optical components and solutions that enhance the security, safety, and other performance attributes of government and commercial customers' products. The ultra-compact, cost-effective MicroNIR spectrometer measures wavelengths of 950 -1650 or 1150 - 2150 nm, weighs less than 60 grams, and is USB powered or wireless. Offering the highest performance-to-price ratio in the industry, the ubiquitous MicroNIR integrates all components into a small unit suitable for convenient, portable use in the field as well as on-line or at-line process monitoring and control. The MicroNIR enables real-time, non-destructive evaluations anywhere. Viavi Solutions (NASDAQ: VIAV) innovates and collaborates with customers to build and operate the highest-performing and highestvalue networks in the world. Learn more about at www.osp.viavisolutions.com and follow us on Twitter, Facebook, and YouTube.

Wasatch Photonics

3022 Stirrup Creek Dr., Ste 311 Durham, NC 27703

www.wasatchphotonics.com

Wasatch Photonics, Inc. is the leader in high performance Volume Phase Holographic Gratings (VPHGs) and Volume Phase Holographic Optical Elements (VHOEs). Products developed by our world class design team include; Raman sensors and instrumentation, advanced holographic components for spectroscopy, hyperspectral imaging, astronomy and OCT. Company headquarters and the holographic component manufacturing facility are located in Logan, Utah. Instrumentation is manufactured at our Systems Division facility located in Research Triangle Park, NC. High efficiency VPH Gratings combined with low F number optics allow unprecedented throughput for our Raman spectrometers. Our Raman systems provide ultimate sensitivity for process control, rapid SERS tag identification and unknown substance identification for homeland security.

WITec Instruments Corp.

130G Market Place Blvd Knoxville, TN 37922

www.WITec-Instruments.com

WITec is a manufacturer of high resolution optical and scanning probe microscopy solutions for scientific and industrial applications. A modular product line allows the combination of different microscopy techniques such as Raman, NSOM or AFM in one single instrument for flexible analyses of optical, chemical and structural properties of a sample.

Booth #26

Booth #82

Booth #105

Workshops are a valuable component of the SciX conference and are conducted by leading experts. There is an additional charge for most workshops. See registration form for costs.

FINDING YOUR WAY THROUGH THE PAT MAZE

Martin Warman and Frank Qi, Vertex Pharmaceuticals

Sunday 1:00-5:00 pm

Introduction

The PAT guidance has been around for over 10 years now, even though the term PAT has clear definitions under ICH, ASTM etc it yet it still means different things to different folks.

Purpose

The purpose of this training course is to allow attendees to understand the meaning behind the guidance, move the initial focus from the tools, and allow attendees to first establish the 'way', 'where', 'when', before looking at the 'which' and 'how'.

Who Will Benefit From The Training?

This is not aimed at scientists trying to learn the fundamentals of the techniques. Instead the application of the techniques will be discussed, and case studies shared, to answer real-world examples, where the first step was to appropriately describe the problem.

The course is intended for analysts and spectroscopists looking to better understand types of application, and therefore how to interact with process specialists (formulators and chemical engineers) and allow them to better interact with other specialties within crossfunctional teams. The course will also be useful for process specialists trying to understand how PAT could be used to help in Process Understanding during process development and optimization, and In Process Control. The intention is that attendees will also come away with an understanding of how process understanding, the application of appropriate in-process controls can be built into a Control Strategy to allow real-time release.

Outcomes

The intention of this course is not to instruct attendees on which applications and tools to use. The intention is that attendees leave the training better equipped to identify potential opportunities within their own processes, but also able to analyze those opportunities to better describe the needs of the application, how best to collect the information to answer those needs, but also the thought process behind looking at those needs from more than one angle to understand what the data is indicating about the process – rather than the more traditional approach of ensuring all data gives the 'same answer'.

LIBS FUNDAMENTALS AND APPLICATIONS Amy Bauer, *TSI* Sunday, 1:00-5:00 pm

This course will cover the basics of LIBS and how this rapidly growing spectroscopic method can be used both in the lab and for industrial problems. After a brief introduction, different instrument configurations and analysis methods are covered in the context of application examples. Emphasis will be placed on identifying good LIBS applications, choosing suitable hardware, and expectations for measurement data. Ample time will be allowed for questions and discussion of particular problems of interest to the attendees.

FUNDAMENTALS AND PRACTICAL APPLICATIONS OF RAMAN SPECTROSCOPY David Tuschel. HORIBA Scientific

Monday, 9:00 am-1:00 pm

Monday, 9:00 am-1:00 pm

Who should take this course?

In this course, you will learn the basics of applied Raman spectroscopy. The topics and content will be of value to researchers in industry and academia, analytical chemists, laboratory technicians, teachers, graduate students and materials scientists. The instructor will teach Raman spectroscopy at the introductory level and cover those topics which will allow the student to practically apply the material learned in the laboratory, workplace and classroom. Students will learn about:

- Raman scattering through the classical description
- Laser excitation wavelength dependence
- Raman sampling
- Dispersive grating based Raman spectrometers
- Spectral resolution and range
- Signal detection and wavelength dependence
- Interpretation of Raman spectra of organic compounds
- Spectral assignment of functional groups
- Interpretation of Raman spectra of inorganic compounds
- Spectral differences of crystals, glasses and amorphous materials
- Application of "Raman crystallography"

Course Outline

- Raman Spectroscopy
 - Chemical bond polarizability
 - Excitation wavelength dependence
 - Raman active normal vibrations
 - Group theory and spectral selection rules
 - Polarization
 - Raman sampling

Instrumentation for Raman Spectroscopy

- Dispersive grating based spectrometer
- Spectral resolution and free spectral range
- Signal detection
- Instrumental wavelength and polarization dependence
- Spectral quality, band shape, and band fitting
- Laser focus and Raman sampling

Interpretation of Raman Spectra - Organic Molecules

- Aliphatic compounds
- Alkenes and aromatics
- Carboxylic acids, esters and amides
- Nitrogen and sulfur containing groups
- Polymers
- Interpretation of Raman Spectra Inorganic Molecules, Crystals, Glasses and Amorphous Materials
- Coordination compounds
- Semiconductors
- Nanomaterials
- Gems and minerals
- Glasses and amorphous materials

Raman imaging

- Hyperspectral data and imaging rendering
- Spatial resolution
- Confocality
- 3D Raman imaging

Application of "Raman Crystallography"

- Crystal classes and Raman tensors
- Raman polarization selection rules
- Polarization/Orientation Micro-Raman Spectroscopy

CHEMOMETRICS WITHOUT EQUATIONS Barry Wise, Eigenvector Monday 9:00 am-4:30 pm

One day including time for hands-on exercises with PLS_Toolbox and Solo software.

Chemometrics without Equations concentrates on two areas of chemometrics: 1) exploratory data analysis and pattern recognition, and 2) regression. Participants will learn to safely apply techniques such as Principal Components Analysis (PCA), Principal Workshops are a valuable component of the SciX conference and are conducted by leading experts. There is an additional charge for most workshops. See on-site registration form for costs.

Components Regression (PCR), and Partial Least Squares (PLS) Regression. Examples will include problems drawn from process monitoring and quality control, predicting product properties, and others. The target audience includes those who collect and/or manage large amounts of data that is multivariate in nature. This includes bench chemists, process engineers, and managers who would like to extract the maximum information possible from their measurements.

Chemometrics Without Equations (or Hardly Any) is designed for those who wish to explore the problem solving power of chemometric tools, but are discouraged by the high level of mathematics found in many software manuals and texts. Course emphasis is on proper application and interpretation of chemometric methods as applied to real-life problems. The objective is to teach in the simplest way possible so that participants will be better chemometrics practitioners and managers.

Course Outline

- Introduction
 - \circ what is chemometrics?
 - resources
 - Pattern Recognition Motivation
 - what is pattern recognition?
 - relevant measurements
 - some statistical definitions
 - Principal Components Analysis
 - what is PCA?
 - scores and loadings
 - \circ interpretation
 - $\circ \quad \text{supervised and unsupervised pattern recognition} \\$
 - examples
- Regression
 - what is regression?
 - classical least squares (CLS)
 - o inverse least squares (ILS)
 - principal components regression (PCR)
 - partial least squares regression (PLS)
 - examples
- Summary

HOW TO BE A PERSON OF INFLUENCE Richard Osibanjo, *Intel* Monday, 1:00 – 4:00 pm

Do you want to become a person people listen to? It is a myth that you need a formal position in order to make a difference in your organization. Great leaders influence their teams to do things they never though they were capable off. Influence comes by connecting with your team members. Influence is not a gift it has to be earned. When you grow in influence with people, they will give you permission to lead them. There can be no significant progress in your personal and professional lives without influence. In this workshop, participants will learn how to grow in influence and use it to make significant changes in their communities. No matter what your goals are in life or what you want to accomplish, you can achieve them quicker, you can become more productive, and the contribution you make can in your circle can make a difference in your circle, if you learn how to become a person of influence.

FAST CATCHUP

Ellen Miseo, Hamamatsu ; Joseph Dorscheimer, Thermo Fisher; Mary Kate Donais, Saint Anselm College; James Rydzak, GlaxoSmithKline; Edita Botonjic-Sehic, Morpho Detection Tuesday, 9:00am-12:00 pm

9:00-9:20

Ellen Miseo, Technology Development, Hamamatsu Corporation

Title: Analytical Instruments –It's easy, build it and people will use it. Right?

9:20-9:40

Joseph Dorsheimer, New England Technical Sales Representative, Thermo Fisher Scientific

Title: A Crash Course in How Scientific Instruments are Sold 9:40-10:00

2:40-10:00

Mary Kate Donais, Professor, Dept. of Chemistry Saint Anselm College

Title: Academics – Not Just "Chalk Talks" Anymore 10:00–10:20

James Rydzak, *S Sr. Scientific Investigator, GlaxoSmithKline* Title: Vibrational Spectroscopy and PAT in the Pharmaceutical Industry.

10:20-10:40

Edita Botonjic-Sehic, Sr. Engineering Program Manager, Morpho Detection, LLC

Title: Explosives Detection and government contracts

10:40-12:00

Open Discussion

MULTI-BLOCK, MULTI-SET, MULTI-LEVEL DATA FUSION

Barry Wise, *Eigenvector* Tuesday, 9:00 am–1:00 pm

Workshop Objectives:

The goal of the workshop is to familiarize the attendees with modeling methods that are useful for investigating and describing data sets with unconventional structures. Attendees will also learn how to use modeling software to explore these data sets and make use of them for data discovery and process monitoring purposes. Abstract:

Most multivariate analysis methods, including Principal Components Analysis (PCA) and Partial Least Squares (PLS) regression, are intended for use with 2-way data, i.e. data that fits into conventional two dimensional tables. However, many analytical and process data sets do not fit the 2-way paradigm. This includes batch and semi-batch process data, but also a wide variety of situations where three dimensional data cubes are associated with a vector or matrix of data.

This workshop considers a number of model forms that can be used on data sets that do not fit the conventional 2-way approaches, *e.g.* PCA or PLS, but also the multi-way approaches, such as Parallel Factor Analysis (PARAFAC) and Multi-way (unfold) PCA (MPCA). This includes instances where data is in distinctly different blocks that share a common mode, in which case the multi-block variants of PCA and PLS may be appropriate. Another case is when the data is semi-batch, such as where processes are run for periods of time and then "reset" e.g. when catalysts are regenerated or the process equipment is cleaned. In these cases tools such as Simultaneous Components Analysis (SCA) or Multi-level SCA (MLSCA) may be used to understand the difference between runs and the variation within runs. Multilevel PLS variants are also potentially useful. Finally, instances where data sets consisting of blocks with different numbers of Workshops are a valuable component of the SciX conference and are conducted by leading experts. There is an additional charge for most workshops. See on-site registration form for costs.

modes must be fused are considered. For example a 3-way data set might share a mode with a 2-way data set such as when a number of batch data records must be related to multiple quality parameters. In these instances models based on coupled matrix and tensor factorizations (CMTF) may be applied.

Attendees will work on hands-on exercises using PLS_Toolbox or Solo software.

Course Outline

- Introduction
 - Definition of multi-block, multi-set and multilevel
 - o Goals of Data Fusion
- Review of Multivariate and Multi-way Models
 - Principal Components Analysis (PCA)
 - Partial Least Squares (PLS) Regression
 - Multi-way (unfold) PCA and PLS
 - Parallel Factor Analysis (PARAFAC)
 - Multi-way PLS (N-PLS)
 - Introduction to PLS_Toolbox/Solo
 - Hands-on exercises
- Multi-set and Multi-Level Models
 - Simultaneous Components Analysis (SCA)
 - ANOVA SCA (ASCA)
 - o Multi-level SCA (MLSCA)
 - Multi-level PLS
 - Hands-on exercises
- Data Fusion Models
 - o Coupled Matrix-Tensor Factorizations (CMTF)
 - Approaches for identifying CMTF models
 - Alternating Least Squares (ALS)
 - Direct optimization
 - o Hands-on exercises

EMOTIONAL INTELLIGENCE Richard Osibanjo, *Intel* Tuesday, 1:00-4:00 pm

In today's competitive and diverse workforce, it is not sufficient to only be a technical expert. Your behavioral and technical competence is what makes the difference between the good and great. Your IQ will get you a job, while your emotional quotient (EQ) will keep you from being fired. It's your EQ that enables you get along and work effectively with different personalities. Research studies have shown that EO accounts for up to 80% of success in life. While there is debate on the 80%, there is consensus that effective leaders are better off and more productive having a high degree of EQ. EQ studies have also shown that science/engineering disciplines have the lowest scores when it comes to emotional intelligence. The good news is that unlike IQ, EQ can be learned. The four primary components of emotional intelligence are self-awareness, selfmanagement, social awareness and relationship management. In this workshop you will learn the basics of emotional intelligence and build a solid foundation for understanding each component. You will become more self-aware, learn to embrace and celebrate your authentic self. Your ability to solve problems, resolve conflict and build high performing teams will be increased as a result of attending this workshop. High performing teams and individuals possess strong EQ skills in each of these four areas, and they practice these skills daily. Anyone can become more emotionally intelligent with the right training and practice.

MULTIVARIATE DATA ANALYSIS WITH THE UNSCRAMBLERTM

Heather Brooke, CAMO Smart Software Wednesday, 9:00 am-4:30 pm

This course is ideal for people who are:

- new to multivariate analysis, those wanting a refresher on methodology
- process engineers looking at strategies for implementing multivariate statistical process control
- working with sensory or other survey based data
- spectroscopists who want to have a better understanding of the fundamentals of multivariate data as applied to other non-spectroscopic situations

Course outline

- What is Multivariate Analysis
- Motivation for using Multivariate Analysis
- Data Collection and Visualization
- Exploratory Data Analysis
- Outlier detection using PCA
- An introduction to Multivariate Regression
- Interpretation of Multivariate Regression Models
- Correct Validation Practices
- Summary and Overview

PROFESSIONAL ANALYTICAL CHEMISTS IN INDUSTRY: WHAT DOES AN ANALYTICAL CHEMIST DO? Diane Parry, Procter & Gamble Wednesday, 9:00 am-3:00 pm

This seminar begins with a discussion of the education requirements and salaries that an analytical chemist may expect in industry. The different roles (including scientific consultant, methods developer, and problem solver) of the industrial analytical chemist are explained. A majority of time is spent on problem solving, both the process and solving real-world problems. Students will learn a "framework" for approaching problems. Time will be available to ask questions on these topics and other related subjects. The Course text includes supplementary material on finding a job, summer employment, etc. The entire course, especially the problem solving, is structured for extensive participation and interaction.Additional information is available at http://www.pg.com/science/prof chemists.jhtml.

The Course is intended primarily for undergraduate students to educate them about careers as analytical chemists in industry. However, graduate students, high school teachers, and college faculty have indicated it was worth their time to attend.

- Typical Course Schedule
- 1. Course Introduction and Personal Perspectives
- 2. Perspectives: The Industrial Analytical Chemist
- 3. Problem Solving I: The Bulging Drum Problem
- 4. Break
- 5. Questions and Answers
- 6. An Approach to Problem Solving
- 8. Problem Solving II: Potential Issues Concerning Use of Recycled Plastics
- 9. Questions & Answers II
- 10. Problem Solving III: Problem Solving by Student Teams
- 11. Summary and Evaluation

WORKSHOPS

Workshops are a valuable component of the SciX conference and are conducted by leading experts. There is an additional charge for most workshops. See on-site registration form for costs.

IMPACT: THINK GLOBALLY - ACT LOCALLY Richard Osibanjo, Intel Wednesday, 1:00-4:00 pm

You have a passion for Chemistry and want to make a difference in your world. You are not satisfied with just writing papers or being a lab rat. You want to make an impact. Can you imagine what could happen if you decided to pursue your dreams? You will be remembered for the problems you solve or the ones you create. People who solve big problems are the ones that will be remembered. Isaac Newton discovered the Newton's Laws of Motion. Louis Pasteur discovered vaccines for anthrax and rabies. Marie Curie was the pioneer researcher on radioactivity. The courage and hard work of our great predecessors was a down payment for what we enjoy now. We can't afford to settle and play it safe. There is a genius in you. What is that dream that keeps coming to your mind? Your ideas could help solve challenging issues such as Ebola, poverty, and illiteracy. Your techniques and novel work can help transform lives and make our world a better place. Great leaders think locally and act globally. This workshop will help you map your blueprint in pursuing your dreams based on your talents and strengths. You will learn how to take charge of your world by developing your strengths and managing your weaknesses. You will learn how to take your idea from the chalkboard to reality. Impactful leadership is making a significant difference in the lives of people around you. You only need to follow your heart and think the unthinkable. When you know where you are going, the world will open its doors to you. If you want to make an impact in your generation then this workshop is for you. The next step is yours!



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Come Celebrate with the 2015 ANACHEM Award Winner and Editor of the Journal *Analytical Chemistry* Jonathan Sweedler

Wednesday, 3:00 pm, Exhibit Hall C/D



	SUNDAV		Advocating for Women in Science, 552A
4:10 – 6:00 pm	"What's Hot" Vendor Presentations, Ballroom B/C, page 55		Non-linear Optical Spectroscopy for Surface Science, 553A
6:15 pm	KEYNOTE LECTURE . Pre-adaptation: How	3:00 pm	POSTER VIEWING AND BREAK, Ballroom A
	Basic Research Helps Oceanographers Meet Global Challenges; Robert S. C. Munier , <i>Ballroom B/C</i> , page 55	3:50 pm	SYMPOSIA , page 63 Bioapplications of ICP-MS, <i>550A/B</i> Vibrational Spectroscopy: Toward Clinical
7:15 – 9:15 pm	Welcome Mixer, SAS Sponsored Student Poster Session, Coblentz Student Awards, FACSS Student and Tomas Hirschfeld Scholar Awards, Ballroom A		Applications, 555A Chemometric Keys for the Interpretation of Forensic Evidence, 551B Nuclear Forensics, 551A
	MONDAY MORNING		Near-IR, 556B LIBS for Pharmaceutical and Biological
7:50 am	Opening Address		Diagnostics, Ballroom E
8:00 am	KEYNOTE LECTURE . Forensic Microscropy and the Lost Art of Observation, Christopher Palenik , <i>Ballroom B/C</i> , page 56		 Pharmaceutical Applications of Low Wavenumber Spectroscopy, 552B Hot Topic Discussion Session – TERS Resolution,
9:15 am	SYMPOSIA, page 56 RSC/ACS Symposium: Analysis with Photons – Laser & Synchrotron Spectroscopy Science and Applications, 554A/B Eundamentals and Novel Applications of LA-ICP-		555B Pharmaceutical Raman, 556A Careers and Diversity in Analytical Science Discussion Panel, 552A In-situ Surface Science, 553A
	MS: Part I, <i>550A/B</i>		TUESDAY MORNING
	Beyond PCA and PLS: New Frontiers in Chemometrics, 551B	8:00 am	PLENARY LECTURES, Ballroom B/C, page 66 Coblentz Society Craver Award. Ji-Xin Cheng
	Analysis of Counterfeit Drugs and New Psychoactive Substances, 551A Inductrial LIPS, Ballroom F	8:30 am	FACSS Charles Mann Award for Applied Raman Spectroscopy. Sanford Asher
	 Sensing recentiques for Counterfeit Drug Detection, 552B SERS, 555B Extending the Scope of Raman: ROA and Other Recent Advances, 556A Novel Teaching Methods in Analytical Chemistry, 552A Advanced Techniques for Infrared Spectroscopy on Structure-Function Relations of Proteins, 556B Characterization and Surface Science of Nanomaterials, 553A 		 ICP-MS in the Analysis of Nanomaterials, 550A/B Craver Award Session Honoring Ji-Xin Cheng, 554A/B Metabolomis and Personalized Medicine, 555A Chemometric Tools to Discover the Next Magic Bullet via Biological Spectroscopy, 551B GC-MS Based Detection of Emerging Flame Retardants in the Environment, 552B Explosive Detection II: Trace, On-site and <i>in-situ</i> 551A
11:00 am	POSTER SESSION AND BREAK, Ballroom A, page 58 Atomic Spectroscopy I Forensic and Security LIBS I Materials Characterization Nanomaterials		Nanoscale IR: I, 556B New Hardware and Novel Methods in LIBS, Ballroom E Continuous/Flow PAT, 553A Emerging Raman Techniques and Applications I, 555B Bioanalytical Applications of Plasmonics, 556A
	MONDAY AFTERNOON	11:00 am	POSTER SESSION AND BREAK , <i>Exhibit Hall</i>
1:20 pm	 SYMPOSIA, page 61 Fundamentals and Novel Applications of LA-ICP- MS: Part II, 550A/B Award Session Honoring 2015 ACS 		Atomic Spectroscopy II Chemometrics LIBS II Raman
	Spectrochemical Award Winner Frank Bright, 554A/B Biomedical and Forensic Applications of	11:40 am	What's Hot Exhibitor Presentations, <i>Exhibit C/D</i> , page 70
	Vibrational Spectroscopy, 555A		TUESDAY AFTERNOON
	Ensuring Public Safety by Chemometric	Noon	Complimentary lunch in exhibit hall for all
	Authentication of Food and Botanicals, 551B	1.20	registered conferees
	Explosive Detection 1, 551A Standards, Protocols and Quantitative Analysis, Ballroom E	1:20 pm	STMPOSIA, page /0 Innovative Atmospheric-Pressure Plasma Ionizatio Sources, 550A/B
	 Sensing Techniques for Counterfeit Drug Detection II, 552B Bioanalytical SERS I, 555B Raman Microscopy, 556A 		FACSS Charles Mann Award Session Honoring Sanford Asher, 554A/BChemometrics in Pharmaceutical Industry, 551B

PROGRAM OVERVIEW

	TUESDAY AFTERNOON, continued	11:40 am	What's Hot Exhibitor Presentations, <i>Exhibit Hall C/D</i> , page 81
	Contaminants in the Environment, 552B		WEDNESDAV AFTEDNOON
	Mass Spectrometry in Forensics, 551A Nanoscale IR II, 556B	Noon	Complimentary lunch in exhibit hall for all
	Electro- and Liquid Phase-separation Techniques, 552A	1:20 pm	SYMPOSIA, page 81 Microfluidic Electrophoresis Modes for Mass
	Advances in Applications of Handheld/Portable Spectrometers, 553A		Spectrometric Analysis, 552A A Lifetime of Spectroscopy: Celebrating Work of Edward Steers, 5504/B
	Emerging Raman Techniques and Applications II, 555B		Meggers Award Symposium Honoring Eric Brauns, 554A/B
	Raman Imaging/Microscopy II, 555A Nanostructured Materials for Plasmonics I, 556A		Pathogens, 555A Quantum Cascade Lasers - Applications, 556B
3:00 PM	POSTER VIEWING AND BREAK, <i>Exhibit Hall C/D</i>		LIBS for Forensic and Homeland Security, Ballroom E
3:50 pm	 SYMPOSIA, page 73 Atmospheric Pressure Plasmas & Liquid Cathode Glow Discharges, 550A/B Chemometrics for Spectroscopic/Spectrometric 		 Ambient Ionization Methods: Developments and Applications, 552B In Situ Analysis of Industrial Processes and Reactions during R&D, 553A
	Data, 554A/B Diabetes and Its Complications, 555A Ambient Ionization and Non-chromatographic Approaches in Forensics and Homeland Security.	3:00 pm	Spatially Offset Raman Spectroscopy, <i>555B</i> Chemistry in Art and Archaeology, <i>551B</i> New Plasmonic Materials and Techniques, <i>556A</i> POSTER VIEWING AND BREAK
	551A Nanoscale IR III, 556B	3:50 pm	<i>Exhibit Hall C/D</i> SYMPOSIA , page 83
	Miniaturization, 552A LIBS for Environmental and Food Monitoring, Ballroom E SAS DAT Tasknigel Section: DAT in the		RSC/ACS Symposium: Analysis with Photons – Laser & Synchrotron Spectroscopy Scince and Applications II, 554A/B Biogedemons in Floateria Fields, 5524
	Pharmaceutical Industries I, 553A Forensic Applications of Raman Spectroscopy, 555B		Fundamentals and Novel Applications of Glow Discharge Spectroscopy II, 550A/B Translation and Commercialization of Analytical
	Analytical Chemists Easing World Poverty, 551B Nanostructured Materials for Plasmonics II, 556A		Technologies, 555A Difficult Data Sets, 556B
	WEDNESDAY MORNING		Ballroom E
8:00 am	PLENARY LECTURES, <i>Ballroom B/C</i> , page 76 SAS's Lester W. Strock Award. R. Kenneth Marcus		Direct Inject Mass Spectrometry, 552B Dedicated (24/7) Online Analysis of Industrial
8:30 am	SAS's Applied Spectroscopy William F. Meggers Award. Eric Brauns		Chiral Analysis, <i>551A</i> Biomedical Raman Spectroscopy, <i>555B</i>
9:15 am	SYMPOSIA, page 76 Microfluidics and Electrophoresis for Bioanalytical		THURSDAY MORNING
	Fundamentals and Novel Applications of Glow Discharge Spectroscopy: Part I, 5504/B	8:00 am	PLENARY LECTURES, <i>Ballroom B/C</i> , page 87 ANACHEM Award. Jonathan Sweedler
	Lester Strock Award Symposium Honoring R.	8:30 am	AES Mid Career Award. Adam Woolley
	Kenneth Marcus, 554A/B Super-Resolution Microscopy and Imaging, 555A	9:15 am	SYMPOSIA, page 87 Bioanalytical Dielectrophoresis, <i>552A</i>
	Chemometrics/Data Analysis for Forensics, 551A New Developments in QCL Technology, 556B Standoff LIBS, <i>Ballroom E</i>		Atmospheric Pressure innovative Sources: Micro & Microwave Plasmas (M&M), 550A/B ANACHEM Award Symposium Honoring Jonathan
	Mass Spectrometric Techniques in Environmental Analysis, 552B		Sweedler, 552B Musculoskeletal Diseases, 555A
	SAS PAT Technical Section: PAT in the Biopharmaceutical Industries II, 553A Bioanalytical SERS II, 555B		Biomedical Applications of IR Spectroscopy and Imaging, 556B Historical LIBS, Ballroom F
11:00 am	Bioanalytical Applications of Phasmonics II; 556A POSTER SESSION AND BREAK, Exhibit Hall		Advances in On-line Process Analysis, 553A Amyloids and Aggregates: What Do We Know
	C/D, page 78 Biomedical and Bioanalytical		About Structure, 551A IRDG Raman Session – Biological Applicationsof Raman Spectroscopy, 555B
	Environmental/Oceanographic Molecular: IR/Near IR Raman		Compact Raman Applications, 556A
48			Future Meeting: September 18 – 23, 2016 Minneapolis, MN

PROGRAM OVERVIEW

11.00 am	DOSTED SESSION Dalluson 1 mags 90			
11:00 am	Mass Spectrometry	FRIDAY MORNING SPECIAL PLENARY SESSION 555-556		
	Microfiluidics Molecular Imaging	8:00 am	Announcement of Innovation Award Winners	
Pharmaceutical Raman SERS	Pharmaceutical Raman SERS	8:15 am	A Trans-Spectral Celebration of the International Year of Light: From X-Rays to THz Spectroscopy, Page 94	
	THURSDAY AFTERNOON			
1:20 pm	SYMPOSIA , page 91 AES Mid-Career Symposium in Honor of Adam Woolley, <i>552A</i> Ontical Diagnostics and Therapeutics in Cancer.	10:15 am	SciX 2016 preview	
	 Softar Diagnostics and Therapeutics in Calcer, 555A Chemometrics and Experimental Design, 553A Decoding Circulating Biomarkers with Spectroscopy: Quo Vadis?, 556B Fundamental Studies for Analytical Development, Ballroom E Recent Advances in IMS-MS Techniques and Measurements, 552B BioAnalytical Techniques for Higher Order Structure, 551A Biological/Biomedical Raman, 555B General Applications of Low Wavenumber Spectroscopy, 556A 			
3:00 PM	POSTER VIEWING AND BREAK, Ballroom A			
3:50 pm	PLENARY SESSION, <i>Ballroom B/C</i> , page 93 FACSS Distinguished Service Award FACSS Innovation Awards			

WEDNESDAY EVENING EVENT, 6:00 PM AN ALL INCLUSIVE EVENT Ballroom A



1920s Great Gatsby Theme Party

Enjoy an evening set in the 1920s with cigar/candy girls dressed in fanciful 20's flapper costumes and Troupe Monte Carlo who will entertain with period dances, such as the Charleston. Casino tables will be available for a night of chance playing craps, roulette, black jack, and poker. The evening would not be complete without a DJ playing a wide variety of music and the opportunity to perform Karaoke. Be sure to dress in your best 20's attire and enjoy an evening of food, beverage, and entertainment with your colleagues.

ATOMIC SPECTROSCOPY Monday (9:15 am session) RSC/ACS Symposium: Analysis with Photons-Laser & Synchrotron Spectroscopy Science & Applications, 554 A/B Fundamentals and Novel Applications of LA-ICP-MS: Part I, 550 A/B Monday (1:20 pm session) Fundamentals and Novel Applications of LA-ICP-MS: Part II, 550A/B Monday (3:50 pm session) Bioapplications of ICP-MS, 550A/B Nuclear Forensics, 551A Tuesday (9:15 am session) ICP-MS in the Analysis of Nanomaterials, 550A/B Tuesday (1:20 pm session) Innovative Atmospheric-Pressure Plasma Ionization Sources, 550A/B Tuesday (3:50 pm session) Atmospheric Pressure Plasmas & Liquid Cathode Glow Discharges, 550A/B Wednesday (9:15 am session) Fundamentals and Novel Applications of glow Discharge Spectroscopy I, 550A/B Lester Strock Award Symposium Honoring R. Kenneth Marcus, 554A/B Wednesday (1:20 pm session) A Lifetime of Spectroscopy: Celebrating Work of Edward Steers, 550A/B Wednesday (3:50 pm session) Fundamentals and Novel Applications of Glow Discharge Spectroscopy II, 550A/B Isotopic Analysis in Laser Induced Plasma, Ballroom E Thursday (9:15 am session) Atmospheric Pressure Innovative Sources: Micro & Microwave Plasmas (M&M), 550A/B AWARDS Monday (1:20 pm session) Award Session Honoring 2015 ACS Spectrochemical Award Winner Frank Bright, 554A/B Tuesday (9:15 am session) Craver Award Session Honoring Ji-Xin Cheng, 554A/B Tuesday (1:20 pm session) FACSS Charles Mann Award Session Honoring Sanford Asher, 554A/B Tuesday (3:50 pm session) Kowalski Award Honoring Thomas Bocklitz: Chemometrics for Spectroscopic/Spectrometric Data, 554A/B Wednesday (9:15 am session) Lester Strock Award Symposium Honoring R. Kenneth Marcus, 554A/B Wednesday (1:20 pm session) Meggers Award Symposium Honoring Eric Brauns, 554A/B Thursday (9:15 am session) ANACHEM Award Symposium Honoring Jonathan Sweedler, 552B Thursday (1:20 pm session) AES Mid-Career Symposium Honoring Adam Woolley, 552A Thursday (3:50 pm session) FACSS Innovation Award, Ballroom B/C **BIOLOGICAL/BIOMEDICAL** Monday (9:15 am session)

Advanced Techniques for Infrared Spectroscopy on Structure-Function Relations of Proteins, 556B

Monday (1:20 pm session) Biomedical and Forensic Applications of Vibrational Spectroscopy, 555A Bioanalytical SERS I, 555B Monday (3:50 pm session) Vibrational Spectroscopy: Toward Clinical Applications, 555A Tuesday (9:15 am session) Craver Award Session Honoring Ji-Xin Cheng, 554A/B Metabolomics and Personalized Medicine, 555A Bioanalytical Applications of Plasmonics, 556A Tuesday (1:20 pm session) FACSS Charles Mann Award Session Honoring Sanford Asher, 554A/B Tuesday (3:50 pm session) Diabetes and Its Complications, 555A Wednesday (9:15 am session) Super-Resolution Microscopy and Imaging, 555A SAS PAT Technical Section: PAT in the Biopharmaceutical Industries II. 553A Bioanalytical SERS II, 555B Bioanalytical Applications of Plasmonics II, 556A Wednesday (1:20 pm session) Meggers Award Symposium Honoring Eric Brauns, 554A/B Pathogens, 555A Wednesday (3:50 pm session) RSC/ACS Symposium - Analysis with Photons - Laser & Synchrotron Spectroscopy Science and Applications II, 554A/B Translation and Commercialization of Analytical Technologies, 555A Biomedical Raman Spectroscopy, 555B Thursday (9:15 am session) ANACHEM Award Symposium Honoring Jonathan Sweedler, 552B Musculoskeletal Diseases, 555A IRDG Raman Session - Biological Applications of Raman Spectroscopy, 555B Thursday (1:20 pm session) Optical Diagnostics & Therapeutics in Cancer, 555A BioAnalytical Techniques for Higher Order Structure, 551A Biological/Biomedical Raman, 552B AES Mid-Career Symposium Honoring Adam Woolley, 552A **CHEMOMETRICS** Monday (9:15 am session) Beyond PCA and PLS: New Frontiers in Chemometrics, 551B Monday (1:20 pm session) Ensuring Public Safety by Chemometric Authentication of Food and Botanicals, 551B Monday (3:50 pm session) Chemometric Keys for the Interpretation of Forensic Evidence, 551B Tuesday (9:15 am session) Chemometric Tools to Discover the Next Magic Bullet via Biological Spectroscopy, 551B Tuesday (1:20 pm session) Chemometrics in Pharmaceutical Industry, 551B Tuesday (3:50 pm session) Chemometrics for Spectroscopic/Spectrometric Data, 554A/B Wednesdav (9:15 am session) Chemometrics/Data Analysis for Forensics, 551A Thursday (1:20 pm session) Chemometrics and Experimental Design, 553A

TECHNICAL PROGRAM OVERVIEW

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GC-MS Based Detection of Emerging Flame Retardants in the
Environment, 552B
Tuesday (1:20 pm session)
Environment, 552B
Wednesday (3:50 pm session)
Dedicated (24/7) Online Analysis of Industrial Processes and Reactions, 553A
ELECTROPHORESIS AND MIROFLUIDICS
Tuesday (1:20 pm session)
Electro- and Liquid Phase-Separation Techniques, 552A Tuesday (3:50 pm session)
Miniaturization, 552A
Weanesaay (9:15 am session) Microfluidies and Electrophonesis for Biognalytical
Applications 5524
Wednesdav (1:20 pm session)
Microfluidic Electrophoresis Modes for Mass Spectrometric
Analysis, 552A
Wednesday (3:50 pm session)
Biopolymers in Electric Fields, $332A$
<i>Inursuuy (7:13 um)</i> Bioanalytical Dielectronhoresis 5524
ANACHEM Award Symposium Honoring Jonathan Sweedler,
552B
Thursday (1:20 pm session)
AES Mid-Career Symposium Honoring Adam Woolley, 552A
FORENSICS AND SECURITY
Monday (9:15 am session)
Analysis of Counterfeit Drugs and New Psychoactive Substances, 551A
Sensing Techniques for Counterfeit Drug Detection, 552B
Monday (1:20 pm session)
Biomedical and Forensic Applications of Vibrational
Explosive Detection L 551A
Sensing Techniques for counterfeit Drug Detection II. 552B
Monday (3:50 pm session)
Chemometric Keys for the Interpretation of Forensic Evidence, 551B
Nuclear Forensics, 551A
Tuesday (9:15 am session)
Explosive Dtection II: Trace, on-site and <i>in-situ</i> , 551A
<i>I uesuay (1:20 pm session)</i> Mass Spectrometry in Forensics 5514
Tuesday (3:50 nm session)
Ambient Ionization and Non-Chromatographic Approaches in
Forensics and Homeland Security, 551A
Wednesday (9:15 am session)
Chemometrics/Data Analysis for Forensics, 551A
Wednesday (1:20 pm session)
LIBS for Forensic and Homeland Security, <i>Ballroom E</i>
LASER INDUCED BREAKDOWN SPECTROSCOPY
Monday (9:15 am session)
Industrial LIBS, Ballroom E Monday (1:20 pm session)
Standards, Protocols and Quantitative Analysis, <i>Ballroom E</i>
Monday (3:50 pm session)
LIBS for Pharmaceutical and Biological Diagnostics, <i>Ballroom</i> E
Tuesday (9:15 am session)
New Hardware and Novel Methods in LIBS, Ballroom E
,

Fuesday (1:20 pm session) Handheld LIBS. Ballroom E
Fuesday (3:50 pm session)
LIBS for Environmental and Food Monitoring, <i>Ballroom E</i> Forensic Applications of Raman Spectroscopy, 555B
Vednesday (9:15 am session) Standoff LIBS, Ballroom E
Vednesday (1:20 pm session)
LIBS for Forensic and Homeland Security, <i>Ballroom E</i> Vednesday (3:50 pm session)
Isotopic Analysis in Laser Induced Plasmas, Ballroom E
Thursday (9:15 am session) Historical LIBS, Ballroom E
Thursday (1:20 pm session) Fundamental Studies for Analytical Development <i>Ballroom F</i>
AASS SPECTROMETRY
Manday (0.15 am sassian)
Fundamentals and Novel Applications of LA-ICP-MS: Part I, 550 A/B
Monday (1:20 pm session)
Fundamentals and Novel Applications of LA-ICP-MS: Part II, 550A/B
Monday (3:50 pm session)
Bioapplications of ICP-MS, 550A/B
UCD MS in the Analysis of Nonomotonials 5504/P
GC-MS Based Detection of Emerging Flame Retardants in the
Environment, 552B
uesday (1:20 pm session)
Innovative Atmospheric-Pressure Plasma Ionization Sources, 5504/R
Fuesday (1:20 pm session)
LC-MS Based Detection of Perfluorinated Contaminants in the
Environment, 552B
uesday (1:20 pm session)
Mass Spectrometry in Forensics, 551A
uesday (3:50 pm session)
Ambient Ionization and Non-Chromatographic Approaches in Forensics and Homeland Security 5514
Vednesday (9:15 am session)
Mass Spectrometric Techniques in Environmental Analysis, 552B
Vednesday (1:20 pm session)
Microfluidic Electrophoresis Modes for Mass Spectrometric Analysis, 552A
Ambient Ionization Methods: Developments and Applications, 552B
Vednesday (3:50 pm session) Direct Inject Mass Spectrometry, 552B
Thursday (9:15 am session)
Atmospheric Pressure Innovative Sources: Micro & Microwave
Plasmas (M&M), 550A/B ANACHEM Award Symposium Honoring Jonathan Sweedler, 552B
Recent Advances in IM-MS Techniques and Measurement, 552B
MOLECULAR (IR AND NEAR IR)
Monday (9:15 am session)
Advanced Techniques for Infrared Spectroscopy on Structure-
Function Relations of Proteins, 556B
Nonday (1.20 pm sassion)

bonday (1:20 pm session)Biomedical and Forensic Applications of Vibrational Spectroscopy, 555A

MOLECULAR (IR AND NEAR IR) - continued
Monday (3:50 pm session)
Vibrational Spectroscopy: Toward Clinical Applications, 555A
Near IR, 556B
Tuesday (9:15 am session)
Metabolomics and Personalized Medicine, 555A
Nanoscale IR I, 556B
Tuesday (1:20 pm session)
Nanoscale IR II, 556B
Tuesday (3:50 pm session)
Diabetes and Its Complications, 555A
Nanoscale IR III, 556B
Wednesday (9:15 am session)
Super-Resolution Microscopy and Imaging, 555A
New Developments in QCL Technology, 556B
Wednesday (1:20 pm session)
Meggers Award Symposium Honoring Eric Brauns, 554A/B
Pathogens, 555A
Quantum Cascade Lasers – Applications, 556B
Wednesday (3:50 pm session)
RSC/ACS Symposium – Analysis with Photons – Laser &
Synchrotron Spectroscopy Science and Applications II,
<i>554A/B</i>
Translation and Commercialization of Analytical Technologies,
Difficult Data Sets, 556B
Thursday (9:15 am session)
Musculoskeletal Diseases, 555A
Biomedical Application sof IR Spectroscopy and Imaging, 556B
Thursday (1:20 pm session)
Optical Diagnostics & Therapeutics in Cancer, 555A
Decoding Circulating Biomarkers with Spectroscopy: Quo
rhakmaceutical srectikoscory
Monday (9:15 am session)
Sensing Techniques for Counterfeit Drug Detection I, 552B
Monday (1:20 pm session)
Sensing Techniques for counterfeit Drug Detection II, 552B
Monday (3:50 pm session)
LIBS for Pharmaceutical and Biological Diagnostics, Battroom
E Dhamma courtical Amplications of Low Wayanumban
Superture Structure State State State Structure Structure Structure Structure State
Dharmanautical Daman 5564
Tuasday (1:20 pm sassion)
Chemometrics in Dharmaceutical Industry 551B
Tuesday (3:50 pm session)
SAS PAT Technical Section: PAT in the Pharmaceutical
Industries I 5534
Wednesday (9.15 am session)
SAS PAT Technical Section: PAT in the Biopharmaceutical
Industries II 5534
Wednesday (3:50 pm session)
Chiral Analysis 5514
Thursday (9:15 am session)
Amyloids and Aggregates: What Do We Know About Structure
551A
Thursday (1:20 pm session)
BioAnalytical Techniques for Higher Order Structure, 551A

PROCESS ANALYTICAL SPECTROSCOPY Tuesday (9:15 am session) Continuous/Flow PAT, 553A Tuesday (1:20 pm session) Chemometrics in Pharmaceutical Industry, 551B Advances in Applications of Handheld/Portable Spectrometer, 553A Tuesday (3:50 pm session) SAS PAT Technical Section: PAT in the Pharmaceutical Industries I, 553A Wednesday (9:15 am session) SAS PAT Technical Section: PAT in the Biopharmaceutical Industries II, 553A Wednesday (1:20 pm session) In situ Analysis of Industrial Processes and Reactions during R&D, 553A Wednesday (3:50 pm session) Dedicated (24/7) Online Analysis of Industrial Processes and Reactions, 553A Thursday (9:15 am session) Advances in On-line Process Analysis, 553A RAMAN Monday (9:15 am session) SERS, 555B Extending the Scope of Raman: ROA and Other Recent Advances, 556A Monday (1:20 pm session) Bioanalytical SERS I, 555B Raman Microscopy, 556A Monday (3:50 pm session) Hot Topic Discussion Session - TERS Resolution, 555B Pharmaceutical Raman, 556A Tuesday (9:15 am session) Emerging Raman Techniques and Applications, 555B Tuesday (1:20 pm session) FACSS Charles Mann Award Session Honoring Sanford Asher, 554A/B Emerging Raman Techniques and Applications II, 555B Raman Imaging/Microscopy II, 555A Tuesday (3:50 pm session) Forensic Applications of Raman Spectroscopy, 555B Wednesday (9:15 am session) Chemometrics/Data Analysis for Forensics, 551A SAS PAT Technical Section: PAT in the Biopharmaceutical Industries II, 553A Bioanalytical SERS II, 555B Wednesday (1:20 pm session) Spatially Offset Raman Spectroscopy, 555B Wednesday (3:50 pm session) Biomedical Raman Spectroscopy, 555B Raman in Cultural Heritage, 556A Thursday (9:15 am session) IRDG Raman Session - Biological Applications of Raman Spectroscopy, 555B Compact Raman Applications, 556A Thursday (1:20 pm session) Biological/Biomedical Raman, 555B General Applications of Low Wavenumber Spectroscopy, 556A

TECHNICAL PROGRAM OVERVIEW

SPECIAL TOPICS

 Monday (9:15 am session)
 Novel Teaching Methods in Analytical Chemistry, 552A
 Advanced Techniques for Infrared Spectroscopy on Structure-Function Relations of Proteins, 556B

 Monday (1:20 pm session)
 Advocating for Women in Science, 552A

Monday (3:50 pm session)

Careers and Diversity in Analytical Science Discussion Panel, 552ATuesday (1:20 pm session)

LC-MS Based Detection of Perfluorinated Contaminants in the Environment, *552B*

Tuesday (3:50 pm session)

Analytical Chemists Easing World Poverty, 551B

Wednesday (1:20 pm session) Chemistry in Art and Archaeology, 551B

Friday (8:00 am session)

A Trans-Spectral Celebration of the International Year of Light: From X-Rays to THz Spectroscopy, 555-556

SURFACE PLASMON RESONANCE

Tuesday (9:15 am session)

Bioanalytical Applications of Plasmonics, 556A Tuesday (1:20 pm session) Nanostructured Materials for Plasmonics I, 556A Tuesday (3:50 pm session) Nanostructured Materials for Plasmonics II, 556A Wednesday (9:15 am session) Bioanalytical Applications of Plasmonics II, 556A Wednesday (1:20 pm session)

New Plasmonic Materials and Techniques, 556A

SURFACE SCIENCE

Monday (9:15 am session)

Characterization and Surface Science of Nanomaterials, 553A Monday (1:20 pm session)

Non-linear Optical Spectroscopy for Surface Science, 553A Monday (3:50 pm session)

In-situ Surface Science, 553A

Tuesday (9:15 am session)

GC-MS Based Detection of Emerging Flame Retardants in the Environment, 552B

SCIX 2015 AND FACSS THANKS ITS MEMBER ORGANIZATIONS FOR THEIR SUPPORT TO THE SciX PROGRAM

ACS, Analytical Division AES Electrophoresis Society American Society of for Mass Spectrometry ANACHEM The Coblentz Society

Council for Near Infrared Spectroscopy

The Infrared and Raman Discussion Group International Society of Automation – Analysis Division North American Society for Laser-Induced Breakdown Spectroscopy Royal Society of Chemistry Analytical Division Society for Applied Spectroscopy The Spectroscopical Society of Japan

PROGRAM HIGHLIGHTS

SUNDAY	MONDAY	TUESDAY	WEDNESDAY	THURSDAY	FRIDAY
	Ballroom Prefunction	Ballroom Prefunction	Ballroom Prefunction	Ballroom Prefunction	Ballroom Prefunction
	7:30 am Wake Up	7:30 am Wake Up Coffee			
	Coffee				and Muffins
	Ballroom B/C	Ballroom B/C	Ballroom B/C	Ballroom B/C	8:00 – 10:30 am
	7:50 am	8:00 am	8:00 am	8:00 am	Announcement of
	Opening Remarks	Coblentz Society Craver	SAS's Lester W. Strock	ANACHEM Award	Innovation Award
	Glen Jackson	Award	Award	Jonathan Sweedler	
		Ji-Xin Cheng	R. Kenneth Marcus	University of Illinois	A Trans-Spectral
	8:00 am	Purdue University	Clemson University		Celebration of the
	Keynote Lecture		-	8:30 am	International year of the
	Christopher Palenik	8:30 am	8:30 am	AES Mid Career Award	Light: From X-Rays to
	Microtrace LLC	FACSS Charles Mann	Applied Spectroscopy	Adam Woolley	the THz Spectroscopy
		Award for Applied	William F. Meggers	Brigham Young	
		Raman Spectroscopy	Award	University	Preview of 2016
		Sanford Asher	Eric Brauns		Conference
		University of Pittsburgh	University of Idaho		
	9:00 – 4:30 pm	9:00 am – 4:00 pm	9:00 am – 4:30 pm		
	Workshops	Workshops	Workshops		
		Exhibit Hall C/D	Exhibit Hall C/D		
		9:00 am – 4:30 pm	9:00 am – 4:00 pm		
		Exhibits Open	Exhibits Open		
	9:15 – 10:55 am	9:15 – 10:55 am	9:15 – 10:55 am	9:15 – 10:55 am	
	Oral Symposia	Oral Symposia	Oral Symposia k	Oral Symposia	
	Ballroom A	Exhibit Hall C/D	Exhibit Hall C/D	Ballroom A	
	11:00 – 12:00 pm	11:00 – 12:00 pm	11:00 – 12:00 pm	11:00 – 12:00 pm	
	Poster Session and	Poster Session and Break	Poster Session and Break	Poster Session and Break	1
	Break				
		Exhibit Hall C/D	Exhibit Hall C/D		
		11:40 am – 1:10 pm	11:40 am – 1:10 pm		
		What's Hot Vendor	What's Hot Vendor		
		Presentations	Presentations		
	Noon	Noon	Noon	Noon	
	Lunch on own	Complimentary lunch in	Complimentary lunch in	Lunch on own	
		Exhibit Hall	Exhibit Hall		
1:00 – 5:00 pm	1:20 – 3:00 pm	1:20 – 3:00 pm	1:20 – 3:00 pm	1:20 – 3:00 pm	
Workshops	Oral Symposia	Oral Symposia	Oral Symposia	Oral Symposia	
	Ballroom A	Exhibit Hall C/D	Exhibit Hall C/D	Ballroom A	
	3:00 - 3:50	3:00 - 3:50	3:00 - 3:50	3:00 - 3:50	
	Poster Viewing and	Poster Viewing and	Poster Viewing and	Poster Viewing and	
	Break	Break	Break	Break	
Ballroom B/C	3:50 – 5:30 pm	3:50 – 5:30 pm	3:50 – 5:30 pm	Ballroom B/C	
4:10 – 6:00 pm	Oral Symposia	Oral Symposia	Oral Symposia	3:50 – 5:30 pm	
What's Hot				Plenary Session	
Vendor				FACSS DSA Awards	
Presentations				Innovation Award	
(raffle)				Session	
Ballroom B/C	Exhibit Hall C/D				
6:15 pm	5:30 – 7:30 pm				
Keynote Lecture:	Exhibit Opening				
Robert S. C.	Reception				
Munier	±				
Woods Hole					
Oceanographic					
Institute					
Ballroom A		Ballroom B/C	Ballroom A		
7:15 – 9:15 pm		6:00 pm	6:00 pm		
Welcome Mixer		Raman Reception	Wednesday Evening		
and SAS		Sponsored by Kaiser	All inclusive event		
Sponsored Student		Optical Systems, Inc.			
Poster Session					
Coblentz Student					
Awards					1
FACSS Student					1
and Tomas					
Hirschfeld Scholar					
Awards		D-11			
		Ballroom A			
		SAS Recention			
		SAS Reception			1

TECHNICAL PROGRAM

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 LegoTM"
- 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



(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

8:00 am Keynote Lecture

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; <u>Paul</u> <u>Farnsworth¹</u>, Lance Moses¹, Jessica Ramsey¹; ¹Brigham Young University
- 9:35 (4) All-Optical Laser Ablation-based Analytical Techniques: Status, Achievements and Directions; <u>Vassilia</u> <u>Zorba¹</u>, Jhanis Gonzalez¹, Huaming Hou¹, George Chan¹, Xianglei Mao¹, Richard Russo¹; ¹Lawrence Berkeley National Laboratory
- 9:55 (5) Laser SIMS Advancements; <u>David Willingham¹</u>, Benjamin Naes¹, Mindy Zimmer¹; ¹Pacific Northwest National Laboratory
- 10:15 (6) Recent Advances in Quantifying Actinide Isotope Ratios by RIMS; <u>Brett Isselhardt</u>¹, Michael Savina^{1, 2}, Andrew Kucher¹; ¹Lawrence Livermore National Laboratory; ²Argonne National Laboratory
- 10:35 (7) Real Time Isotopic Analysis of Atmospheric Greenhouse Gases Using Mid-IR Laser Spectroscopy; <u>David Nelson¹</u>, Barry McManus¹, Joanne Shorter¹, Tara Yacovitch¹, Scott Herndon¹, Mark Zahniser¹; ¹Aerodyne 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; <u>Bodo Hattendorf</u>¹, Marcel Burger¹, Luzia Gyr¹, Gunnar Schwarz¹, Alexander Gundlach-Graham¹, Hao Wang¹, Detlef Günther¹; ¹ETH Zurich, Laboratory for Inorganic Chemistry
- 9:35 (9) Advances in High Repetition Rate Femtosecond Laser Ablation; <u>Fanny Claverie</u>¹, Ariane Donard^{1, 2}, Amélie Hubert², Fabien Pointurier², Nagore Grijalba^{1,3}, Nora Unceta³, Christophe Pécheyran¹; ¹LCABIE, IPREM UMR UPPA/CNRS 5254, University of Pau and Pays de l'Adour, Pau, France; ²CEA-DIF, Bruyères le Châtel, Arpajon; ³Department 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 Almirall¹, Tricia Hoffman¹; ¹Florida International University

- 10:15 (11) High-resolution for Direct Isotopic Analysis; Martin Resano¹, Esperanza García-Ruiz¹, Maite Aramendía¹, Eduardo Bolea-Fernandez², Frank Vanhaecke², Flavio Nakadi²,Marcia Veiga²; ¹University of Zaragoza; ²Department of Analytical Chemistry, Ghent University, Belgium; ³Universidade de Sao Paulo
- 10:35 (12) Expanding LA-ICP-MS Capabilities with Simultaneous LIBS and LAMIS; <u>Richard Russo</u>^{1,2}, Jhanis Gonzalez^{1,2}, Xianglei Mao^{1,2}, George Chan¹, Vasillia Zorba¹, Jong Yoo², Alexander Bol'shakov², Derrick Quarles²; ¹Lawrence Berkeley National Laboratory; ²Applied 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.; <u>Ludovic Duponchel</u>¹; ¹Lille University
- 9:35 (14) Multi-block Data Analysis: New Extensions and Applications in Chemometrics; <u>Douglas Rutledge¹</u>, Delphine Jouan-Rimbaud Bouveresse¹; ¹AgroParisTech
- 9:55 (15) Classical Least Squares Methods for Target Detection in Hyperspectral Imaging; <u>Neal Gallagher</u>¹; ¹Eigenvector Research, Inc.
- 10:15 (16) Homeopathic ICA: A Simple Approach to Expand the Use of Independent Component Analysis; <u>Willem</u> <u>Windig¹</u>, Michael Keenan², Barry Wise¹; ¹Eigenvector Reseach, Inc.; ²8346 Roney Rd. Wolcott, NY 14590
- 10:35 (17) **Comparative Study of Classification Trees for the Authentication of Marijuana**; <u>Peter Harrington¹</u>, Xinyi Wang², Steve Baugh¹; ¹Ohio University; ²Cannaprint

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**; <u>Iain</u> <u>Oswald</u>¹, Oliver Sutcliffe², Niamh Nic Daeid³; ¹University of Strathclyde; ²Manchester Metropolitan University; ³University of Dundee
- 9:35 (19) Evaluation of Two Wavelengths, 785 and 1064 nm, for the Identification of New Psychoactive Substances using Handheld Raman Spectroscopy; <u>Amira Guirguis</u>¹, Sarah Girotto¹, Benedetta Berti¹, Jacqueline Stair¹; ¹University of Hertfordshire
- 9:55 (20) Forensic Examinations to Determine Illicit Drugs Commonly Seized in the Philippines: From Evidence to Judgment; <u>Ronald Jefferson Narceda</u>¹; ¹Philippine Drug Enforcement Agency

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

- 10:15 (21) Improved Identification Algorithms for Detection of Counterfeit Medicines by Raman Spectroscopy; <u>Latevi</u> <u>Lawson¹</u>, Jason Rodriguez¹; ¹FDA
- 10:35 (22) Drug Quality and Dissolution Testing at All Points in the Supply Chain: Integration of Scalable Technology in the Health System; Muhammad Zaman¹, Nga Ho¹, Darash Desai¹; ¹Boston University

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

- 9:15 (23) **LIBS Outside the Lab**; <u>Christian Bohling</u>¹, Jens-Uwe Günther¹, Angelika Feierabend¹, Andreas John¹; ¹Secopta GmbH, Berlin
- 9:35 (24) Stimulated Emission and Lasing in a Laser-Induced Plasma; <u>Lev Nagli¹</u>, Michael Gaft¹; ¹Laser Distance Spectrometry Ltd
- 9:55 (25) The Determination of Bioavailability Concentrations of Nutrients in Soils using Chemometric Analysis of LIBS Data; Josette El Haddad¹, Aissa Harhira¹, Luc English², Gilles Clément², Charles Nault², Alain Blouin¹, Mohamad Sabsabi¹; ¹National Research Council Canada - Energy, Mining and Environmentt; ²LOGIAG Inc.
- 10:15 (26) LIBS Process Analyzer; <u>Francois Doucet¹</u>, Lutfu Ozcan¹; ¹ELEMISSION Inc.
- 10:35 (27) Laser Induced Breakdown Spectroscopy for Gold Analysis in Ore Samples; <u>Kheireddine Rifai</u>^{1,2}, Marcel Laflamme¹, Marc Constantin¹, Mohamad Sabsabi², Alain Blouin², François Vidal³, Paul Bouchard², Konstontinos Fytas¹; ¹Université Laval; ²National Research Council Canada - Energy, Mining and Environment; ³IRNS - 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; <u>Neville Broad</u>^{1,2}; ¹Authenticate Limited (UK); ²University of Kent (UK)
- 9:35 (29) **Combating Adulterated Drug Products**; <u>Connie</u> <u>Ruzicka¹</u>, Kelly Park¹, Katherine Alejo¹; ¹US Food and Drug Administration
- 9:55 (30) Challenges of Counterfeit Drug Detection in the Field; <u>Pauline Leary</u>¹, John Reffner²; ¹Smiths Detection; ²John Jay College of Criminal Justice
- 10:15 (31) The Creation of Paper-based Devices to Detect Select Pharmaceuticals; <u>Toni Barstis</u>¹; ¹Saint Mary
- 10:35 (32) Rapid Identification of Counterfeit Medicines from the World Market using Dual Laser Handheld Raman Spectroscopy; <u>Sulaf Assi</u>¹; ¹Bournemouth 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 Liu¹; ¹University of Washington
- 9:35 (34) New Reporters for bioLogical SERS Measurements; <u>Colin Campbell</u>¹, Patrick Thomson¹, Kate Fisher¹; ¹University of Edinburgh

- 9:55 (35) High Throughput Optofluidic Surface Enhanced Raman Spectroscopy (SERS) Interrogation: Proof of Concept via Lectin Detection of Cancerous Cells; <u>Marjorie</u> <u>Willner</u>¹, Jonathan Simpson², Kay McMillan², Michele Zagnoni², Duncan Graham², Peter Vikesland¹; ¹Virginia Polytechnic Institute and State University; ²University of Strathclyde
- 10:15 (36) Ultrasensitive Detection with SERS and SEHRS; Jon Camden¹; ¹University of Notre Dame
- 10:35 (37) Surface-enhanced Raman Scattering (SERS) Spectroscopy for Intracellular Chemical Imaging and Protein Analysis; <u>Katsumasa Fujita</u>¹; ¹Osaka 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; <u>Vladimir</u> <u>Baumruk</u>¹, Marketa Pazderkova^{1, 2}, Vaclav Profant¹, Lucie Bednarova², Petr Malon¹; ¹Charles University in Prague, Faculty of Mathematics and Physics; ²Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences
- 9:35 (39) Vibrational Chiroptical Spectroscopy in Natural Product Chemistry: Have We Achieved Enough?; Joao <u>Marcos Batista Junior</u>¹; ¹Federal University of Sao Carlos -UFSCar
- 9:55 (40) Insights into the Vibrational Nature of Carbohydrates from Raman Optical Activity; <u>Shaun</u> <u>Thomas Mutter</u>¹; ¹University 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; <u>Martha Vardaki¹</u>, Benjami Gardner¹, Nicholas Stone¹, Pavel Matousek²; ¹School of Physics, University of Exeter; ²Central Laser Facility, STFC Rutherford Appleton Laboratory
- 10:35 (42) Standoff UV Raman Spectroscopy: Spatial Heterodyne Raman Spectrometer for Planetary Applications; <u>Nirmal Lamsal</u>¹, S. Michael Angel¹, Shiv K. Sharma², Tayro Acosta-Maeda²; ¹University of South Carolina; ²University 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 Harrison¹; ¹San Diego State University
- 9:35 (44) Arduino Powered Instrument Design and Construction in Undergraduate Analytical Chemistry Courses; <u>Celeste Morris¹</u>; ¹Northern Kentucky University
- 9:55 (45) Multiperspective Views in Teaching Laboratory Techniques; <u>Kevin Davies</u>¹; ¹Florida Gulf Coast University
- 10:15 (46) **Social Media in the Blended Classroom**; <u>Kate</u> <u>Hayden</u>¹; ¹Birmingham-Southern College, Birmingham AL
- 10:35 (47) Perspectives from the Flip: The Active-Learning Experience in Analytical Chemistry; Jared Baker¹; ¹Elmira 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; <u>Teizo Kitagawa¹</u>; ¹University of Hyogo
- 9:25 (49) Coupling Mechanism in the Reaction of Cytochrome C Oxidase Revealed by Newly Developed Time-Resolved IR Measurements; <u>Satoru Nakashima</u>¹; ¹Graduate School of Life Science, University of Hyogo
- 9:55 (50) Infrared Spectroscopic Study on the Structure and Dynamics of Sodium Pump Rhodopsin; <u>Keiichi Inoue</u>^{1,2}; ¹Nagoya Institute of Technology; ²PRESTO, JST
- 10:15 (51) Infrared Studies of the Photosynthetic Oxygen Evolving Complex; <u>Bridgette Barry</u>¹, Udita Brahmachari¹, Zhanjun Gup¹; ¹Georgia Institute of Technology
- 10:35 (52) Novel Time-Resolved IR Spectroscopies to Elucidate the Mechanism of Channelrhodopsin; Joachim Heberle¹; ¹FU 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; <u>Melissa Hines</u>¹; ¹Cornell University
- 9:35 (54) Atomic Scale Spectrometry and Structure -Correlating Atom Probe Tomography and Transmission Electron Microscopy; <u>David Diercks</u>¹, Brian Gorman¹; ¹Colorado School of Mines
- 9:55 (55) **Single Atom Alloys as a Strategy for Selective Heterogeneous Hydrogenations**; <u>Charles Sykes</u>¹; ¹Tufts University
- 10:15 (56) **Epitaxial Graphene: Not so Plane and Simple**; <u>Phillip</u> <u>First¹</u>; ¹Georgia Institute of Technology
- 10:35 (57) Photopatterned Electroless Gold Deposition: Optimizing Film Patterning and Nanoscale Structure for Applications; <u>Y M Nuwan Bandara</u>¹, Buddini Karawdeniya¹, Julie Whelan¹, Brian Velleco¹, Jason Dwyer¹; ¹University 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; <u>Jidong Lu¹</u>, Meirong Dong¹, Jun LI¹, Xuan Dong¹, ¹South 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; <u>Meirong Dong</u>¹, Jidong Lu¹, Jianhua Yu¹, Bo Zhang¹, Yue Pan¹; ¹South China University of Technology

Poster Board #3

(60) Excited State Decay of N2+ at Stratospheric Pressures; <u>Kumarasiri Konthasinghe</u>², Andreas Muller², Adam Hopkins¹; ¹Alakai Defense Systems; ²University of South Florida

Poster Board #4

(61) **Cold Atmospheric Plasma: An Inside Look Through Optical Diagnostics**; <u>Liesl Krause</u>^{1,2}, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University; ²Department 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**; <u>Michael Marino¹</u>, Payson Dieffenbach¹, Liesl Krause², Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University; ²Department of Electrical and Computer Engineering, College of Engineering, Villanova University

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; <u>Bharati Pardeshi</u>¹; ¹PDEA

Poster Board #7

(64) Chlorine Isotope Determination by High-Resolution Continuum Source Graphite Furnace Molecular Absorption Spectrometry; <u>Esperanza García-Ruiz¹</u>, Flavio V. Nakadi², Marcia A.M.S. da Veiga², Maite Aramendía^{1,3}, Martín Resano¹; ¹University of Zaragoza; ²Universidade de Sao Paulo; ³Centro 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**; <u>Patrick Skrodzki</u>^{1,2}, Niral Shah¹, Jason Becker^{1,2}, Sivanandan Harilal¹, Mark Phillips¹, Brian Brumfield¹,Nicole LaHaye¹; ¹Pacific Northwest National Laboratory; ²Purdue University

Poster Board #9

(66) Develpment of High-Density Microplasma Emission Source using 3-D Molding Process Based on

Microsterolithography; <u>Ken Kakegawa</u>¹, Ryoto Harigane², Mari Aida¹, Hidekazu Miyahara¹, Shoji Maruo², Akitoshi Okino¹; ¹Department of Energy Sciences, Tokyo Institute of Technology; ²Department 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; <u>Ehsan Rezaei</u>¹, Charles Nguyen¹, Anastasia Desyatova Desyatova¹, Deepak Rudrappa², Paul Blum², Joseph Turner¹; ¹Mechanical and Materials Engineering, University of Nebraska-Lincoln; ²School of Biological Sciences, University of Nebraska-Lincoln

Poster Board #11

(68) **The Use of XYZ Sample Manipulator in Quadrupole Glow Discharge Mass Spectrometer**; <u>Maciej Miśnik^{1,2}</u>, Piotr Konarski¹, Aleksander Zawada^{1,3}; ¹Institute of Tele and Radio Technology, ul. Ratuszowa 11, 03-450 Warszawa; ²Gdańsk University of Technology, ul. G. Narutowicza 11/12, 80-233 Gdańsk; ³Military 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; <u>Edward Steers</u>², Zdenek Weiss¹, Sohail Mushtaq², Volker Hoffmann⁴, Viktoria Weinstein²; ¹LECO Instrumente Plzeň spol. s r.o.; ²London Metropolitan University, London; ³Imperial College London; ⁴IFW Dresden *Poster Board #13*

(70) Does Asymmetric Charge Transfer Play an Important Role as the Ionization Mode in Low Power-Low Pressure GD-MS?; <u>Edward Steers</u>¹, Sohail Mushtaq¹, Glyn Churchill², DeAnn Barnhart², Volker Hoffmann³, Karol Putyera⁴, Juliet Pickering; ¹London Metropolitan University; ²Nu Instruments

Ltd.; ³IFW Dresden; ⁴Evans 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 Hussain¹, Amer Jamil⁴; ¹Government College University Faisalabad Pakistan; ²COmsats Institute of Technology Islamabad Pakistan; ³Koc University, Istanbul, Turkey; ⁴University 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; <u>Zhenyu</u> Lu¹, Brianna Cassidy¹, Stephanie Dejong¹, Katherine Witherspoon¹, Michael Myrick¹, Stephen Morgan¹; ¹University of South Carolina

Poster Board #16

(73) An Experimental Study of the Forensic Luminol Test for Detection of Bloodstains; <u>Brianna Cassidy</u>¹, Zhenyu Lu¹, Kathrine Witherspoon¹, Jennifer Martin¹, Stephanie DeJong¹, Raymond Belliveau¹, Michael Myrick¹, Stephen Morgan¹; ¹University of South Carolina

Poster Board #17

(74) Lost in Translation: Bridging Vibrational Spectroscopy Knowledge from Scientists to End Users; Luisa T.M. Profeta¹, Alan Ford¹, Alen Tomczak¹, Jack Burton¹, Ken Pohl¹; ¹Alakai Defense Systems

Poster Board #18

(75) **Novel Concept for Forensic Analysis of Biomarkers**; <u>Jan</u> <u>Halamek</u>¹; ¹Department of Chemistry, University at Albany, SUNY

Poster Board #19

(76) **New and Practical Methods to Characterize Organic Gunshot Residue**; <u>Sydney Brooks</u>¹, Brittany Yeager¹, Suzanne Bell¹; ¹West Virginia University

Poster Board #20

(77) **The Surprising Effect of Temperature on the Weathering of Gasoline**; <u>Ashley Cochran¹</u>, Heather Birks¹, Tyler Williams¹, Glen P. Jackson¹; ¹West Virginia University an Board #21

Poster Board #21

(78) Raman and Laser Induced Fluorescence Spectroscopy on Ageing Fingerprints; <u>Lars Landström</u>¹, Christian Lejon¹, Therese Mikaelsson¹, Göran Kidfelt², Milja Kanerva², Cecilia Vahlberg²,Kent Rosengren², Per Ola Andersson¹; ¹CBRN Defence and Security, Swedish Defence Research Agency (FOI); ²Nationellt Forensiskt Center (NFC)

Poster Board #22

(79) **Detection of Trace Evidence Particles by Mid-Infrared Laser Reflectance Imaging**; <u>Raymond Belliveau</u>¹, Stephanie DeJong¹, Lu Zhenyu¹, Brianna Cassidy¹, Stephen Morgan¹, Michael Myrick¹; ¹University of South Carolina, Department of Chemistry and Biochemistry

Future Meeting: September 18 – 23, 2016, Minneapolis, MN

Poster Board #23

(80) A Raman 'Spectroscopic Clock' for Bloodstain Age Determination: The First Week After Deposition; <u>Kyle C.</u> <u>Doty</u>¹, Gregory McLaughlin¹, Igor K. Lednev¹; ¹University at Albany

LIBS Posters

Poster Board #24

(81) Self-Absorption Measurements of Resonant Aluminum Lines; <u>David Surmick¹</u>, Christian Parigger¹; ¹University of Tennessee Space Institute

Poster Board #25

(82) Laser-Induced Plasma Diagnostics with the Hydrogen Balmer beta Line; <u>Ghaneshwar Gautam</u>¹, Christian Parigger¹; ¹University 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**; <u>Ola Ahmed</u>, Hisham Imam², Abdel Rahman Zekri³; ¹National Cancer institute, Cairo University, Egypt; ²National institute of laser enhanced science (NILES), Cairo University, Egypt; ³National Cancer institute, Cairo University, Egypt transmersity, Egypt

Poster Board #27

(84) **Discrimination of Polymers from Plasma Parameters using Laser Induced Breakdown Spectroscopy**; <u>M Atif</u>; ¹King Saud University

Poster Board #28

(85) **The Role of Gas Dynamics on the Formation of AlO in Laser-Ablation Plumes**; <u>Sivanandan Harilal</u>¹, Brian Brumfield¹, Jeremy Yeak², Mark Phillips¹; ¹Pacific Northwest National Laboratory; ²PM & AM Research

Poster Board #29

(86) Multiblock Analysis Applied to LIBS and XRF Data of Geological Materials; <u>Faten Ammari</u>¹, Léna Bassel¹, Catherine Ferrier³, Delphine Lacanette-Puyo⁴, Rémy Chapoulie¹, Bruno Bousquet²; ¹Université Bordeaux Montaigne, IRAMAT-CRP2A, UMR 5060 CNRS; ²Université de Bordeaux, CELIA, UMR 5107 CNRS; ³Université de Bordeaux, PACEA, UMR 5199 CNRS; ⁴Université 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; <u>Heather Johns</u>¹, David Kilcrease¹, James Colgan¹, Elizabeth Judge¹, James Barefield¹, Samuel Clegg¹; ¹Los Alamos National Laboratory

Poster Board #31

(88) **Temporally and Spatially-Resolved Absorption Spectroscopy of Atomic Oxygen in an Air Spark**; <u>Brian</u> <u>Brumfield¹</u>, Sivanandan Harilal¹, Mark Phillips¹; ¹Pacific Northwest National Laboratory

Poster Board #32

(89) Laser-induced Breakdown Spectra of Rocks at Variable Ablation and Collection Angles; <u>Elly Breves</u>¹, Kate Lepore¹, M. Darby Dyar¹, Steven C. Bender², Robert L. Tokar²; ¹Mount Holyoke College; ²Planetary Science Institute

Poster Board #33

(90) Application of the Laser-Induced Breakdown Spectroscopy Technique in Steel and Metal Industry; <u>Vincenzo Palleschi</u>^{1,2}, Emanuela Grifoni¹, Stefano Legnaioli^{1,2}, Stefano Pagnotta¹, Giulia Lorenzetti¹; ¹Applied and Laser Spectroscopy Laboratory, ICCOM-CNR, Pisa, Italy; ²National 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); <u>Jinesh Jain</u>¹, Alexander Bol'shakov², Hervé Sanghapi¹, Christina Lopano¹, Dustin McIntyre¹, Richard Russo²; ¹National Energy Technology Laboratory; ²Applied 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; <u>Patrick Skrodzki</u>¹, Jason Becker¹, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center 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 Becker¹, Patrick Skrodzki¹, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center 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; <u>Takeyoshi Goto¹</u>, Yukihiro Ozaki¹; ¹Kwansei Gakuin Unversity

Poster Board #38

(95) Electronic Transitions of Hydrated Amino Acids in the Wavelength Region 145–300 nm Studied by Far-Ultraviolet Spectroscopy; <u>Takeyoshi Goto¹</u>, Yukihiro Ozaki¹; ¹Kwansei Gakuin Unversity

Poster Board #39

(96) **Thermal Analysis of Thermally Reversible Gels Made of a Bio-based, Biodegradable Polymer**; <u>Brian Sobieski¹</u>, Liang Gong¹, John Rabolt¹, Isao Noda¹, Bruce Chase¹, Steve Aubuchon^{1,2}; ¹University of Delaware; ²TA Instruments

Poster Board #40

(97) Temperature Dependence of FUV Spectra for Aqueous Solutions of Alkali Halide to the Freezing-point of Eutectic; <u>Yusuke Morisawa¹</u>, Yuka Nishikawa¹, Akifumi Ikehata²; ¹Kinki University; ²NFRI, NARO

Poster Board #41

(98) **Computing Molar Extinction Coefficient of Capsaicin Using Absorbance Spectroscopy in the Visible Range**; <u>Abraham Lopez</u>¹, José Javier Báez Rojas¹, Jorge Castro Ramos¹, Karen Esmonde-White²; ¹National Institute of Astrophysics Optics and Electronics; ²University of Michigan, Medical School

Poster Board #42

(99) Measuring Thermal Properties of Oilseeds using Unilateral Nuclear Magnetic Resonance sensor; <u>Maria G. A.</u> <u>Carosio¹</u>, André de S. Carvalho², Luis F. Cabeça³, Luiz A. Colnago¹; ¹EMBRAPA Instrumentation; ²Institute of Chemistry of São Carlos; ³Federal Technological University of Parana

Poster Board #43

(100) Moving Window Two-Dimensional Correlation Spectroscopy of the Early Stage Crystallization of Polyethylene; <u>Ying Jin</u>, Anthony Kotula¹, Angela Hight Walker¹, Kalman Migler¹, Young Jong Lee¹, ¹National Institute of Standards and Technology

Poster Board #44

(101) **Spectroscopic Markers for Uranyl Phosphates: A Vibrational Study**; <u>Dale L. Perry</u>¹, Nataliya Kalashnyk², Eric Faulques³, Florian Massuyeau³; ¹Lawrence Berkeley National Laboratory, University of California, Berkeley; ²Institut Matériaux Microéléctronique Nanosciences de Provence (IM2NP), Université d' Aix-Marseille, UMR CNRS 7334; ³Institut des Matériaux Jean Rouxel, Université de Nantes, UMR CNRS 6502

Poster Board #45

(102) Elemental Characterization of Glass Tesserae via X-Ray Fluorescence Spectrometry; <u>Andrew Sparks</u>¹, Mary Kate Donais¹; ¹Saint Anselm College

Poster Board #46

(103) First Electronic Transition of Water Molecules in Binary Solutions Studied by Far-Ultraviolet Spectroscopy; <u>Kodai Kishibe</u>¹, Takeyoshi Goto¹, Hiroto Tanaka¹, Yukihiro Ozaki¹; ¹Graduate School of Science and Technology, Kwansei Gakuin University

Poster Board #47

(104) Thermal Behavior and Lamella Structures of Poly(3hydroxybutyrate-co-3-hydroxyvalerate) Studied by Low-Frequency Raman, Terahertz Spectroscopy, and Small Angle X-ray Scattering; Dian Marlina¹, Mengfan Wan¹, Koh Yoshida¹, Hiromichi Hoshina², Harumi Sato³, Yukihiro Ozaki¹; ¹Graduate School of Science and Technology, Kwansei Gakuin University; ²RIKEN; ³Graduate 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; <u>Swati</u> <u>Naik</u>¹, Gabriel Caruntu¹; ¹Central Michigan University

Poster Board #48

(106) Coupling Single Molecule Spectroscopy and Electrochemistry in Zero-Mode Waveguides; <u>Lawrence</u> <u>Zaino</u>, Dane Grismer, Donghoon Han, Paul Bohn¹; ¹University of Notre Dame

Poster Board #50

(107) Measurement of Spatially Confined Nanoclusters of Porphyrins Using Conductive-Probe Atomic Force Microscope; <u>Xianglin Zhai</u>¹, Neepa KuruppuArachchige¹, Pedro Derosa², Jayne Garno¹; ¹Louisiana State University; ²Louisiana Tech University

Poster Board #51

(108) **Turn-On Fluorescence as a Strategy for Monitoring the Catalyzed Reduction of Nitrite by Pd-on-Au Nanoparticles**; <u>Anthony Stender</u>¹, Emilie Ringe¹; ¹Rice University

Poster Board #52

(109) Studies of Electronic States of CNT/Rubber Nanocomposites by using Attenuated Total Reflectance Spectroscopy in the Ultraviolet Region; <u>Yusuke Morisawa</u>¹, Kenta Kobashi², Ichiro Tanabe², Harumi Sato³, Takeyoshi Goto², Yukihiro Ozaki²; ¹Department of Chemistry, School of Science and Engineering, Kinki University; ²Department of Chemistry, School of Science and Technology, KwanseiGakuin University; ³Graduate School of Human Development and Environment, Kobe University

TECHNICAL PROGRAM – MONDAY Posters 11:00 am – 12:00 pm ♦ Orals 1:20 – 3:00 pm

Poster Board #53

(110) Investigation of Electronic States of Nano Carbon/Polymer Nanocomposites by Attenuated Total Reflectance-Ultraviolet Spectroscopy; <u>Kenta Kobashi</u>¹, Ichiro Tanabe¹, Yusuke Morisawa², Harumi Sato³, Takeyoshi Goto¹, Yukihiro Ozaki¹; ¹Graduate School of Science and Technology, Kwansei Gakuin Univ; ²Graduate School of Science and Technology, Kinki Univ; ³Graduate School of Human Development and Environment, Kobe Univ

Poster Board #54

(111) **Structural and Magnetic Properties of Cobalt Substituted Magnetite/Ferrihydrite Composites**; <u>Dale L.</u> <u>Perry</u>³, K. I. Camacho¹, N. Pariona¹, Arturo I. Martinez¹, E. Baggio-Saitovitch²; ¹Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional Unidad Saltillo; ²Centro Brasileiro de Pesquisas Físicas, Río de Janeiro; ³Lawrence 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 Pisonero¹, David Blanco², Natalia Beltrán², Nerea Bordel¹; ¹Department of Physics, University of Oviedo; ²Department 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; <u>Takafumi Hirata</u>¹; ¹Kyoto University
- 2:00 (114) State of the Art in Bio-Imaging by LA-ICP-MS; <u>Philip Doble¹</u>; ¹UTS
- 2:20 (115) Development of a Laser Ablation–Inductively Coupled Plasma–Mass Spectrometry Cell and Deconvolution Approaches for Fast High Resolution 3D Imaging; <u>Stijn J. M. Van Malderen¹</u>, Johannes T. van Elteren², Frank Vanhaecke¹; ¹Department of Analytical Chemistry, Ghent University, Belgium; ²Analytical 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; <u>Nicole LaHaye^{1,2}</u>, Jose Kurian³, Prasoon Diwakar², Lambert Alft³, Sivanandan Harilal¹; ¹Pacific Northwest National Laboratory; ²Purdue University; ³Technische 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?**; <u>Gary M.</u> <u>Hieftje¹</u>, Elise A. Dennis¹, Alexander Gundlach-Graham², Steven J. Ray¹; ¹Indiana University; ²ETH Zürich
- 1:40 (118) Interplay of Chromatography and Spectroscopy with Carbon Nanoparticles; <u>Luis Colon¹</u>, Zuqin Xue¹, Karina Tirado-González¹, Amaris Borges-Muñoz¹; ¹University at Buffalo - SUNY

- 2:00 (119) Quantum Dots and Upconverting Nanoparticles: Using Paper Platforms for Multiplexed Optical Sensing by Resonance Energy Transfer; <u>Ulrich Krull</u>¹, M. Omair Noor¹, Feng Zhou¹, Samer Doughan¹, Yi Han¹, Anna Shahmuradyan¹, Uvaraj Uddayasankar¹; ¹University of Toronto Mississauga
- 2:20 (120) Genome-Inspired Aptamers: Affinity Derived from Nature; Linda McGown¹; ¹Rensselaer Polytechnic Institute
- 2:40 (121) Seeing the Light: Studies of the Ocular Surface; <u>Frank Bright¹</u>; ¹SUNY-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}; ¹Leibniz Institute of Photonic Technology; ²Institute of Physical Chemistry and Abbe Center of Photonics
- 1:40 (123) Practical Considerations in using Raman Spectroscopy for Aging of Blood Stains; <u>Anita Mahadevan-</u> <u>Jansen¹</u>, Kiana Jansen¹, Maggie O'Connor¹, Maurice Aalders, Isaac Pence¹; ¹Vanderbilt University
- 2:00 (124) Unsupervised and Supervised Multivariate Statistical Analysis of a Large Lung Spectral; <u>Max Diem</u>¹; ¹Northeastern University
- 2:20 (125) Advanced Statistics of Raman Spectroscopic Data for Disease Diagnostics and Forensic Purposes; <u>Lenka</u> <u>Halamkova¹</u>, Kyle C. Doty¹, Gregory McLaughlin¹, Elena Ryzhikova¹, Oleksandr Kazakov¹, Igor K. Lednev¹; ¹University at Albany, SUNY
- 2:40 (126) **Speed Acquisition Improvement in Raman Imaging via Compressive Sensing**; <u>Nicolas Spegazzini</u>¹, Rishikesh Pandey¹, Ishan Barman², Ramachandra Rao Dasari¹; ¹Massachusttes Institute of Technology; ²Johns 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; <u>Federico Marini</u>¹; ¹University of Rome La Sapienza
- 1:40 (128) Instrumental Approaches and Chemometric Analyses for Establishing Authenticity of Botanical Products; <u>Paula N. Brown</u>¹, Michael Chan¹, Jamie Finley¹, Christina E. Turi², Andrew R. Lewis³; ¹British Columbia Institute of Technology; ²University of British Columbia; ³Simon Fraser University
- 2:00 (129) A UV-Vis-PCA Approach to Botanical Identity Confirmation using DNA Validated Botanical Reference Materials; Jeremy Stewart¹; ¹Gaia Herbs, Inc
- 2:20 (130) Chemometrics in the United States Pharmacopeia; Lucy L. Botros¹, Jeffrey C. Moore¹, Alan R. Potts¹; ¹U.S. Pharmacopeial Convention
- 2:40 (131) Spectral Fingerprinting: Following the Transition from Raw Botanical to Finished Product; James Harnly¹; ¹US 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 Zang¹; ¹University of Utah
- 1:40 (133) Fluorescence Detection of Explosives: A Study Towards Optimization of an Array of Thin Film Optical Sensors; <u>William Euler</u>¹, Hui Qi Zhang¹, Mingyu Liu¹, Matthew Mullen¹; ¹University of Rhode Island
- 2:00 (134) **Issues in Explosive Detection: Sampling**; <u>Jimmie</u> <u>Oxley</u>¹; ¹University of Rhode Island
- 2:20 (135) **HPIMS in Explosive Detection and Forensic Applications**; <u>Ching Wu</u>¹, Anthony Midey¹, Adam Griachen¹, Mark Osgood¹; ¹Excellims Corporation
- 2:40 (136) **HMTD Decomposition:** A Kinetic Study; <u>Lucus</u> <u>Steinkamp</u>¹, Lauryn DeGreeff², Kevin Johnson², Greg Collins², Susan Rose-Pehrsson²; ¹National Research Council; ²Nova 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; <u>Zhe Wang</u>¹, Zongyu Hou^{1, 2}, Tingbi Yuan^{1,2}; ¹State Key Lab of Power Systems, Department of Thermal Engineering, Tsinghua-BP Clean Energy Center, Tsinghua University; ²China Guodian Science and Technology Research Institute
- 2:00 (138) Choices and Improvements in Baseline Removal in LIBS Spectroscopy; <u>Melinda (Darby) Dyar¹</u>, Thomas Boucher², Stephen Giguere², CJ Carey², Sridhar Magadevan²; ¹Mount Holyoke College; ²University of Massachusetts at Amherst
- 2:20 (139) Analysis of Wear Metals in Engine Oil using LIBS; Markus Gaelli¹, Amy Bauer¹; ¹TSI 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; <u>Kate Lepore¹</u>, Elly Breves¹, M. Darby Dyar¹; ¹Mount 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 Jasper¹, Martin Pavane², Dean Eyler³, Ila Sharma⁴, Albert Lee⁴; ¹Nature's Fingerprint / MIT LLC; ²Cozen O; ³Gray Plant Mooty; ⁴Chemir Analytical Services
- 1:40 (142) A Tiered Analytical Approach for Investigating Poor Quality Emergency Contraceptives; <u>Facundo</u> <u>Fernandez</u>¹, Maria Eugenia Monge¹, Prabha Dwivedi¹, Manshui Zhou¹, David Jenkins², Paul Newton^{3,4}; ¹Georgia Institute of Technology; ²Product Quality and Compliance, FHI 360; ³Lao-Oxford-Mahosot Hospital-Wellcome Trust Research Unit, Microbiology Laboratory, Mahosot Hospital; ⁴WorldWide Antimalarial Resistance Network, Churchill Hospital
- 2:00 (144) Meeting Authentication Challenges with Spectroscopic Solutions; Jeffry Denault¹, Robert Beal¹; ¹Eli Lilly and Company

2:20 (145) Raman Spectral Fingerprinting for Biologics Counterfeit Drug Detection; <u>Ravi Kalyanaraman¹</u>, Anna Luczak¹, Jeremy Peters¹, Varsha Ganesh¹; ¹Bristol-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**; <u>Duncan Graham</u>¹, Jonathan Simpson¹, Derek Craig¹, Karen Faulds¹; ¹University of Strathelyde
- 1:40 (147) **Metabolite Identification by Sheath-Flow SERS**; <u>Zachary Schultz¹</u>, Matthew Bailey¹, Kevin Jacobs¹; ¹University of Notre Dame
- 2:00 (148) Development of SERS for Monitoring Small Molecule Metabolites; <u>Mark McDermott</u>^{1,2}, Shereen Elbayomy^{1,2}, Albert Cao^{1,2}; ¹University of Alberta; ²National Institute for Nanotechnology
- 2:20 (149) **Stimulated Raman Spectroscopy for SERS of Biological Systems**; <u>Renee Frontiera</u>¹, W. Ruchira Silva¹, Emily L. Keller¹; ¹University 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; <u>Chloe</u> <u>Westley</u>¹, Yun Xu¹, Andrew Carnell², Nicholas Turner¹, Royston Goodacre¹; ¹Department of Chemistry, University of Manchester, Manchester Institute of Biotechnology; ²Department 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; <u>Koichi Iwata</u>¹, Ashok Samuel², Soshi Yabumoto², Kenichi Kawamura³; ¹Gakushuin University; ²National Chiao Tung University, Taiwan; ³Tokyo Instruments
- 1:40 (152) Linear and Non-Linear Fiber-Based Ramanspectroscopy for Biophotonic Applications; Juergen <u>Popp</u>^{1,2}; ¹Leibniz Institute of Photonic Technology; ²Institute 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; <u>Katherine Hollywood</u>¹, LornaAshton², Katherine Lau³, Saba Khan¹, Nicholas Lockyer¹, Mark Dunne¹,Karen Cosgrove¹, Alan Dickson¹, Royston Goodacre¹; ¹University of Manchester, UK; ²Lancaster University, UK; ³Renishaw PLC, UK
- 2:20 (154) Rapid, Quantitative Spectroscopic Imaging using Coherent Anti-Stokes Raman Scattering; <u>Marcus</u> <u>Cicerone¹</u>; ¹National Institute of Standards and Technology
- 2:40 (155) **Bioorthogonal Stimulated Raman Imaging for Biomedicine**; <u>Wei Min¹</u>, Lu Wei¹; ¹Columbia 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 Maurer¹; ¹Central Connecticut State University
- 1:40 (157) Challenges in Managing a Diverse Workforce; <u>Fred</u> <u>LaPlant¹</u>; ¹3M

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

- 2:00 (158) Don't Call Us Dropouts (please)! Choosing Nontraditional Career Paths in the Sciences; <u>Emily</u> Monosson¹; ¹Independent
- 2:20 (159) Adventures Abroad! Pursuing International (European) Academic Positions; Ingeborg Iping Petterson¹; ¹Biomedical Physics, University of Exeter
- 2:40 (160) **How a Frozen Banana Shaped My Career Path**; <u>Heather Brooke¹</u>; ¹CAMO 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**; <u>Paul Cremer</u>¹; ¹Penn State University
- 1:40 (162) Protein Structures and Folding at Interfaces Probed by Chiral Sum Frequency Generation Vibrational Spectroscopy; <u>Elsa Yan¹</u>; ¹Yale University
- 2:00 (163) Molecular structure at Solid Surfaces: Understanding the Role of Bulk Effects; <u>Dennis Hore</u>¹; ¹University of Victoria
- 2:20 (164) Direct Small-Molecule Detection in a Primary Antibody Assay using Second > Harmonic Generation; John Conboy¹; ¹University of Utah
- 2:40 (165) What Makes Aqueous Foams Stable? A Combined Oscillating Bubble and Vibrational Sum-Frequency Spectroscopy Study; <u>Patrick Koelsch</u>¹, Matthias J. Hofmann², Robert Weikl², Hubert Motschmann²; ¹University of Washington, Department of Bioengineering; ²University 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; <u>Anna</u> <u>Donnell</u>¹, Alexey Porollo², George Deepe¹, Joseph Caruso¹; ¹University of Cincinnati; ²Cincinnati Childrens' Hospital
- 4:10 (167) **The Use of Stable Isotope Labeling in Mass Spectrometry Based Bioanalysis**; <u>Stephan Hann</u>^{1,2}, Teresa Mairinger¹, Eva Oburger³, Markus Puschenreiter³, Gunda Koellensperger⁴; ¹Division of Analytical Chemistry, Department of Chemistry, BOKU Vienna, Austria; ²Austrian Center of Industrial Biotechnology (ACIB); ³Institute of Soil Research, BOKU Vienna, Austria; ⁴Institute of Analytical Chemistry, University of Vienna, Austria
- 4:30 (168) Applications of ICPMS and MC-ICPMS at Chemical Metrology, National Research Council Canada; Lu Yang¹; ¹National Research Council Canada
- 4:50 (169) ICP-MS for Multiplex Analysis of Copy Number Variations In Tumor Cells; <u>Maria Montes-Bayon</u>¹, Tamara Iglesias¹, Marta Espina^{1,2}, L. Maria Sierra^{1,2}, Elisa Blanco-González¹; ¹University of Oviedo; ²Oncology 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)?; <u>Shi Jiao¹</u>, John W. Olesik¹; ¹Ohio 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; <u>Torsten Frosch</u>¹, Timea Boegoezi¹, Stefan Hanf¹, Tobias Jochum¹, Juergen Popp^{1,2,3}; ¹Leibniz Institute of Photonic Technology; ²Friedrich Schiller University, Institute for Physical Chemistry; ³Friedrich Schiller University, Abbe Centre of Photonics
- 4:10 (172) **IR Imaging: Applications in Wound and Transplant Pathology**; <u>Michael Walsh</u>¹, Bennett Davidson¹, Hari Sreedhar¹, Vishal Varma¹, Peter Nguyen¹, Sanjeev Akkina¹, Aliya Husain², Suman Setty¹, Andre Kajdacsy-Balla¹, William Ennis¹; ¹University of Illinois At Chicago; ²University of Chicago
- 4:30 (173) Shining Light Inside Middle Ear: What Raman Spectroscopy Tells Us about Infection?; <u>Rishikesh Pandey</u>¹, Nicolas Spegazzini¹, Tulio A Valdez², Ishan Barman³, Ramachandra Rao Dasari¹; ¹MIT; ²Connecticut Children; ³Johns Hopkins University
- 4:50 (174) Multi-centre Raman Spectral Histopathology of Deparaffinised Oesophageal Tissues.; Jennifer Dorney¹, Martin Isabelle², Gavin Rhys-Lloyd², Catherine Kendall², Riana Gaifulina³, Aaran Lewis³,Geraint Thomas³, Katherine Lau⁴, David Reece⁴, Nick Stone¹; ¹University of Exeter, Exeter; ²Gloucester Hospital, Gloucester, United KIngdom; ³University College London; ⁴Renishaw PLC UK
- 5:10 (175) Addressing Variability of Tissue Raman Spectroscopy for Clinical Diagnostics; <u>Isaac Pence</u>¹, Anita Mahadevan-Jansen¹; ¹Vanderbilt 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; <u>Stephen L.</u> <u>Morgan¹</u>, Nathan C. Fuenffinger¹; ¹University of South Carolina
- 4:10 (177) Development and Evaluation of a Searchable Database for the Characterization and Comparison of Forensic Evidence using Spectrochemical Methods; <u>Tatiana Trejos</u>¹, Claudia Martinez¹, Ruthmara Corzo¹, Kiran Subedi¹, Rhett Williamson¹, Peter Torrione², Jong Yoo³, Jose Almirall¹; ¹Florida International University; ²CoVar Applied Technologies; ³Applied Spectra, Inc
- 4:30 (178) A Bayesian Approach to Interpretion of Multielement Data; James Curran¹; ¹University of Auckland
- 4:50 (179) Chemometric Approaches for the Analysis of Chemical Attribute Signatures Generated from Forensically Relevant Samples; <u>Adam B. Hall¹</u>; ¹Northeastern University; ²Boston University School of Medicine; ³IonSense, 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. <u>Derrick Quarles Jr.</u>¹, Charles Sisson¹, Jhanis J. Gonzalez^{1,2}, Richard E. Russo^{1,2}; ¹Applied Spectra, Inc.; ²Lawrence 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; <u>Albert Fahey¹</u>, Kamron Fazel¹, Kenneth Grabowski¹, Evan Groopman¹; ¹Naval Research Laboratory
- 4:10 (182) X-Ray Microscopy of Nuclear Materials; Jesse Ward¹, Greg Eiden¹, Andrew Duffin¹; ¹Pacific Northwest National Laboratory
- 4:30 (183) Advances in Analysis of Samples for Nuclear Non-Proliferation at CEA/DIF; <u>Bruno Bernard-Michel¹</u>, Fabien Pointurier¹, Maxime Bridoux¹, Anne-Laure Fauré¹, Amélie Hubert¹, Olivier Marie¹, Anne-Claire Pottin¹; ¹CEA-DIF, Bruyères le Châtel
- 4:50 (184) Discrimination of Uranium ore Concentrates from Several Countries by Chemometric Data Analysis; Josette El Haddad¹, Aissa Harhira¹, Alain Blouin¹, Mohamad Sabsabi¹, Marvin Zaluski², Chunsheng Yang², Christopher Drummond², Slobodan Jovanovic³, Tanya Hinton³, Ali El-Jaby³; ¹National Research Council Canada - Energy, Mining and Environment; ²National Research Council Canada -Information and Communications Technologies; ³Canadian Nuclear Safety Commission
- 5:10 (185) DC Arc Spectroscopy Plasma Characterization for Direct Solid Analysis of Nuclear Materials; <u>Benjamin T.</u> <u>Manard¹</u>, John Matonic¹, Robert Jump¹, Dennis Montoya¹, Alonso Castro¹, Ning Xu¹; ¹Los Alamos National Laboratory

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Monday Afternoon, Room 556B				
	NEAR IR			
	Organizer and Presider: Franklin E. (Woody) Barton			
3:50	(186) NIR With Problem Data Sets; <u>Franklin Barton</u> ¹ ,			
	James de Haseth ¹ ; ¹ Light Light Solutions Instruments, Inc.			
4:10	(187) A New Look at the Derivative Quotient Method in			
	Regression ; <u>David Hopkins</u> 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			
	<u>OBrien</u> 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			
2.00	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 Breckenridge¹; ¹Bristol-Myers Squibb

- 4:50 (193) Identification of Meat Species by using Laser Induced Breakdown Spectroscopy; <u>Gonca Bilge</u>¹, Banu Sezer¹, Hasan Murat Velioğlu², Kemal Efe Eseller³, Halil Berberoğlu⁴, İsmail Hakkı Boyacı¹; ¹Hacettepe University, Department of Food Engineering; ²Namık Kemal University, Department of Agricultural Biotechnology; ³Atılım University, Department of Electrical & Electronics Engineering; ⁴Gazi University, Department of Physics
- 5:10 (194) Study of Plasma and Identification of Hazardous Elements in the Polystyrene using Laser Induced Breakdown Spectroscopy; <u>W. Aslam Farooq</u>¹; ¹King 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 Wasylyk¹, Ming Huang¹, Robert Wethman¹; ¹Bristol-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; <u>Alain Hedoux¹</u>, Laurent Paccou¹, Yannick Guinet¹; ¹University Lille 1, UMET - UMR CNRS 8207
- 4:30 (197) Chemical Imaging of Crystalline Components in Pharmaceutical Dosage Forms by Using Low Frequency Raman Spectroscopy; <u>Toshiro Fukami</u>¹, Motoki Inoue¹, Hiroshi Hisada¹, Tatsuo Koide²; ¹Meiji Pharmaceutical University; ²National 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; <u>Mark</u> <u>Sullivan¹</u>, Elaine Harrop Stone², Monwara Hoque², Xiao Hua Zhou¹, Richard McKay¹; ¹Advantest America Inc; ²Merlin Powder Characterisation Ltd
- 5:10 (199) Low Wavenumber Raman Spectroscopy Applications in API Phase Discovery and Characterization; <u>Courtney Maguire</u>¹, Andrew Brunskill¹; ¹Merck 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**; <u>Richard Van Duyne¹</u>; ¹Northwestern University
- 4:10 (201) **Resolution and Enhancement in TERS Microscopy**; <u>Satoshi Kawata¹</u>, Atsushi Taguchi¹; ¹Osaka University
- 4:30 (202) Molecular Structure Changes on the Nanometre Scale Investigated and Induced by TERS; <u>Volker</u> <u>Deckert</u>^{1,2}; ¹University of Jena; ²Leibnitz Institute of Photonic Technology
 4:50 Discussion
- 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; <u>Don Pivonka¹</u>, William Rocco¹, Dilip Modi¹; ¹Incyte Inc.
- 4:10 (204) Quantification of Residual Crystallinity in Pharmaceutical Formulations using Transmission Raman Spectroscopy; <u>Mark Mabry</u>¹; Julia Griffen¹, Matthew Bloomfield², Andrew Owen¹, Darren Andrews¹, Pavel Matousek³; ¹Cobalt Light Systems, Ltd; ²Cobalt Light Systems, Inc; ³Central 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 Seabrooks¹, Nicole Canfield¹, Justin Pennington¹; ¹Merck
- 4:50 (206) Screening of Antibiotics Using Portable Spectrometers; Jason Rodriguez¹, Latevi Lawson¹, Hirsch Srivastava¹, Megha Mohan¹; ¹FDA
- 5:10 (207) Prediction of Bead Coating Thickness using Raman Quantitative Model; <u>Hanzhou Feng</u>¹, James Drennen¹, Carl Anderson^{1,2}; ¹Duquesne University, Graduate School of Pharmaceutical Sciences; ²Duquesne 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 Maurer¹; ¹Central Connecticut State University
- 4:10 (209) Are You the Only Professional Woman in the Organization?; <u>Ellen Miseo</u>¹; ¹Hamamatsu Corp.
- 4:30 (210) A Nontraditional Career Path; <u>Emily Monosson</u>¹; ¹Independent/Ronin Institute
- 4:50 (211) **Discussion Panel**; <u>Fred LaPlant</u>¹; ¹3M
- 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; <u>Colin Ingram</u>¹; ¹Andor 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; <u>Eric Stach</u>¹; ¹Brookhaven National Laboratory
- 4:30 (214) *In situ* Probing of Environmental Liquid Surfaces and Interfaces using Microfluidics: Toward Multimodal and Mesoscale Imaging; <u>Xiao-Ying Yu</u>¹, Zihua Zhu²; ¹Fundamental and Computer Sciences Directory; ²W. 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; <u>Franklin (Feng) Tao¹</u>, Shiran Zhang¹, Luan Nguyen¹, Junjun Shan¹; ¹University 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 Cheng¹; ¹Purdue University



8:30 am – FACSS Charles Mann Award for Applied Raman Spectroscopy (217) UV Resonance Raman Spectroscopic Studies of Protein Structure and Dynamics; <u>Sanford</u> <u>Asher¹</u>, David Punihaole¹, Elizabeth M. Dahlburg¹, Ryan S. Jakubek¹, Zhenmin Hong¹; ¹University 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**; <u>Olga</u> <u>Borovinskaya</u>¹, Martin Tanner¹; ¹TOFWERK AG
- 9:35 (219) Analytical Insights into Human Risk Assessments of Noble Metal Nanomaterials; Petra Krystek¹; ¹VU University Amsterdam
- 9:55 (220) Single Particle ICP-MS in a Multitechnique Approach to Elucidate the Fate of Silver Nanoparticles in Burnt Patients; <u>Marco Roman^{1,4}</u>, Chiara Rigo¹, Vincenzo Vindigni², Hiram Castillo-Michel³, Warren R.L. Cairns⁴; ¹University Ca; ²Burns Center, University Hospital of Padua; ³European Synchrotron Radiation Facility (ESRF), Grenoble; ⁴Institute 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 Bettmer¹, Juan Soto-Alvaredo¹, Carlos López-Chaves², Maria Montes-Bayón¹, Cristina Sanchez-González², Juan Llopis-González²; ¹University of Oviedo; ²University of Granada
- 10:35 (222) Cloud Point Extraction for Silver Nanoparticle and Ion Quantification; <u>Nicole Hanks</u>¹, Joseph Caruso¹, Peng Zhang¹; ¹University 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; <u>Ning Fang</u>¹, Kuangcai Chen², Ashley Augspurger²; ¹Georgia State University; ²Iowa State University
- 9:35 (224) **High Speed Molecular Imaging by Phosphorescence Lifetime Multiphoton Microscopy**; <u>Scott Howard</u>¹; ¹University of Notre Dame
- 9:55 (225) Ultrafast Nanoscopy of Energy and Charge Transport; Libai Huang¹; ¹Purdue University
- 10:15 (226) Gigapixel Fluorescence Histology for Rapid 'No-Cut' Surgical Pathology; J. Quincy Brown¹; ¹Tulane University
- 10:35 (227) **TERS Characterization of Membrane Receptors**; Zachary Schultz¹, Hao Wang¹; ¹University 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**; <u>Rima Kaddurah-</u> <u>Daouk</u>^{1,2}; ¹Duke University Medical Center; ²On behalf of the Pharmacometabolomics Research Network

- 9:35 (229) Stable Isotope Resolved Metabolomics (SIRM) on Fresh Human Tissues as a Preclinical Drug Testing Platform; <u>Andrew Lane</u>¹, Teresa Fan¹, Alexander Belshoff², Richard Higashi¹, Jeremiah Martin¹, Michael Bousamra²; ¹University of Kentucky; ²University of Louisville
- 9:55 (230) **Personalized Medicine in Human Space Flight**; <u>Michael A Schmidt</u>¹; ¹Sovaris Aerospace, LLC
- 10:15 (231) Metabolomic Applications in Nutritional Research; Lorraine Brennan¹; ¹UCD Institute of Food and Health
- 10:35 (232) NMR as an Important Analytical Tool for Identifying Drug Metabolites in Support of Drug Discovery; <u>Yingzi Wang</u>¹, Xiaoliang Zhuo¹, John Leet¹, Stella Huang¹, Joseph Cantone¹, Dieter Drexler¹, Kim Johnson¹, Benjamin Johnson¹, Michael Reily¹, Adrienne Tymiak¹; ¹Bristol-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; <u>Barry</u> <u>Lavine¹</u>, Maissa Gaye², David Clemmer², Tao Ding¹, H Shion³, W. Chen³, A. Hussein³, Y. Hu^{,4}, S. Zhou^{,4}, Yehia Mechref⁴; ¹Department of Chemistry, Oklahoma State University; ²Department of Chemistry, Indiana University; ³Waters Corporation, Pharmaceutical Life Sciences; ⁴Department of Chemistry & Biochemistry, Texas Tech University
- 9:35 (234) Medical Applications of Multivariate Statistical Process Control; <u>Lionel Blanchet</u>^{1,2}, Jasper Engel³, Frederik-Jan van Schooten¹; ¹Department of Toxicology, Maastricht University Medical Center, the Netherlands; ²Top Institute Food and Nutrition (TIFN), Wageningen, the Netherlands; ³NERC Metabolomics Facility, School of Biosciences, Birmingham University
- 9:55 (235) Sparse Deconvolution of High-Density Super-Resolution Images; Cyril Ruckebusch¹, Romain Bernex¹, Siewert Hugelier¹, Olivier Devos², ¹, Johan de Rooi², Paul Ailers²; ¹LASIR CNRS Université de Lille, France; ²Department of Biostatistics, Erasmus Medical Center, Rotterdam, The Netherlands
- 10:15 (236) Multivariate Curve Resolution of Mass Spectrometry Imaging (MSI) of Biological Tissues; <u>Roma</u> <u>Tauler¹</u>, Carne Bedia¹, Joaquim Jaumot¹; ¹IDAEA-CSIC
- 10:35 (237) Investigations on the Analysis Workflow for Biomedical Application of Raman Spectroscopy; <u>Thomas</u> <u>Bocklitz</u>¹, Jürgen Popp^{1,2}; ¹University of Jena, Institute of Physical Chemistry; ²Institue 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; <u>Carrie McDonough</u>¹, Rainer Lohmann¹; ¹Graduate School of Oceanography, University of Rhode Island
- 9:35 (239) A Great Lakes Perspective on Flame Retardants: Lessons from the Integrated Atmsopheric Deposiiton Network.; <u>Marta Venier</u>¹, Amina Salamova¹, Todd Nettesheim², Ron Hites¹; ¹Indiana University; ²Environmental Protection Agency Great Lakes National Program office; ⁴Indiana University
- 9:55 (240) Emerging Flame Retardants in North American Aquatic Ecosystems; <u>Da Chen¹</u>, Rebecca Sutton², Jeremy Moore³, Doug Adams⁴, Yan Wu¹, Hillary Marler¹, Hillary Marler¹; ¹Southern Illinois University; ²San Francisco Estuary Institute; ³US Fish and Wildlife Service; ⁴Cape Canaveral Scientific, Inc.
- 10:15 (241) Strategies and Techniques for Identifying Unknown Compounds in Environmental Samples; <u>Eric J Reiner</u>^{1,3}, Karl J Jobst ³, Miren Pena-Abaurrea¹, Anne L Myers¹, Li Shen², Alina Muscalu², Ralph Ruffolo², Xavier Ortiz², Paul A Helm²; ¹University of Toronto; ²Ontario Ministy of the Environment and Climate Change; ³McMaster 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; <u>Geneviève Granger</u>¹, Nathalia Bukar¹, Jean-François Masson¹, Andreea R. Schmitzer¹; ¹Département de Chimie, Université de Montréal, Montréal, Canada
- 9:35 (243) Generation and Quantitation of Parts per Quadrillion Levels of TNT and RDX; <u>Braden Giordano</u>¹, Benjamin Andrews², Adam Lubrano²; ¹U.S. Naval Research Laboratory; ²Nova Research, Inc.
- 9:55 (244) Analysis and Delivery of Vapor from Binary Explosive Mixtures for Instrumental and Canine Detection; <u>Susan Rose-Pehrsson^{1,2}</u>, Lauryn DeGreeff¹, Frank Lucus Steinkamp³, Braden Giordano¹, Christopher Katilie^{1,2}; ¹U.S. Naval Research Laboratory; ²Nova Research, Inc.; ³National Research Council
- 10:15 (245) **Trace Explosive Detection using Zinc Oxide Nanowire Catalysts**; <u>Zachary Caron</u>¹, Otto Gregory¹; ¹University of Rhode Island, Department of Chemical Engineering
- 10:35 (246) In-situ Detection of Energetic Materials Based on Surface Plasmon Spectroscopies; <u>Thibault Brulé</u>¹, Geneviève Granger¹, Natalia Bukar¹, Marc Vidal¹, Jean François Masson¹; ¹Département 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**; <u>Rolando Rebois</u>¹, Ariane Deniset-Besseau¹, Delphine Onidas¹, Alexandre Dazzi¹; ¹Laboratoire de Chimie Physique - Université Paris-Sud

- 9:35 (248) AFM-IR Spectroscopy and Imaging of Polymer Nanofibers and Thin Films at the Nanoscale; John Rabolt¹, Liang Gong¹, Isao Noda^{1,3}, Bruce Chase¹, C. J. McBrin¹, Curtis Marcott^{1,2}; ¹Department of Materials Science and Engineering, University of Delaware; ²LightLightSoluions; ³Department 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; <u>Martin Wagner</u>¹, Karina Carneiro², Stefan Habelitz², Thomas Mueller¹; ¹Bruker Nano Surfaces; ²University of California, Preventive and Restorative Dental Sciences
- 10:15 (250) Introducing nano-FTIR Imaging and Spectroscopy at 10 nm Spatial Resolution; <u>Tobias Gokus</u>¹, Andreas Huber¹, Florian Huth¹; ¹Neaspec GmbH
- 10:35 (251) Characterization of a Polyethylene–Polyamide Multilayer Film using Nanoscale Infrared Spectroscopy and Imaging; <u>Mauritz Kelchtermans</u>¹, Michael Lo², Eoghan Dillon², Kevin Kjoller², Craig Prater², Curtis Marcott³; ¹ExxonMobil Chemical Europe, Belgium; ²Anasys Instruments; ³Light 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 Laserna¹; ¹Universidad de Malaga
- 9:55 (253) Pathways Towards High-Resolution Chemical Analysis and Imaging with Femtosecond LIBS; <u>Vassilia</u> <u>Zorba¹</u>; ¹Lawrence Berkeley National Laboratory
- 10:15 (254) New Hybrid Calibration-Free/Artificial Neural Networks Approach for Quantitative Analysis; <u>Vincenzo</u> <u>Palleschi</u>¹; ¹National Research Council
- 10:35 (255) New Methodology for Quantitative Laser-Induced Breakdown Spectroscopy Based on CSigma graphs. Application to Fused Glass Samples; <u>Carlos Aragon^{1,2}</u>, Jose Antonio Aguilera^{1,2}; ¹Departamento de Fisica, Universidad Publica de Navarra; ²Institute 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 Marquardt¹, Thomas Dearing², Michael Roberto³, Olav Bleie⁴; ¹University of Washington; ²MarqMetrix Inc; ³Infometrix; ⁴Univ. of Bergen, Norway
- 9:35 (257) Recent Advances in Automatic Continuous Online Monitoring of Polymerization reactions (ACOMP); <u>Wayne</u> <u>Reed</u>², Michael F. Drenski¹; ¹Advanced Polymer Monitoring Technologies, Inc.; ²Tulane University
- 9:55 (258) Development of NIR Methodology for Process Monitoring and Control using an Offline Calibration Approach; <u>Evan Hetrick</u>¹, Zhenqi Shi¹, Lukas Barnes¹, David Myers¹, Bryan Castle¹, Salvador Garcia Munoz¹, Ian Leavesley¹; ¹Eli Lilly and Company
- 10:15 (259) *In situ* ATR-FTIR: A Technological Shift in Continuous Processing; <u>Dom Hebrault</u>¹; ¹Dom Hebrault
- 10:35 (260) Getting More Out of Process Measurements with Diode Array Spectrometers: Instrumental and Analysis Approaches; <u>Robert Lascola¹</u>, Patrick O'Rourke¹, Elizabeth Evans¹, Edward Kyser¹; ¹Savannah 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 Ozaki¹, Wei Ji¹, Yue Wang², Ichiro Tanabe¹, Bing Zhao²; ¹Department of Chemistry, School of Science and Technology, Kwansei Gakuin University; ²State Key Laboratory of Supramolecular Structure and Materials, Jilin University
- 9:35 (262) Coherent Raman Spectroscopy with Optical Frequency Combs; <u>Takuro Ideguchi</u>^{1,2}, Simon Holzner², Birgitta Bernhardt², Guy Guelachvili³, Theodor Hänsch^{2,4}, Nathalie Picqué^{2,3,4}; ¹The University of Tokyo; ²Max-Planck-Institut für Quantenoptik; ³Institut des Sciences Moléculaires d'Orsay, CNRS; ⁴Ludwig-Maximilians-Universität München
- 9:55 (263) Functionalised Nanoparticles for the Detection of Explosives and Small Molecule by SERS; <u>Karen Faulds</u>¹, Rachel Norman¹, Duncan Graham¹, Neil Shand²; ¹University of Strathelyde; ²Defence Science and Technology Laboratory FACSS Student Award
- 10:15 (264) Raman Spectroscopy of Single Electrospun Nanofibers; <u>Marie Richard-Lacroix</u>¹, Christian Pellerin¹;

¹University of Montreal

10:35 (265) Spectroscopy on Mars - Searching for Signs of Life; <u>Ian Hutchinson¹</u>, Richard Ingley¹, Howell Edwards¹, Nick Waltham²; ¹University of Leicester; ²Rutherford 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; <u>Andreas Dahlin¹</u>; ¹Chalmers University of Technology
- 9:35 (267) Head-to-Head Comparison of the Performance of SERS and ELISA Diagnostic Tests for Infectious Disease; <u>Marc Porter¹</u>, Lars Laurentius¹, Nicholas Owens¹, Alexis Crawford¹, Jennifer Granger¹; ¹University of Utah
- 9:55 (268) Single Nanoparticle SPRI Microscopy and Plasmonic Nanocone Arrays For Biosensing; <u>Robert M.</u> <u>Corn¹</u>, Adam Maley¹, Millie Fung¹; ¹Dept. of Chemistry, University of California-Irvine
- 10:15 (269) Microdialysis SPR: Sensing in Whole Blood; Jean-Francois Masson¹; ¹Département 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; <u>Gustav Emilsson¹</u>, Kunli Xiong¹, Andreas Dahlin¹; ¹Dept. 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 Yu¹; ¹National Institute of Standards and Technology Poster Board #2 (272) Identification of Stroke Metalloprotein Biomarkers and Metal Profile in Human Blood Plasma; Keaton Nahan¹, Julio Landero¹, Opeolu Adeoye², Joseph Caruso¹; ¹University of Cincinnati, McMicken College of the Arts and Sciences; ²University of Cincinnati, Medical Center Poster Board #3 (273) Determination of Calcium, Magnesium, and Aluminum in Pine from the Southern Appalachians; David Butcher¹, Alyssa Bailey¹; ¹Western Carolina University Poster Board #4 (274) Calculation of Ion Beam Formation behind the Skimmer Cone of an ICP-MS; Ross Spencer¹; ¹Brigham 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 <u>Tu¹</u>, Tiebang Wang¹, Xiaoyi Gong¹; ¹Merck & Co., Inc. **Poster Board #6** (276) Challenges in Trace Element Analysis of Cobalt Precursors; Lisa Milstein Mey-Ami¹, Phil Clancy¹, Fuhe Li¹, Hugh Gotts¹; ¹Air 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 Haferl¹, Haopeng Wang¹, Kaveh Jorabchi¹; ¹Georgetown University

Poster Board #8

(278) Absorption Spectroscopy of 238U in Laser-Induced Plasma; Jason Becker¹, Brian Brumfield¹, Nicole LaHay¹, Patrick Skrodzki¹, Mark Phillips¹, Sivanandan Harilal¹; ¹PNNL ter Board #9

Poster Board #9

(279) Development and Validation of a New Method to Measure Activity of the Na+, K+ ATPase Using ICP-MS QQQ; <u>Cory Stiner¹</u>, Julio Landero¹, Judith Heiny¹; ¹University of Cincinnati

Poster Board #10

(280) A Green and Fast Approach to Arsenic Speciation; <u>Maria C. Hespanhol da Silva</u>^{1,3}, Julio A. Landero², Joseph A. Caruso²; ¹Universidade Federal de Viçosa; ²University of Cincinnati; ³Conselho Nacional de Desenvolvimento Científico e Tecnológico

Poster Board #11

(281) Effect of Laser Wavelength and Ambient Pressure on Late-Time Bulk Particle Emission; <u>Niral Shah</u>¹, Patrick Skrodzki¹, Brian Brumfield¹, Nicole LaHaye¹, Sivanandan Harilal¹, Mark Phillips¹; ¹Pacific Northwest National Laboratory ar Board #12

Poster Board #12

(282) **Method Development and Validation for the Analysis of Polyacrylic Lithography Reagents by ICPMS**; <u>Phil</u> <u>Clancy</u>¹, Hugh Gotts¹, Scott Anderson¹; ¹Air Liquide-Balazs NanoAnalytical

Chemometrics Posters

Poster Board #13

(283) Combining Statistics and Chemometrics for Guidance of Continuous Improvement Efforts; <u>Mark Henson</u>¹, ¹Shire 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**; <u>Olof Svensson</u>¹, Halldis Thoroddsen², Álvaro Díaz-Bolado¹, Anders Sparén¹, Mats Josefson¹; ¹AstraZeneca R&D Mölndal, Mölndal, Sweden; ²Chalmers University of Technology, Göteborg, Sweden

Poster Board #16

(286) Fluorescence Excitation Spectroscopy and Imaging Multivariate Optical Computing for the Characterization of Natural Phytoplankton Populations; <u>Shawna Tazik</u>¹, Joseph Swanstrom¹, Cameron M. Rekully¹, Stefan T. Faulkner¹, Nicholas S. Viole¹, Timothy J. Shaw¹, Tammi L. Richardson², Michael L. Myrick¹; ¹University of South Carolina, Department of Chemistry and Biochemistry; ²University of South Carolina, Marine Science Program and Department of Biological Sciences

Poster Board #17

(287) A Convex Optimization Approach to Calibration Transfer; <u>Thomas Boucher</u>¹, Melinda Dyar², CJ Carey¹, Stephen Giguere¹, Sridhar Mahadevan¹; ¹University of Massachusetts Amherst; ²Mount Holyoke College

Poster Board #18

(288) A Framework for Fully Customized Baseline Removal; <u>Stephen Giguere¹</u>, M. Darby Dyar², CJ Carey¹, Thomas Boucher¹, Sridhar Mahadevan¹; ¹College of Information and Computer Sciences, University of Massachusetts, Amherst; ²Department of Astronomy, Mount Holyoke College

Poster Board #19

(289) Characterizing Calibration Data Sets by Fusion of Dissimilarity Merits Including Outlier Detection; <u>Brett</u> <u>Brownfield¹</u>, John Kalivas¹; ¹Idaho State University Poster Board #20

(290) Investigation of Cyclodextrin Complexes with PAHs using Steady-State Fluorescence and Parallel Factor Analysis; Joseph Chiarelli, Jonathan Kenny; ¹Tufts University Poster Board #21

(291) MATSA: A User-Friendly Software Program for Magnetic Audio Tape Spectral Analysis; <u>Nathan C.</u> <u>Fuenffinger¹</u>, Brianna M. Cassidy¹, Zhenyu Lu¹, Michael L. Myrick¹, Eric M. Breitung², Stephen L. Morgan¹; ¹University of South Carolina; ²Library of Congress

Poster Board #22

(292) An Effective Approach to Building a Calibration Matrix for a Multi-Component Mixture; <u>Huggins Z.</u> <u>Msimanga¹</u>, Mihyang Song², Newsha Tavakoli³, Truong Thach Ho Lam⁴; ¹Kennesaw State University; ²Mercer University College of Pharmacy; ³Georgia Institute of Technology; ⁴Philadelphia College of Osteopathic Medicine

Poster Board #23

(293) Clustering in Spectroscopy - How Important is the Review Process?; <u>Michael Boruta</u>¹; ¹ACD/Labs LIBS Posters

Poster Board #24

(294) Comparison of Metal Concentrations in Soil with LIBS, XRF, and ICP-MS; Jay Clausen¹; ¹US Army Corps of Engineers ERDC-CRREL

Poster Board #25

(295) **Optimization of Liquid Jet System for Laser-Induced Breakdown Spectroscopy Analysis**; <u>Pavel Porizka</u>², Katarina Skocovska¹, Jan Novotny², David Prochazka², Karel Novotny^{2,3}, Jozef Kaiser²; ¹Faculty of Mechanical Engineering, Brno University of Technology; ²CEITEC BUT - Central European Institute of Technology, Brno University of Technology; ³CEITEC 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; <u>Pavel Porizka</u>¹, Jan Novotny¹, Gabriela Vitkova¹, David Prochazka¹, Jakub Klus¹, Michal Brada¹, Ales Hrdlicka^{1,2}, Karel Novotny^{1, 2}, Jozef Kaiser^{1, 2}; ¹CEITEC BUT - Central European Institute of Technology, Brno University of Technology; ²CEITEC MU -Central European Institute of Technology, Masaryk University, rn Barned 427

Poster Board #27

(297) The Effects of Laser Pulse Energy, Spot Size, and Wavelength on Laser Produced Plasmas in Transverse Magnetic Fields; <u>Payson Dieffenbach</u>¹, Michael Marino¹, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University

Poster Board #28

(298) **Analyzing Ice with LIBS**; <u>Jay Clausen</u>¹, Richard Hark², Alexander Bol'shakov³, John Plummer⁴; ¹USACE ERDC CRREL; ²Juanita College; ³Applied Spectra Inc.; ⁴JR Plumer Associates LLC

Poster Board #29

(299) Spectroscopic Analysis of Cerium, Cesium and Strontium (Nuclear Surrogates) using Laser Induced Breakdown Spectroscopy (LIBS); <u>Charles Ghany^{1,2}</u>, Hervé Sanghapi^{1,2}, Chet Bhatta^{1,2}, Bader Alfaraj^{1,2}, Fang Yueh^{2,3}, Jagdish Singh^{2,3}; ¹Mississippi State University; ²Institute for Clean Energy Technology; ³JPS 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).; <u>Chet Bhatt</u>^{1,2,3}, Charles Ghany^{1,2,3}, Bader Alfarraj^{1,2,3}, Fang Yueh^{1,2}, Jagdish Singh^{1,2,3}; ¹Mississippi State University; ²Institute of Clean Energy Technology (ICET); ³Department of Physics and Astronomy, MSU

Poster Board #31

(301) **Overview of Some Theoretical Modeling of LIBS Emission Spectra**; <u>David Kilcrease</u>¹, Heather Johns¹, James Colgan¹, Beth Judge², James Barefield Il², Roger Wiens³, Sam Clegg⁴; ¹Theoretical Division, Los Alamos National Laboratory; ²Chemical Diagnostics and Engineering, Los Alamos National Laboratory; ³Space and Remote Sensing Division, Los Alamos National Laboratory; ⁴Physical Chemistry and Applied Spectroscopy, Los Alamos National Laboratory

Poster Board #32

(302) A Study of Wheat Flour Tortillas using Laser Induced Breakdown Spectroscopy (LIBS); <u>Charles Ghany</u>^{1,2}, Hervé Sanghapi^{1,2}, Chet Bhatta^{1,2}, Bader Alfaraj^{1,2}, Fang Yueh^{2,3}, Jagdish Singh^{2,3}; ¹Mississippi State University; ²Institute for Clean Energy Technology; ³JPS 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; <u>A.A. Bol'shakov</u>¹, X.L. Mao², J.J. Gonzalez^{1,2}, R.E. Russo^{1,2}; ¹Applied Spectra Inc; ²Lawrence Berkeley National Laboratory

Poster Board #34

(304) Evaluation of Optical Depths of Sr Emission Lines in Laser Induced Breakdown Spectroscopy (LIBS); <u>Bader</u> <u>Alfarrai</u>, Herve Sanghapi, Charles Ghany, Chet Bhatt, Fang Yueh, Singh Jagdish; ¹ICET-MSU

Poster Board #35

(305) **Femtosecond Laser Ablation: A Molecular Dynamics Study**; <u>Alexander Miloshevsky</u>¹, Mark Phillips², Gennady Miloshevsky¹, Sivanandan Harilal²; ¹Purdue University; ²Pacific Northwest National Laboratory

Poster Board #36

(306) Simultaneous Measurement of Conserved Scalars in Flames using LIBS; <u>Wendong Wu¹</u>, Richard Axelbaum¹; ¹Washington University in St.Louis

Poster Board #37

(307) Adaptive Multi-Sensor Data Fusion Model for *in-situ* Mars Exploration; <u>Tajana Schneiderman</u>¹, Pablo Sobron²; ¹The Ohio State University; ²The SETI Institute

RAMAN Posters

Poster Board #38

(308) Application of Low and Mid Frequency Raman for Characterization of Amorphous-Crystalline Indomethacin.; <u>Michaella Raglione Raglione¹</u>, John Wasylyk², Peter Larkin³; ¹The University of Delaware; ²Bristol Myers Squibb; ³Cytec Poster Board #39

(309) High Throughput Integrated Raman Probe with Elongated Core Collection Fiber-optic; <u>Robert Chimenti</u>¹; ¹Innovative Photonic Solutions

Poster Board #40

(310) Improved Material Identification in the Field using a Long Wavelength Handheld Raman Spectrometer; <u>Claire</u> <u>Dentinger¹</u>, Claude Robotham¹, Eric Roy¹; ¹Rigaku Raman Tehcnologies

Poster Board #41

(311) Calorimetry-Derived Vectors to Resolve Pure Raman Spectral Components of Phospholipid Vesicle Phase Transitions; Jay Kitt¹, Joel Harris¹; ¹University of Utah

Poster Board #42

(312) Advances in Kaiser Raman Analyzers for *in situ* Studies of Small Volume Liquid-phase Reactors; <u>Ian Lewis</u>¹, Sean Gilliam¹, Lisa Ganster¹; ¹Kaiser Optical

Poster Board #43

(313) State of the Art Microanalysis using Raman Microscopy; Peng Wang¹, Thomas Tague¹, Sergey Shilov¹; ¹Bruker Optics Inc

Poster Board #44

(314) **High-Speed Compressive Raman and Fluorescence Imaging of Pharmaceutical Composites**; <u>Owen Rehrauer</u>¹, Bharat Mankani¹, Greg Buzzard¹, Brad Lucier¹, Dor Ben-Amotz¹; ¹Purdue University

Poster Board #45

(315) Impact of Radiation Environment on the Performance of Analytical Instrumentation for Planetary Missions; <u>Arthur</u> <u>Smalley¹</u>, Ian Hutchinson¹, Richard Ingley¹, Melissa McHugh¹; ¹University of Leicester

Poster Board #46

(316) **Transmission Raman Spectroscopy using a Spatial Heterodyne Raman Spectrometer**; <u>K. Alicia Strange</u> (<u>Fessler</u>)¹, Kelly Paul¹, S. Michael Angel¹; ¹The University of South Carolina

es	entati	ions 11:40 am – 1:10 p	m	• Orals 1:20	– 3:00 pm		
	Poster	r Board #47					
	(317) Raman Analysis of Ancient Carbonaceous Matter of						
	Ŕ	Relevance to Martian Geolo	ogy;	Richard Ingley ¹ , 0	Cédric		
	Ν	Malherbe ² , Ian Hutchinson ¹ ,	Joh	n Parnell ⁴ ; ¹ Univer	sity of		
	L	Leicester; ² University of Lièg	ge; ³	University of Leic	ester;		
	4	^t University of Aberdeen					
	Poster	r Board #48			.		
	(.	(318) Wide-Field, Hyperspe	ectra	al Raman Spectro	scopy Using		
	a E	a Fiber Array Spectral 1 ra. Hotorodyno Spectrometer:	Notl	nor Coupled with			
	I. N	Nelson ¹ S. Michael Angel ² :	¹ Ch	emImage Sensor S	vstems:		
	2 ₁	University of South Carolina	e chi a	eminage Bensor B	ystems,		
	Poster	r Board #49	*				
	(.	(319) How Low Can You G	0? I	Modelling a Rama	ın		
	S	Spectrometer to Determine	hov	w Instrument Par	ameters		
	A	Affect Lower Sensitivity Li	mits	s; <u>Liam Harris¹,</u> Iai	n		
	H	Hutchinson ¹ , Richard Ingley ¹	, Но	owell Edwards ¹ ; ¹ U	Jniversity of		
	L	Leicester					
	Poster	r Board #50 (220) On timining the Desifer			* D		
	(. S	(320) Optimising the Perior Spectroscopy Instrument E	ma or I	lice of a Stand-Of	I Kaman		
	A	Annlications: Melissa McHu	υι ι ισh ¹	Ian B Hutchinso	n ¹ Richard		
	I	Inglev ¹ , Nick Nelms ² , Howel	1 G.	M. Edwards ¹ : ¹ Un	iversity of		
	L	Leicester; ² European Space R	lese	arch and Technolo	gy Centre,		
	E	European Space Agency					
	Poster	r Board #51					
	(3	(321) Synthesis and Charac	teri	sation of Novel Sl	ERS Active		
	P	Phosphate Capped Gold Na	nop	particles; <u>Peter W</u>	hite ¹ , Wassie		
	N	Mersha', Mark Baron'; 'Univ	/ers	ity of Lincoln			
	Poster	r Board #32 (222) The Analysis of Plue (Sala	ont Duos by SED	Susing		
	() T	(522) The Analysis of Diue (Freated Silver Nanonarticle	501V 261 I	Peter White ¹ Thon	5 using		
	N	Mark Baron ¹ : ¹ University of	Lino	coln	ius i uroriek ,		
1			_ 1	•10 nm			
	WHA	AT'S HOT VENDOR PRE	SEI	NTATIONS. Exhi	ibit Hall C/D		
		Presider: Brian Dal	ble,	Arete Associates	5		
	Com	plimenary lunch is available	in t	he exhibit hall for	all conferees		
	11:40	Princeton "LightField -	— T	he Future of Scien	tific Imaging		
		and Spectroscopy Softw	are'	,	00		
	11:50	Ondax "New Low-frequ	uenc	⊳y THz-Raman® P	robe for <i>in</i> -		
		situ Measurements"					
	12:00	B&W Tek "The Latest	in P	ortable Raman			
	12 10	Instrumentation"		17 . (200		
	12:10	Phonens"	osco	py and imaging of	2D		
	12.20	Ocean Ontics "Flame: 1	Rlaz	ving a New Path in	NIR		
	12.20	Spectroscopy"	Diaz	ing a new I ath in			
	12:30	Innovative Photonic So	oluti	ions "High Throug	thout		
		Integrated Raman Probe	s"	0 0			
	12:40	Renishaw "Innovative I	Ram	an imaging"			
	12:50	Kaiser Optical Systems	s "I	lluminating Your (Chemistry		
	1 00	with Raman"					
	1:00	BIOLOOIS "A BIOLOOIS I	ort	able Raman Micro	scope: An		
		R&D 100 Market Disruj	pter				
		Tuesday Aftern	oon	Room 550A/B			
	INNOVATIVE ATMOSPHERIC-PRESSURE PLASMA						
	IUNIZATION SOUKCES						
	1.20 (222) Ambient Legislation and a Develop (DADT, D. 1.						
	Cody ^{1, 1} IFOL USA Inc						
	1.40 (324) Laser Induced Plasma for Ambient Ionization. Inc.						
	1.10	Riedel ¹ : ¹ BAM Federal Ins	stitu	te for Materials Re	esearch and		

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

- 2:00 (325) Expanding Analytical Frontiers of the Solution-Cathode Glow Discharge; <u>Andrew Schwartz</u>¹, Kelsey Williams², Jacob Shelley², Steven Ray¹, Gary Hieftje¹; ¹Indiana University, Department of Chemistry; ²Department of Chemistry and Biochemistry, Kent State University
- 2:20 (326) Laser Ablation Sample Transfer for Tissue Proteomics and Genomics; <u>Kermit Murray¹</u>, Fabrizio Donnarumma¹; ¹Louisiana State University
- 2:40 (327) Correlation-based Technique to Facilitate Detection, Identification, and Differentiation of Many Analytes in Direct Mass Spectrometry Approaches; Jacob Shelley¹, Yi You¹, Sunil Badal¹, Allyson Beechy¹; ¹Department 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 Champion¹; ¹Northeastern University
- 1:40 (329) Plasmonically Enhanced Raman Spectra of Cells and Body Fluids: SERS Applications in Diagnostics and Forensics; Lawrence Ziegler¹; ¹Boston University
- 2:00 (330) Predictability and Sensitivity of ROA Spectroscopy for Structure Elucidation of Protein Therapeutics; <u>Rina</u> <u>Dukor</u>¹; ¹BioTools Inc
- 2:20 (331) Enhanced Vibrational Optical Activity: Making Small Big; Laurence Nafie¹; ¹Syracuse University
- 2:40 (332) Raman Spectroscopy of Amyloid Fibrils; Igor Lednev¹, Valentin Sereda¹; ¹University 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**; <u>Yang (Angela) Liu</u>¹; ¹Pfizer Worldwide Research & Development
- 1:40 (334) Validation of Bioanalytical Methods: DoE Methodology; <u>Roujian Zhang</u>¹;Qiang Qin¹, Benhur Ogaby¹, Binbing Yu¹, Lingmin Zeng¹, ¹MedImmune
- 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; <u>Guiyang Li¹</u>, Zai-qing Wen¹, Guoxiang Chen²; ¹Amgen Inc; ²MedImmune, LLC
- 2:20 (336) Utilizing CoA and Spectroscopic Data To Aid Model Maintenance of Real Time Release Methods; <u>Dongsheng</u> <u>Bu</u>¹, Yan Zhang¹, Dimuthu Jayawickrama¹, Gary McGeorge¹; ¹Bristol-Myers Squibb
- 2:40 (337) Development and Validation of API Characterization Methods via On-line Raman Measurements for Real-Time Release Testing; John-David McElderry¹, Chunsheng Cai¹, Justin Pritchard¹, Frank Qi¹, Kelly Swinney¹; ¹Vertex 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; <u>Christopher</u> <u>Higgins¹</u>, Simon Roberts¹; ¹Colorado 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; <u>Xianming Zhang</u>¹, Andrea Weber¹, Cindy Hu¹, Wenlu Zhao², Minggang Cai², Pete August², Rainer Lohmann², Chad Vecitis¹, Elsie Sunderland¹; ¹School of Engineering and Applied Sciences, Harvard University; ²Graduate School of Oceanography, University of Rhode Island
- 2:00 (340) Analytical Challenges on Newly Identified Commercial Fluorosurfactants and Extractable Organofluorine in Human; <u>Leo Yeung¹</u>, Scott Mabury¹; ¹University of Toronto - Department of Chemistry
- 2:20 (341) Perfluorophosphinates and Other Perfluorinated Acids in Northern Pike and Double-Crested Cormorants; <u>Amila De Silva¹</u>; ¹Environment Canada
- 2:40 (342) Pilot Whales as an Indicator of Temporal Patterns in PFASs in North Atlantic Seawater; <u>Elsie Sunderland¹</u>, Bjarni Mikkelsen², Maria Dam³, Rosanna Bossi⁴; ¹Harvard University; ²The Faroese Museum of Natural History; ³Environment Agency, Faroe Islands; ⁴Aarhus 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**; <u>Yang Cui</u>¹, Eric Bergles¹, Mike Chai¹, Charlie Zhang¹, William Yang¹; ¹BaySpec, Inc.
- 1:40 (344) You Can't Tell a Book by Its Cover: Analytical Adventures in Anthropodermic Bibliopegy; <u>Daniel Kirby</u>¹, Anna N. Dhody², Beth Lander², Richard R. Hark^{3,4}; ¹Peabody Museum of Archaeology and Ethnology; ²The College of Physicians of Philadelphia; ³Brown University, John Hay Library; ⁴Juniata College, Department of Chemistry
- 2:00 (345) GC-MS and GC-IR Studies on Substituted Cathinones: Bath Salt-type Aminoketone Designer Drugs; <u>Randall Clark¹</u>, Jack DeRuiter¹, Younis Abiedalla¹, Karim Abdel-Hay¹; ¹Auburn University
- 2:20 (346) Probabilistic Detection of Firearms Discharge Residue on Skin Using Ion Mobility Spectrometry and Neural Networks; <u>Suzanne Bell</u>¹; ¹West Virginia University
- 2:40 (347) A Case Study in the Determination of Geographical Origin for Dalbergia, a CITES Listed Wood Species; James Jordan¹, Michael Doughten², Tyler Coplen², Haiping Qi², Ed Espinoza³; ¹National Geospatial-Intelligence Agency; ²U.S. Geological Survey; ³U.S. Fish & Wildlife Forensics Laboratory



- 1:20 (348) Measuring Correlated Composition and Optical Properties at the Nanoscale with the PTIR Technique: Application to Perovskites Solar Cells; <u>Andrea Centrone</u>¹; ¹NIST, Center for Nanoscale Science and Technology
- 1:40 (349) Assessing the Chemical, Mechanical and Structural Properties of Shale at Nanoscale; Jing Yang¹, Andrew Pomerantz¹; ¹Schlumberger-Doll Research Center, Schlumberger
- 2:00 (350) **IP-Enhanced Infrared Photoexpansion Nanospectroscopy in Air and Aqueous Solutions**; <u>Mikhail</u> <u>Belkin¹</u>, Mingzhou Jin¹, Feng Lu¹; ¹The 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**; <u>Craig Prater</u>¹, Eoghan Dillon¹, Qichi Hu¹, Honghua Yang¹, Curtis Marcott³, Feng Lu², Mingzhou Jin², Mikhail Belkin², Kevin Kjoller¹; ¹Anasys Instruments; ²The University of Texas at Austin; ³Light Light Solutions
- 2:40 (352) **Resonance Tracking in Resonance Enhanced Infrared Nanoscopy**; <u>Georg Ramer</u>¹, Anna Balbekova¹, Andreas Schwaighofer¹, Bernhard Lendl¹; ¹Vienna 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**; <u>Rodrigo Martinez-Duarte</u>¹; ¹Clemson University
- 1:40 (354) Experimental Evidence of Deterministic Absolute Negative Mobility for Organelles and Colloids; <u>Alexandra</u> <u>Ros¹</u>, Jinghui Luo¹, Katherine Muratore², Edgar Arriaga²; ¹Arizona State University; ²University of Minnesota
- 2:00 (355) **DNA Fractionation using Surface Dielectrophoresis**; <u>Ghislain Tchantchou</u>¹, Jeremy Buhain¹, Sagnik Basuray¹; ¹New Jersey Institute of Technology
- 2:20 (356) Ultrafast Immunoassays by Coupling Dielectrophoretic Biomarker Enrichment on Nano-Slit Device with Electrochemical Detection; <u>Nathan Swami</u>¹, Walter Varhue¹, Bankim Sanghavi¹, Kuo-Tang Liao², Chia-Fu Chou²; ¹Electrical Engineering, University of Virginia; ²Institute of Physics, Academia Sinica, Taiwan
- 2:40 (357) Particle Separation Employing Dielectrophoresis; Blanca Lapizco-Encinas¹; ¹Rochester Institute of Technology

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

- 1:20 (358) Portable LIBS from Research to Reality; Francois
- Doucet¹, Lutfu Ozcan¹; ¹ELEMISSION Inc. 1:40 (359) Handheld LIBS for Metal Alloy Analysis; <u>Phillip</u> <u>Tan¹</u>, Greg Petersen¹, Jacob Scheckman¹; ¹TSI Incorporated
- 2:00 (360) A Novel Handheld LIBS Analyzer and Its
 Applications; <u>Sean Wang¹</u>, Jing Li¹, Katherine Bakeev¹, Qun Li¹; ¹B&W Tek, Inc.
- 2:20 (361) Advances in Handheld LIBS Instrumentation for Soil and Geochemical Monitoring; <u>Brendan Connors</u>¹, Morgan Jennings¹, Justin Spott¹, David Day¹; ¹SciAps, Inc.
- 2:40 (362) Metals Analysis When to Use Portable XRF, LIBS, or OES, a presentation by Oxford Instruments; <u>David</u> <u>Clifford</u>¹; ¹Oxford Instruments

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

- 1:20 (363) Ultra-miniaturized Hyperspectral Imager; <u>William</u> <u>Yang¹</u>; ¹BaySpec, Inc.
- 1:40 (364) Developing Screening Methods for Drug Compounds Using Portable Ion Mobility Spectrometry; Connie Ruzicka¹; ¹US Food and Drug Administration
- 2:00 (365) Portable/Handheld Infrared Spectrometers becoming a Reality for the Food Industry; <u>Luis Rodriguez-Saona¹</u>; ¹The Ohio State University
- 2:20 (366) **The Versatility of Portable Raman in Process Development**; <u>Thomas Padlo¹</u>, Katherine Bakeev¹, Philip Zhou¹; ¹B&W Tek, Inc.

2:40 (367) **Progress in Portable Visible Spectrometry**; Alexander Scheeline¹; ¹SpectroClick

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; <u>Johannes Kiefer</u>¹; ¹Universitaet Bremen
- 1:40 (369) Surface Enhanced Raman Optical Activity as a New Chirally-Sensitive Nanoprobe; <u>Ewan Blanch</u>^{1,2}, Saeideh Ostovar pour^{1, 2}, Lisa Rocks³, Karen Faulds³, Duncan Graham³, Vaclav Parchansky⁴,Petr Bour⁴; ¹RMIT University; ²University of Manchester; ³University of Strathclyde; ⁴Charles University
- 2:00 (370) Raman Spectroscopy Detects Invasive Brain Cancer Cells in Humans; <u>Kevin Petrecca¹</u>; ¹McGill University
- 2:20 (371) **Deep UV Raman and TERS Microscopy**; <u>Satoshi Kawata¹</u>; ¹Osaka University
- 2:40 (372) Selective-sampling Raman Micro-Spectroscopy for Tissue Diagnosis; <u>Ioan Notingher</u>¹; ¹University 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**; <u>David Tuschel</u>¹; ¹HORIBA Scientific
- 1:40 (374) *In Situ* Analysis of Materials under Mechanical Stress: A Novel Instrument for Simultaneous Nanoindentation and Raman Spectroscopy; <u>Chris</u> <u>Michaels¹</u>, Yvonne Gerbig¹, Robert Cook¹; ¹NIST
- 2:00 (375) Confocal Raman Microscopy Investigation of Solute Accumulation into Individual C18 Particles; <u>David Bryce</u>¹, Jay Kitt¹, Joel Harris¹; ¹University of Utah
- 2:20 (376) **AFM and Raman Mapping of Neural Stem Cells Before and After Differentiation**; <u>Radu Alex Boitor</u>¹, Faris Sinjab¹, Ioan Notingher¹; ¹The University of Nottingham
- 2:40 (377) Coherent Anti-Stokes Raman Scattering Correlation Spectroscopy and Imaging: <u>Karen Antonio</u>¹, Zachary Schultz¹; ¹University 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; <u>Michael Canva</u>^{1,2}; ¹LCF, Laboratoire Charles Fabry - Institut d; ²LN2, Laboratoire Nanotechnologies Nanosystèmes - U. de Sherbrooke / CNRS
- 1:40 (379) **Optics, Plasmonics and SharpEdgeOnics in Novel Nanoarchitectures**; <u>Michael J. Naughton</u>¹; ¹Boston College
- 2:00 (380) **Plasmonic Gold Nanohole Arrays for Surface-Enhanced Raman Scattering Biosensing**; <u>Nianqiang (Nick)</u> <u>Wu¹</u>, Peng Zheng¹, Xuefei Gao¹; ¹West Virginia University
- 2:20 (381) Mapping the Extracellular Space using Ion-Selective Core-Shell Luminescent Nanoparticles; <u>Denis Boudreau</u>^{1,2}, Jérémie Asselin^{1, 2}, Philippe Legros^{1,2}, Mazeyar Pavinzadeh Gashti¹, Rihab Bouchareb³, Jesse Greener¹, Patrick Mathieu³; ¹Department of Chemistry, Université Laval; ²Center for optics, photonics and lasers, Université Laval; ³Quebec Heart and Lung Institute, Université Laval
 2.400 Webba
- 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**; <u>Allen White</u>¹, Andrew Schwartz², Steven Ray², Gary Hieftje²; ¹Indiana University, Rose-Hulman Institute of Technology; ²Indiana University, Department of Chemistry
- 4:10 (384) Measurements of Solvated Electrons at a Plasma-Liquid Interface via Optical Absorption Spectroscopy; <u>Paul Rumbach¹</u>, David Bartels¹, R. Mohan Sankaran², David Go¹; ¹University of Notre Dame; ²Case Western Reserve University
- 4:30 (385) Design Modifications to a Solution Cathode Glow Discharge and Examples of Industrial Application; <u>Stuart</u> <u>Schroeder</u>¹; ¹Alberta Innovates Technology Futures
- 4:50 (386) **Discharges with Liquid Electrode: Properties and Mechanisms**; <u>Peter Bruggeman¹</u>; ¹University of Minnesota
- 5:10 (387) Highly Sensitive Elemental Analysis for Cd by Solution-Anode Glow Discharge Atomic Emission Spectrometry; <u>Zhenli Zhu</u>¹; ¹China 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; <u>Max Diem¹</u>; ¹Northeastern University
- 4:10 (389) Single Cell Raman Imaging: Problems and Pitfalls When Comparing Images for Quantitative and Qualitative Purposes.; <u>Martin A. B. Hedegaard¹</u>; ¹University 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; <u>Rachel</u> <u>Emerson^{1,2}</u>, John Kalivas¹; ¹Idaho State University; ²Idaho National Laboratory
- 4:50 (391) Issues in Hierarchical Modeling of Complex Chemical Data; <u>Steven Brown¹</u>; ¹University of Delaware
- 5:10 (392) Feasibility of an End-of-Shift Monitor for the Determination of α-Quartz in Mine Dusts; Peter Griffiths¹, Andrew Weakley², Arthur Miller³, Emanuele Cauda⁴; ¹Griffiths Consulting LLC; ²University of California, Davis; ³National Institute of Occupational Safety and Health, Spokane; ⁴National 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; <u>Wolfgang Peti</u>^{1,2,3}; ¹Brown University School of Medicine; ²Brown University; ³University of Copenhagen
- 4:10 (394) Raman Spectroscopy Based Sensing of Alternative Glycemic Markers: Quo vadis?; <u>Rishikesh Pandey</u>¹, Nicolas Spegazzini¹, Niyom Lue¹, Jeon Woong Kang¹, Gary Horowitz², Ishan Barman³, Ramachandra Dasari¹; ¹Massachusttes Institute of Technology; ²Harvard Medical School; ³Johns Hopkins University

- 4:30 (395) Raman-based Blood Glucose Concentration Prediction by Structural Calibration; <u>Nicolas Spegazzini</u>¹, Rishikesh Pandey¹, Jeon Woong Kang¹, Ishan Barman², Ramachandra Rao Dasari¹; ¹Massachusttes Institute of Technology; ²Johns Hopkins University
- 4:50 (396) Early Diagnosis of End Stage Renal Disease Due to Diabetes using IR Imaging; <u>Vishal Varma</u>^{1,2}, Andre Kajdacsy-Balla^{1,4}, Sanjeev Akkina^{3,4}, Suman Setty^{1,4}, Michael Walsh^{1,2,4}; ¹Department of Pathology, University of Illinois at Chicago; ²Department of Bioengineering, University of Illinois at Chicago; ³Department of Medicine, University of Illinois at Chicago; ⁴University 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; <u>Ebrahim Aboualizadeh¹</u>, Christine Sorenson², Reyhaneh Sepehr³, Mahsa Ranji³, Nader Sheibani⁴, Carol Hirschmugl¹; ¹University of Wisconsin-Milwaukee, Department of Physics; ²Department of Pediatrics, University of Wisconsin School of Medicine and Public Health; ³Biophotonics Laboratory, University of Wisconsin Milwaukee, Department of Electrical Engineering and Computer Science; ⁴Department 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); <u>Jack Syage</u>¹, Karl Hanold¹, Andrey Vilkov¹; ¹Morpho Detection, LLC
- 4:10 (399) Characterizing and Databasing Drugs and Drug Analogs to Stay Ahead of Clandestine Designer Drug Laboratories; <u>Kristina Williams</u>¹, Guido Verbeck¹; ¹University of North Texas
- 4:30 (400) Mobilized Open Air Ionization: Detection of Explosives and Dangerous Supplements with a Compact DART-MS; Frederick Li², Joseph Lapointe¹, Joseph Tice¹, Adam Hall³, Brian Musselman¹; ¹IonSense, Inc. Saugus, MA; ²Boston University School of Medicine: Biomedical Forensic Sciences Program, Boston, MA; ³Northeastern 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; <u>Rhett Williamson</u>¹, José Almirall¹; ¹Florida International University
- 5:10 (402) Direct Sample Analysis Using Electrospray Ionization High Performance Ion Mobility-Mass Spectrometry; <u>Adam Graichen¹</u>, Robert Jackson¹, Jianglin Wu¹, Ching Wu¹, Mark Osgood¹; ¹Excellims 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; <u>Mark</u> <u>Rickard¹</u>, Gregory Meyers¹, Carl Reinhardt¹, Jamie Stanley¹; ¹The Dow Chemical Company
- 4:10 (404) NanoMineralogy of Extraterrestrial Samples Using AFM-tip Enhanced Infrared Spectroscopy; <u>Gerardo</u> <u>Dominguez</u>¹, Alex McLeod², Zack Gainsforth³, Priscilla Kelly², Fritz Keilmann⁴, Andrew Westphal³,Mark Thiemens², Dimitri Basov²; ¹California State University, San Marcos; ²University of California, San Diego; ³University of California, Berkeley; ⁴Ludwig-Maximilians-Universität and Center for Nanoscience
- 4:30 (405) Looking Inside Single Cells and Tissue using Nanoscale Infrared Spectroscopy; <u>Curtis Marcott</u>¹, Eoghan Dillon², Qichi Hu², Kevin Kjoller²; ¹Light Light Soluitons; ²Anasys 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 Gong¹, D. Bruce Chase¹, Isao Noda^{1,2}, C.J. McBrin¹, John Rabolt¹; ¹Department of Materials Science and Engineering, University of Delaware; ²Meredian Bioplastics
- 5:10 (407) Photothermal AFM-IR of Bacteria Polyurethane Bilayers: Impact of Local Sample – Cantilever Damping on Quantitative IR Measurements; <u>Daniel Barlow</u>¹, Justin Biffinger¹, Allison Cockrell³, Michael Lo², Kevin Kjoller², Debra Cook², Woo Kyung Lee¹, Pehr Pehrrson¹, Wendy Goodson⁻⁴, John Russell¹; ¹Chemistry Division, Naval Research Lab; ²Anasys Instruments; ³Nova Research, Inc.; ⁴Nanostructured & 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; <u>Cedric</u> <u>Malherbe¹</u>, Melissa Mchugh¹, Ian B. Hutchinson¹, Richard Ingley¹, Howell G. M. Edwards¹; ¹University of Leicester, Department of Physics and Astronomy
- 4:10 (409) Sampling and Preconcentration of Volatile Organic Compounds Using Capillary Microectraction of Volatiles (CMV); <u>Natasha Kreitals</u>¹, Anamary Tarifa¹, Dnisha Hamblin¹, Jose Almirall¹; ¹Florida International University
- 4:30 (410) Sample Delivery of Biphasic Droplets Containing Protein Crystals For Serial Femtosecond Crystallography With An X-Ray Free Electron Laser; <u>Austin Echelmeier</u>¹, Garrett Nelson¹, Bahige G. Abdallah¹, Uwe Weierstall¹, John C. H. Spence¹, Petra Fromme¹, Alexandra Ros¹; ¹Arizona State University
- 4:50 (411) Electrokinetic Biomarker Enrichment in Physiological Media by Coupling Dielectrophoresis with Ion Conductivity Gradients in Nanoslits; <u>Nathan Swami</u>¹, Ali Rohani¹, Walter Varhue¹, Kuo-Tang Liao², Chia-Fu Chou²; ¹Electrical Engineering, University of Virginia; ²Institute of Physics, Academia Sinica, Taiwan
- 5:10 (412) Using Pyrolyzed Paper for Electrochemical Detection in Microfluidic Paper-Based Analytical Devices; <u>Carlos Garcia²</u>, Elizabeth Evans¹, Jason Giuliani¹, Gema Duran³, Angel Rios³, Tomas Benavidez¹; ¹UT San Antonio; ²Clemson University; ³University 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; <u>Dustin McIntyre</u>¹, Christian Goueguel^{,3}, Cantwell Carson³, Herve Sanghapi³, Jinesh Jain²; ¹USDOE NETL; ²AECOM/URS; ³ORISE
- 4:10 (414) Analysis of Bakery and Dairy Products by Laser Induced Breakdown Spectroscopy; <u>Kemal Eseller</u>¹, Gonca Bilge², İsmail Boyaci²; ¹Atilim University; ²Hacettepe University
- 4:30 (415) LIBS Analysis of Plant Samples Advantages and Limitations; <u>Jozef Kaiser¹</u>, Jan Novotný¹, David Prochazka¹, Pavel Pořízka¹, Aleš Hrdlička¹, Karel Novotný¹; ¹Brno University of Technology, CEITEC - Central European Institute of Technology
- 4:50 (416) Laser-Induced Breakdown Spectroscopy: Application to Nuclear Waste Management; Jagdish Singh², Fang Yu Yueh¹; ¹Institute for Clean Energy Technology, Mississippi State University; ²JPS Advanced Technology R&D LLC,
- 5:10 (417) LIBS to the Extreme: High-dose Radiochemical Analyses where ICP Methods Cannot Follow; <u>Rodger</u> <u>Martin¹</u>, Tom Hylton¹; ¹Oak 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 SAS FAT Technical Section Business Meeting
 3:50 (418) Transmission Raman Analysis of Bilayered Tablets;
- 4:10 <u>Gary McGeorge¹</u>, Yan Zhang¹; ¹Bristol-Myers Squibb (419) **PAT Methods Development for the Pharmaceutical**
- Industry; <u>Carl Anderson</u>¹; ¹Duquesne University 4:30 (420) A NIR In-Process Control Method for
- 4:30 (420) A NIR In-Process Control Method for Determination of API Concentration in Tablets Manufactured by a Continuous Process; <u>Frank Qi</u>¹; ¹Vertex
- 4:50 (421) Monitoring Drying Performance of Pharmaceutical API by Raman Spectroscopy and Mass Spectrometry; <u>Ming Huang¹</u>, Daniel Hsieh¹, Robert Wethman¹, John Wasylyk¹; ¹Bristol-Myers Squibb Co.
- 5:10 (422) To Find Needles in Haystacks, Use a Metal Detector; Pharmaceutical Materials Analysis by Nonlinear Optical Stokes Ellipsometry; <u>Garth Simpson¹</u>, Paul Schmitt¹, Niraj Trasi¹, Lynne Taylor¹; ¹Purdue 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 <u>Popp</u>^{1,2}; ¹Leibniz Institute of Photonic Technology; ²Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena
- 4:10 (424) **Developing Deep UV Raman Standoff Spectrometer for Trace Explosives**; <u>Sanford Asher</u>¹, Sergei Bykov¹, Katie Gares¹, Kyle Hufziger¹; ¹University of Pittsburgh
- 4:30 (425) An Application of SERS in Forensics: Hair Dyes; <u>Dmitry Kurouski</u>¹, Richard Van Duyne¹; ¹Northwestern University
- 4:50 (426) **Discrimination of Animal and Human Blood Using Raman Spectroscopy and Chemometrics**; <u>Kyle C. Doty</u>¹, Gregory McLaughlin¹, Igor K. Lednev¹; ¹University at Albany, SUNY

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

5:10 (427) Forensic Analyses by Morphologically Directed Raman Spectroscopy; <u>Brooke Kammrath</u>¹, Andrew Koutrakos^{1, 2}, Josemar Castillo³, Joe Wolfgang³, Deborah Huck-Jones⁴; ¹Henry C. Lee College of Criminal Justice and Forensic Sciences, Dept of Forensic Science, University of New Haven; ²University of Verona; ³Malvern Instruments Inc.; ⁴Malvern 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; <u>Alex Nemiroski</u>¹, Dionysios C. Christodouleas¹, Ashok A. Kumar¹, Jonathan W. Hennek¹, George M. Whitesides¹; ¹Harvard University
- 4:10 (429) Arsenic in Drinking Water: Promoting Awareness through Remediation and Measurement Projects for Students; Julian Tyson¹, Ray Kronquist²; ¹University of Massachusetts; ²Chemists without Borders
- 4:50 (430) **Three Tales from Vietnam**; <u>Alexander Scheeline</u>¹; ¹SpectroClick
- 5:10 (431) Catalyzing Analytical Chemistry and Natural Products Drug Discovery Around the World; <u>Nina</u> <u>Dudnik¹</u>; ¹Seeding 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; <u>Francis Zamborini</u>¹, Prashant Jain², Aiqin Fang¹, Sarah White²; ¹University of Louisville; ²University of Illinois
- 4:10 (433) Identifying Uranium Speciation in Environmental Samples using Raman and SERS; <u>Amanda Haes</u>¹, Grace Lu¹, Tori Forbes¹; ¹University of Iowa
- 4:30 (434) Structure and Plasmons of Single Bimetallic Nanorods during Reaction; Jing Zhao¹, Sravan Thota¹, Shutang Chen¹, Yadong Zhou², Shengli Zou²; ¹University of Connecticut; ²University of Central Florida
- 4:50 (435) Tunable 3D Plasmonic Cavity as an Ultrasensitive SERS Platform; <u>François Lagugné-Labarthet</u>¹, Mohammadali Tabatabaei¹, Mohamadreza Najiminaini¹, Jeffrey Carson¹; ¹Western University
- 5:10 (436) Scanning Angle Raman Spectroscopy Measurements of Thin Films and Buried Polymer Interfaces; <u>Emily</u> <u>Smith</u>^{1,2}, Jonathan Bobbitt^{1,2}, Craig Damin^{1,2}; ¹Ames Laboratory; ²Iowa 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; <u>R. Kenneth Marcus¹</u>; ¹Clemson University



8:30 am – Applied Spectroscopy William F. Meggers Award.

(438) Mid-infrared Diffuse Reflection on Ultrafast Time Scales; <u>Eric Brauns</u>¹; ¹University of Idaho

Orals 9:15 – 10:55 am

Wednesday Morning, Room 552A MICROFLUIDICS AND ELECTROPHORESIS FOR BIOANALYTICAL APPLICATIONS Organizar: Adam Woollay: Presider: Vishal Sabora

- Organizer: Adam Woolley; Presider: Vishal Sahore
- 9:15 (439) Electroosmotic Sampling and Microfluidic Determination of Extracellular Thiols in Brain Tissue Cultures; <u>Stephen Weber</u>¹, Juanfang Wu¹, Jessie Jiang¹, James Landers², Erin Redman³, J.P. Alarie³, J. Michael Ramsey³; ¹University of Pittsburgh; ²University of Virginia; ³University of North Carolina
- 9:35 (440) Fabrics as Platforms for Electrophoretic Separations; <u>Shashi Murthy</u>¹, Tanya Narahari¹, Dhananjaya Dendukuri²; ¹Northeastern University; ²Achira Labs
- 9:55 (441) Nanogels for Reversibly Patterned Electrophoretic Separations; <u>Lisa Holland¹</u>, Brandon Durney¹, Tyler Davis¹, Srikanth Gattu¹; ¹Chemistry Department, West Virginia University
- 10:15 (442) Pressure-Actuated Microfluidic Devices for Pre-Term Birth Biomarker Analysis; <u>Vishal Sahore</u>¹, Suresh Kumar¹, Adam Woolley¹; ¹Brigham Young University
- 10:35 (443) DNA Separation by Sequence; <u>Linda McGown¹</u>, Jia Zhao¹, Steven Cramer¹, Cecily Wilbanks¹, Shekhar Garde¹, Xueru Tepke¹; ¹Rensselaer 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**; <u>Nerea Bordel¹</u>, Jorge Pisonero¹, Cristina González-Gago¹, Alfredo Sanz-Medel¹; ¹University of Oviedo

- 9:35 (445) Quantitative Reconstruction of the GDOES Sputter Depth Profile of a Monomolecular Layer Structure of Thiourea on Copper; JiangYong Wang¹, Yi Liu¹, Wei Jian¹, Siegfried Hofmann², Ken Shimizu³; ¹Department of Physics, Shantou University; ²Max Planck Institute for Intelligent Systems; ³University Chemical Laboratory, Keio University
- 9:55 (446) Application of RF Glow Discharge Optical Emission Spectroscopy for Quantitative Depth Profile Analysis of Chemically Strengthened Glass; <u>Anna Nached</u>¹, Georgiy Guryanov¹, Jamie Vargeson¹; ¹Science and Technology Division, Corning Incorporated
- 10:15 (447) Advances in Glow Discharge Mass Spectrometry for Elemental Analysis for Low Level Detection; <u>Ekbal Patel</u>¹; ¹Mass Spectrometry Instruments Ltd
- 10:35 (448) Consequences of Heterogeneous Surface Composition in Depth-Resolved Glow Discharge Spectrometry; <u>Andrew P. Storey¹</u>, Steven Ray¹, Maxim Voronov², Volker Hoffmann², Wolfgang Buscher³, Carsten Engelhard⁴, Gary Hieftje¹; ¹Indiana University; ²IFW Dresden; ³University of Muenster; ⁴University 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**; <u>Joseph</u> <u>Caruso</u>¹; ¹University of Cincinnati
- 9:35 (450) Ferritin: A Clinical Biomarker and a Protein Cage for Nanoparticles; <u>Maria Montes-Bayon¹</u>, Tobias Konz¹, F. Javier Alonso¹, Alfredo Sanz-Medel¹; ¹University of Oviedo
- 9:55 (451) The Liquid Sampling Atmospheric Pressure Glow Discharge: A Miniaturized Plasma for Giant Problems in Nuclear Forensics; <u>Benjamin T. Manard¹</u>, Ning Xu¹, Alonso Castro¹, R. Kenneth Marcus²; ¹Los Alamos National Laboratory; ²Clemson 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; <u>Steven Ray</u>¹, Elise Dennis², Christie Enke^{2,3}, Gary Hieftje², David Koppenaal⁴; ¹State University of New York at Buffalo; ²Indiana University; ³University of New Mexico; ⁴PNNL
- 10:35 (453) Ken Marcus and the Glow on the Horizon; <u>Gary M.</u> <u>Hieftje¹</u>, Andrew J. Schwartz¹, Steven J. Ray¹; ¹Indiana 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; <u>George Patterson</u>¹, Maria Ingaramo¹, Andrew York¹; ¹National 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; <u>Nicolas</u> <u>Spegazzini¹</u>, Rishikesh Pandey¹, Ishan Barman², Ramachandra Rao Dasari²; ¹Massachusttes Institute of Technology; ²Johns Hopkins University
- 9:55 (456) Absorption Spectroscopy and Imaging from the Visible through Mid-IR with 20 nm Resolution Using AFM Probes; <u>Andrea Centrone¹</u>; ¹NIST, Center for Nanoscale Science and Technology
- 10:15 (457) Fiber Bundle Arrays for Wide-Field, Dynamic SERS Nanoscopy; <u>Eric Languirand</u>¹, Brian Cullum¹; ¹University of Maryland, Baltimore County
- 10:35 (458) *In situ* ATR-FTIR Spectroscopy and Imaging to Monitor the Purification Process of Antibodies; <u>Maxime</u> <u>Boulet-Audet</u>¹, Bernadette Byrne¹, Sergei Kazarian¹; ¹Imperial 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; <u>Nicholas Petraco</u>¹; ¹John 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 Almirall¹, James Curran²; ¹Florida International University; ²University of Auckland
- 9:55 (461) Statistical Method for Comparison of Mass Spectra: Applications for the Identification of Controlled Substances; <u>Ruth Waddell Smith</u>¹, Melissa A. Bodnar-Willard², Victoria L. McGuffin²; ¹Forensic Science Program, Michigan State University; ²Department of Chemistry, Michigan State University
- 10:15 (462) Fusion of UV-visible Absorbance and Fluorescence Data for Forensic Discrimination of Dyed Textile Fibers; <u>Nathan C. Fuenffinger¹</u>, Stephen L. Morgan¹; ¹University of South Carolina; ²University of South Carolina
- 10:35 (463) Infrared Imaging and Multivariate Curve Resolution Applied to the Forensic Examination of Automotive Paints; <u>Barry Lavine</u>¹, Matthew Allen¹, Koichi Nishikida², Mark Sandercock⁰; ¹Department of Chemistry, Oklahoma State University; ²Materials Science Center, University of Wisconsin; ³Forensic 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**; <u>Don Kuehl</u>¹, Richard Sharp¹, Eugene Ma¹, Jinhong Kim¹, Charles Marshall¹; ¹RedShift 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; <u>Mathieu Carras</u>¹, Clément Gilles^{1, 2}, Luis Orbe³, Guillermo Caprintero³, Gregory Maisons¹; ¹mirSense, France; ²III-V Lab, France; ³Universidad Carlos III de Madrid, Spain
- 9:55 (466) Integrated Ring Laser Systems for Spectroscopy based on Quantum Cascade Structures; <u>Schrenk Werner</u>¹, Rolf Szedlak^{1, 2}, Daniela Ristanic¹, Benedikt Schwarz¹, Peter Reininger¹, Andreas Harrer¹,Hermann Detz¹, Donald C. MacFarland¹, Aaron M. Andrews¹, Gottfried Strasser¹; ¹Technische Universität Wien, Center for Micro- and Nanostructures and Institute for Solid State Electronics
- 10:15 (467) Monolithic Quantum Cascade Lasers And Their Applications; <u>Christian Pfluegl</u>¹; ¹Eos Photonics, Inc.
- 10:35 (468) **Broadly-tunable Monolithic THz Quantum Cascade** Laser Sources; <u>Mikhail Belkin¹</u>, ¹The University of Texas at Austin

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

9:15 (469) **Standoff LIBS. Concepts and Scenes**; <u>Javier Laserna</u>¹; ¹Universidad de Malaga

- 9:55 (470) Application of Distance Correction to ChemCam LIBS Measurements; <u>Alissa Mezzacappa</u>¹, Noureddine Melikechi¹, Agnes Cousin², Roger Wiens³, Jeremie Lasue², Samuel Clegg³, Robert Tokar⁴, Steven Bender⁴, Nina Lanza³, Sylvestre Maurice²; ¹Optical Science Center for Applied Research, Delaware State University; ²Institut de Recherche en Astophysique et Planetologie (IRAP), Universite' Paul Sabatier, France; ³Los Alamos National Laboratory; ⁴Planetary Science Institute
- 10:15 (471) Stand-off LIBS using Laser Filamentation: Fundamental Characterization for Quantitative Analysis; <u>Matthieu Baudelet^{1,2}</u>, Matthew Weidman¹, Mark Ramme¹, Khan Lim¹, Magali Durand¹, Martin Richardson¹; ¹Townes Laser Institute, University of Central Florida; ²National Center for Forensic Science, University of Central Florida
- 10:35 (472) Femtosecond Filament-Laser Ablation Molecular Isotopic Spectrometry; <u>George Chan¹</u>, Huaming Hou¹, Xianglei Mao¹, Vassilia Zorba¹, Richard Russo¹; ¹Lawrence 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; <u>Murray Johnston</u>¹; ¹University of Delaware
- 9:35 (474) Rapid Measurement of Nanoparticle and Microparticle Size Distribution and Number Concentration by Inductively Coupled Plasma Mass Spectrometry; <u>Austin Wilson¹</u>, Chuanqiang Sun¹, John W. Olesik¹; ¹Ohio State University
- 9:55 (475) A New Approach for Halogen Isotope Measurements with Focus of Compound-Specific Isotope Ratio Analysis; <u>Matthias Gehre¹</u>, Julian Renpenning¹, Kristina Hitzfeld¹, Tetyana Gilevska¹; ¹Helmholtz 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 Badal¹, Shawn Michalak², George Chan³, Jacob Shelley¹; ¹Department of Chemistry and Biochemistry, Kent State University; ²Stark State College; ³Lawrence Berkeley National Laboratory
- 10:35 (477) **High-Sensitivity Organohalogen Detection and Quantification by PARCI-MS**; <u>Kaveh Jorabchi¹</u>; ¹Georgetown 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; <u>Tony Wang</u>¹, David Meriage¹; ¹Amgen
- 9:35 (479) Micro-Raman Spectroscopy used as a PAT Tool and for Real Time Monitoring of Protein Stability during Freeze Drying; <u>Tatiana Starciuc</u>^{1,2}, Laurent Paccou^{1, 2}, Yannick Guinet^{1,2}, Alain Hedoux^{1,2}; ¹University of Lille 1 Sciences en Technology; ²University Lille 1, UMET - UMR CNRS 8207
- 9:55 (480) *In situ* Raman Spectroscopic Monitoring of Multiple Biochemical Species during Microbial Fermentation Process Development; <u>Karin Balss¹</u>, Sean Gilliam³, Angelica Spinelli¹, Wojciech Czaja²; ¹Janssen Pharmaceuticals; ²Depuy Synthes; ³Kaiser Optical Systems

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

- 10:15 (481) PAT Raman Data Acquisition in Biopharmaceutical Development and Manufacturing Environments using Siemens SIPAT Framework; <u>Stefani Takahashi</u>¹, John Paul Smelko¹, Brandon Berry¹, Robert Song¹; ¹Biogen
- 10:35 (482) CQA Focused Process Analytical Technology for Biologics Manufacturing; <u>Douglas Richardson</u>¹, Zi Chen¹, Maria Khouzam¹, Daisy Richardson¹, John Higgins¹, David Pollard¹; ¹Merck

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; <u>Tuan Vo-</u> <u>Dinh¹</u>, Hsin-Neng Wang¹, Yang Liu¹, Andrew Fales¹; ¹Duke University
- 9:35 (484) Gold Superstructures for SERS-based Bioimaging; Srikanth Singamaneni¹; ¹Washington University in St. Louis
- 9:55 (485) SERS Imaging of Gold Nanoparticles in Biological, Paper, and Granular Matricies; <u>Peter Vikesland¹</u>, Rebecca Lahr¹, Matthew Chan¹; ¹Virginia Polytechnic Institute and State University
- 10:15 (486) Selective Detection of 100 B. Anthracis Ames Spores in 20 Minutes using a Portable SERS Assay; <u>Stuart</u> <u>Farquharson</u>¹, Chetan Shende¹, Wayne Smith¹, Carl Brouillette¹, Jay Sperry³, Todd Sickler², Amber Prugh², Jason Guicheteau²; ¹Real-Time Analyzers, Inc.; ²US Army; ³University of Rhode ISland

10:35 (487) Raman Spectroscopy and SERS Investigations of Rhizosphere and Medically Relevant Bacterial Communities; <u>Sneha Polisetti</u>¹, Nameera Baig³, Jennifer Morrell-Falvey², Joshua Shrout⁴, Mitchel Doktycz², Paul Bohn^{1,3}; ¹Department of Chemical & Biomolecular Engineering, University of Notre Dame; ²BioSciences Division, Oak Ridge National Laboratory; ³Department of Chemistry, University of Notre Dame; ⁴Department 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; <u>Christa Brosseau¹</u>, Lili Zhao¹, Reem Karaballi¹, Jonathan Blackburn²; ¹Saint Mary; ²University of Cape Town, Cape Town, South Africa
- 9:35 (489) **Direct Detection of MicroRNA based on Plasmon Hybridization of Nanoparticle Dimers**; <u>Jennifer Chen</u>¹; ¹York University
- 9:55 (490) Filtration of Antigen-Assembled Gold Nanoparticles for SERS Detection; Jeremy Driskell¹, Arielle Lopez¹, Francis Lovato¹; ¹Illinois State University
- 10:15 (491) Integration of Electrophoretic Capture and Surface Plasmon Resonance Sensing in a Microfluidic Channel; <u>Karl Booksh¹</u>, Ornella Sathoud¹, Joe Smith¹, Casey Kneale¹, Missy Postelwaite¹, Kimberly Hibsman¹; ¹University of Delaware
- 10:35 (492) **Real-time Monitoring Bacterial Growth under Different Flow Rates with Surface Plasmon Resonance Imaging**; <u>Pegah N. Abadian</u>¹, Edgar Goluch¹; ¹Northeastern 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-Carbonneau¹, Jean-François Masson¹; ¹University of Montreal

Poster Board #2

(494) **Histopathological Characterization of Biological Tissues using High-Resolution Infrared Spectroscopic Imaging**; <u>Jayakrupakar Nallala</u>¹, Gavin Lloyd², Neil Shepherd³, Nicholas Stone⁴; ¹Bio-physics, School of Physics, University of Exeter; ²Biophotonics Research Unit, Gloucestershire Royal Hospitals; ³Department of Pathology, Gloucestershire Hospitals; ⁴Bio-physics, School of Physics, University of Exeter

Poster Board #3

(495) Predicting Vascularized Composite Allograft Outcome during Modulated Immunosuppression using Multimodal Imaging; <u>Nicole Crane</u>^{1,2,3}, Rajiv Luthra^{1,3}, Georg Furtmuller⁴, Eric Elster², Gerald Brandacher⁴, W. P. Andrew Lee⁴; ¹Naval Medical Research Center; ²Uniformed Services University of Health Sciences; ³Henry M. Jackson Foundation for the Advancement of Military Medicine; ⁴Johns Hopkins University

Poster Board #4

(496) **From Fiber Spectrometers to Fiber Sensors**; <u>Viacheslav</u> <u>Artyushenko</u>¹; ¹art photonics GmbH

Poster Board #5

(497) Spectroscopic Investigation of the Effects of Bioavailable Ions on Apatite Mineral Composition and Kinetics; <u>Mary Tecklenburg¹</u>, Md. Shah Alam¹, Honey Madupalli¹, Andrew Derry¹, James Lamblin¹, Megan Ling¹; ¹Central 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**; <u>Muhammad</u> <u>Ramzan^{1,2}</u>, Muhammad Asgher¹, Raymond Legge³, Yan Feng²; ¹Department of Chemistry & Biochemistry, University of Agriculture Faisalabad, Pakistan; ²Key State Laboratory of Microbial Metabolism, Shanghai Jiao Tong University, China; ³Department 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; <u>Yelena Pyatski¹</u>, Carol Flach¹, Qihong Zhang¹, Richard Mendelsohn¹; ¹Rutgers University

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

Poster Board #8

(500) New Routes for Tissue Pathology using Ouantum **Cascade Laser Based Imaging Microscopes**; Vishal Varma¹, Hari Sreedhar¹, Peter Nguyen¹, Andrew Graham², Francesca Gambacorta², Kyle Meinke¹, Oluwatobi Adelaja¹, Aliya Husain³, Grace Guzman¹, Michael Walsh¹; ¹University of Illinois at Chicago; ²University of Illinois at Urbana-Champaign; ³University of Chicago

Poster Board #9

(501) Metabolomic Characterization of Leishmania Major and Leishmania Donovani by 1H and 1H-13C HSOC NMR.; Paulo Falco Cobra^{1,2,3}, John Markley^{,3}, Otavio Thiemann⁴, Luiz Colnago²; ¹Instituto de Quimica de Sao Carlos - Universidade de Sao Paulo; ²EMBRAPA Instrumentacao; ³Biochemistry Department - University of Wisconsin - Madison; ⁴Instituto 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 Davies¹; ¹Florida Gulf Coast University

Poster Board #11

(503) Imaging and Feature Selection using GA-FDA Algorithm for the Classification of HSI Biomedical Images; Rupali Mankar¹, Vishal Verma², Michael Walsh², Bueso-Ramos Carlos³, David Mayerich¹; ¹University of Houston; ²Department of Pathology, University of Illinois at Chicago; ³Division 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 <u>Shanmugasundaram</u>¹, Nadya Pavlova^{2, 3}, Andrey Pavlov⁴, Jin Y. Wang⁵, James E. Galen⁵, Alexei Slesarev⁴, Antonio del Castillo-Olivares⁵, Frank T. Robb^{2, 3}, Igor K. Lednev¹; ¹Department of Chemistry, University at Albany, State University of New York, Albany, NY; ²Department of Microbiology and Immunology, University of Maryland, MD; ³Institute of Marine and Environmental Technology, University of Maryland, MD, USA; ⁴Fidelity Systems, Inc., Gaithersburg, MD; ⁵Center 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 Soto¹, Jorge Castro Ramos², Humberto Miguel Sansebastián Aguilar³, Diana Antonieta Sen Salinas⁴; ¹National Institute of Astrophysics, Optics and Electronics (INAOE); ²National Institute of Astrophysics, Optics and Electronics (INAOE); ³H&M Biomedical Technology International; ⁴Center 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-Ramos¹, Adriana May-Salazar², Gabriel Aguilar-Soto¹, Diana Sen-Salazar¹, Francisco Gutierrez-Gonzalez³, Reimer Romero-Hernandez¹,Karen Esmonde-White⁴; ¹Instituto Nacional de Astrofisica Optica y Electronica; ²Instituto Mexicano del Seguro Social; ³Centro para la prevención del cancer; ⁴University 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 Bello¹, Christina Gasbarro¹, Anton Smirnov¹; ¹EIC Laboratories, Inc.

Future Meeting: September 18 – 23, 2016, Minneapolis, MN

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; <u>Christian Goueguel</u>¹, Dustin McIntyre¹, Jinesh Jain², Cantwell Carson¹, Herve Sanghapi³; ¹USDOE, National Energy Technology Laboratory; ²AECOM; ³Institute for Clean Energy Technology Poster Board #17

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

Poster Board #18

(510) Infrared Spectroscopic Assessment of Biomass for **Bioethanol Generation**; Ramyasri Ailavajhala¹, Mugdha Padalkar¹, Uday Palukuru¹, Arash Hanifi¹, Rashid Kaveh¹, Benoit Van Aken¹, Nancy Pleshko¹; ¹Temple 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 White¹, Nicole Lenca², Frank Kero¹, Jason Weisenseel¹, Benjamin Southwell³, Bogdan Bogdanov¹, Craig Young¹, Judy Westrick²; ¹PerkinElmer, Oak Brook Technology Center; ²Wayne State University; ³Lake Superior State University

Poster Board #20

(512) The Photoacoustic Effect from Moving Sources; Wenyu Bai¹, Gerald Diebold¹; ¹Department of Chemistry, Brown University

Poster Board #21

(513) Polyethylene: A Novel Approach for Passively Sampling Fluorotelomer Alcohols; Erik Dixon-Anderson¹, Rainer Lohmann¹; ¹University of Rhode Island Graduate School of Oceanography

Poster Board #22

(514) Oligomerizational Behaviour of Nitrophenol under Simulated Atmospheric Conditions; Hafiz Muhammad Danish Sultan², Farhat Yasmeen¹, Muzafar Abbas¹; ¹University of Engineering and Technology, Lahore; ²University College of Pharmacy, University of Punjab, Lahore

Poster Board #23

(515) Investigation of Fluorescence Yield Variability in Emiliania huxleyi; Stefan Faulkner¹, Cameron Rekully¹, Shawna Tazik¹, Joe Swanstrom¹, Timothy Shaw¹, Tammi Richardson², Michael Myrick¹; ¹University of South Carolina Department of Chemistry and Biochemistry; ²University of South Carolina Department of Biological Sciences

Poster Board #24

(516) Design of Optical Interference Filters for Taxonomic **Classification of Phytoplankton**; Cameron Rekully¹, Shawna Tazik¹, Stefan Faulkner¹, Timothy Shaw¹, Tammi Richardson¹, Michael Myrick¹; ¹University of South Carolina

Poster Board #25

(517) Decrease in Cadmium Levels in Canadian Western Amber Durum from 1995 to 2013; Anja Richter¹; ¹Canadian 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; <u>Sergey Shilov</u>¹, Michael Joerger¹, Thomas Tague¹; ¹Bruker

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

	1
Poster Board #27	Poster Board #39
(519) Non-Destructive Analysis of Surface Coatings using	(531) Infrared Imaging for Identification of Tissue Damage
the Agilent 4300 Handheld FTIR analyzer; Dipak Mainali ¹ ,	in Pathology; Bennett Davidson ^{1,3} , Michael Walsh ³ , William
Leung Tang ¹ ; ¹ Agilent Technologies	Ennis ² , Timothy Koh ³ , Andre Kajdacsy-Balla ³ , Sagar
Poster Board #28	Nadimpali ¹ ; ¹ Department of Bioengineering, College of
(520) Near Infrared Spectral Evaluation of Tissue	Engineering and Medicine, University of Illinois at Chicago:
Engineered Cartilage Correlates to Gene Expression of	² Department of Surgery and Section of Wound Healing and
constructs : Farzad Yousefi ¹ , Ramyasri Ailayaihala ¹ , Uday	Tissue Repair. College of Medicine. University of Illinois at
Palukuru ¹ , Sveda Yusra Nahri ¹ , Nancy Pleshko ¹ : ¹ Department of	Chicago: ³ Department of Pathology and Spectral Pathology Lab.
Bioengineering Temple University PA	College of Medicine. University of Illinois at Chicago
Poster Roard #29	Paman Postars
(521) Differential Excitation Spectroscopy: A New	
Technique : Boyd Hunter ¹ Jason Cox ¹ Paul Harrison ¹ Bill	Poster Board #40
Walters ¹ Michael Miller ² . ¹ Kestrel Corporation: ² Southwest	(532) Probing Triplet-Triplet Energy Transfer Efficiency in
Research Institute	Artificial Photosynthetic Pigments using Resonance Raman
Poster Board #30	Spectroscopy; Elizabeth Kish [*] , Katherine WongCarter [*] , Smitha
(522) Vibrational Spectroscopy of an Imidazolium Ionic	Pillai ⁻ , Gerdenis Kodis ⁻ , Dalvin D. Mendez-Hernandez,
Liquid Confined in a Metal Organic Framework: Johannes	Junming Ho, Ana L. Moore ⁻¹ , Thomas Moore ⁻ , Devens Gust ⁻ ,
Kiefer ¹ Manish Singh ² James Anderson ² Nilesh Dhumal ³	Bruno Robert'; Department of Life Sciences, CEA Saclay,
Hyung Kim ³ : ¹ Universitat Bremen: ² University of Aberdeen:	France; Department of Chemistry and Biochemistry, Arizona
³ Carnegie Mellon University Pittsburgh	State University; Department of Chemistry, Yale University
Destay Degrad #21	Poster Board #41
(523) In situ Spectroscopie Study on Small Molecules	(533) Effects of Molecular Absorption Cross-Section on
Diffusion in Anion Exchange Membranes: Ving Jin ¹ Viochui	Raman System Throughput; <u>Justin Cooper</u> ⁴ , Adam Hopkins ² ;
Liu ¹ Wonyu Zhang ¹ E. Drugn Coughlin ¹ : ¹ Dolumor Science and	¹ Alakai Defense Systems; ² Alakai Defense Systems
Endingering University of Massachusetts Amherst	Poster Board #42
Digineering, Oniversity of Massachusetts Annierst	(534) In-line Quality Control of Cross-linking for
(525) Demovel of Dana Manney Contributions for	Photovoltaic Encapsulants via Raman Spectroscopy; <u>Mark</u>
(525) Kemoval of Done Water by Near Informed (NID)	Kemper ¹ , Christina Hirschl ² , Martin Kraft ² , Bradford Behr ¹ ;
Evaluation of Bone water by Near Infrared (NIK) Spectroscopy Has I'm Vara ¹ Muadha Dadallar ¹ Michael	¹ Tornado Spectral Systems; ² CTR Carinthian Tech Research AG
Spectroscopy; <u>Hee Jin Y ang</u> , Mugana Padaikar, Michael	Poster Board #43
Ispiryan, Chamiin Kajapakse, Nancy Piesnko; Tempie	(535) Transmission Raman Spectroscopy an Alternate Tool
Difference and #24	to Traditional HPLC to Determine the Content Uniformity
(526) Design and Devformance of a New Diamond	of Solid Dosage Forms; <u>Michelle Raikes</u> ¹ , Reggie Saraceno ¹ ,
(526) Design and Performance of a New Diamond	Prince Korah ¹ , Julia Griffen ² ; ¹ Boehringer Ingelheim
Attenuated Total Reflection-video Microscopy Accessory;	Pharmaceuticals; ² Cobalt Light Systems Ltd
David Schering; Cziek	Poster Board #44
Poster Boara #35 (527) Ameliantics of New Informed Transflortion and	(536) Multi-wavelength Dispersive Raman Spectrometer and
(527) Application of Near-Infrared Transflection and	Microscope for Non-destructive Pharmaceutical Ingredient
I ransmission, and Hand-Heid Raman Spectroscopy in	Analysis; <u>Jack Qian</u> ¹ ; 'BaySpec Inc.
Ahmad Shawly 2,4 Ahmad Ihrahim ^{2,4} Eman Elzanfaly ³ Maisan	Poster Board #45
Anned Snawky', Anned Ioranni', Eman Eizaniary, Maissa Salam ² Ahmad El Cin h^2 Stanbar Haa 4 , ¹ Matuchus UCA, Juan	(537) Raman Monitoring of the Carbonization Process of
Salem, Anmed El Gindy, Slephen Hoag; Metronm USA, Inc.;	Metal–Organic Frameworks ; <u>Szetsen Lee</u> ¹ , Yu-Ting Gong ¹ ,
Analytical Chemistry Department, Faculty of Pharmacy, Misr	Bing-Han Li ¹ , Chia-Her Lin ¹ ; ¹ Chung Yuan Christian
International University, Egypt; Analytical Chemistry	University
Department, Faculty of Pharmacy, Cairo University, Egypt;	Poster Board #46
School of Pharmacy, University of Maryland, MD	(538) Characterization of Graphene and Other Two-
Poster Boara #50	Dimensional Materials by Raman Spectroscopy; <u>Pierre</u>
(528) Dynamics of an Internal Protonated water Cluster: an	<u>Negri¹, Tim</u> Prusnick ¹ , Ian Haywood, Olga Milikofu ³ , Tim
Isotope Exchange Study of Photosynthetic Oxygen	Batten ² ; ¹ Renishaw Inc.; ² Renishaw Plc.; ³ Renishaw K.K.
Evolution; Udita Branmachari, Bridgette Barry; Georgia	Poster Board #47
Institute of Technology	(539) Coherent Raman Microscopic Study during the
(520) Conversion Viburtianal Superturgeness Transford Internel	Stretching of a Homologous PE Blend ; <u>Ying Jin</u> ¹ , Ian Ryu ¹ ,
(529) Cryogenic vibrational Spectroscopy Traps an Internal Buston at al Water Cluster in Distance of the Theory Curl	Chad Snyder ¹ , Young Jong Lee ¹ ; ¹ National Institute of
Protonated water Cluster in Photosystem II; <u>Zhanjun Guo</u> ,	Standards and Technology
Bridgette Barry; Georgia Institute of Technology	Poster Board #48
(520) Monitoring the Discussion and Defermention of	(540) Assessing Composition and Morphometry Properties
(550) Monitoring the Disruption and Ketormation of Structure Company Linida Dealting Order in the ATD	of Ostrich Cartilage as Possible Tissue Engineering
Stratum Corneum Lipids Packing Order in vivo with ATR	Scaffolds; C. Erika Ramírez ¹ , Jorge L. Flores ¹ , Verónica M.
IK, <u>Ouangru Mao</u> , M. Cainerine Mack, Hao Ouyang;	Rodríaguez Betancourtt ¹ , JI Delgado-Saucedo ¹ , Héctor Pérez
Johnson α Johnson Consumer Inc.	Ladrón de Guevara', Miguel Guzmán ² , Adán T. Paíno ¹ , Karen
	Esmonde-White ⁺ ; 'Universidad de Guadalajara - CUCEI;
	Higher Technological Institute of Irapuato - ITESI;
	'Universidad de Guadalajara - CULAGOS; ⁴ University of
	Michigan - Medical School

TECHNICAL PROGRAM – WEDNESDAY 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 #49

(541) Automated Chemical ID of Particles using Raman Spectroscopy; <u>Vincent Larat</u>¹, Eunah Lee¹, Bernd Bleisteiner¹, David Tuschel¹, Simon Fitzgerald¹; ¹HORIBA Scientific *Poster Board #50*

(542) Classification of High and Low Glycated Hemoglobin in Diabetic Patients with Raman Spectroscopy and PCA-SVM; <u>Villa Manriquez José Fabián¹</u>, Castro Ramos Jorge², Gutierrez Delgado Francisco³; ¹Instituto Nacional de Astrofísica Optica y Electronica; ²Instituto Nacional de Astrofísica Optica y Electronica; ³Centro de Estudios y Prevención del Cancer a.c. tra Board #51

Poster Board #51

(543) **Comparing Raman Mapping of Colon Tissue with Immunohistochemistry for Tissue Classification**; <u>Aaran</u> <u>Lewis</u>¹, Riana Gaifulina¹, Jennifer Dorney², Martin Isabelle³, Manuel Rodriguez-Justo¹, Naomi Guppy¹, Nick Stone², Catherine Kendall³, Katherine Lau⁴, Geraint Thomas¹; ¹University College London; ²University of Exeter; ³Gloucestershire Hospitals NHS Foundation Trust; ⁴Renishaw PLC

Poster Board #52

(544) Identification of Polymeric Microfibers in Fish Stomach and Great Lakes Waters using Raman

Spectroscopy; <u>Karen Esmonde-White</u>¹, Rachel Cable², Melissa Duhaime²; ¹University of Michigan Medical School; ²University of Michigan

Poster Board #53

(545) Comparison of Machine Learning Methods to Identify Bacteria using Raman Spectroscopy; <u>Cynthia Hanson</u>, Elizabeth Vargis¹; ¹Utah State University

Poster Board #54

(546) Measuring Copolymer Chemical Heterogeneity by Combining SEC with Offline Raman Spectroscopy; <u>Aaron</u> <u>Urbas¹</u>, Andre Striegel¹, Leena Pitkanen¹; ¹National 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; <u>David Chen</u>¹, Shuai Sherry Zhao¹; ¹University of British Columbia
- 1:40 (548) High Peak Capacity Separations of Proteins and Peptides Using Two Dimensional Micro Free Flow Electrophoresis; <u>Michael Bowser</u>¹, Matthew Geiger¹, Alexander Johnson¹, Nicholas Frost¹; ¹University of Minnesota, Department of Chemistry

- 2:00 (549) Multiplexed Separations for Biomarker Discovery in Metabolomics: Urinary Markers of Smoke-Exposure in Firefighters; <u>Philip Britz-McKibbin</u>¹; ¹Department 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; <u>Lingjun Li</u>¹, Xuefei Zhong¹, Shan Jiang¹, Zichuan Zhang¹; ¹University 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. Ivanov¹, Rosa Viner², Marcia R. Santos², Arseniy M. Belov¹, David R. Bush¹, Chitra K. Ratnayake³, Barry L. Karger¹; ¹Northeastern University, Barnett Institute of Chemical and Biological Analysis, Boston, MA; ²Thermo Fisher Scientific, San Jose, CA; ³Sciex, 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 Cantle¹; ¹Nu Instruments
- 1:40 (553) **Pushing the Boundaries in Glow-Discharge Spectrometry— a Tribute to Edward Steers**; <u>Gary M.</u> <u>Hieftje¹</u>, Andrew P. Storey¹, Jacob T. Shelley², Steven J. Ray¹; ¹Indiana University; ²Kent State University
- 2:00 (554) Measurement of Oxygen in Solid Samples using Analytical Glow Discharges with Optical or Mass Spectrometric Detection; <u>Volker Hoffmann</u>¹, Edward Steers², Sohail Mushtaq², Juliet Pickering³, Cristina Gonzalez Gago⁴, Petr Smid⁴, Thomas Hofmann⁴, Cornel Venzago^{, 4}, Wolfgang Gruner¹; ¹IFW Dresden; ²London Metropolitan University; ³Imperial College, London; ⁴AQura GmbH
- 2:20 (555) Investigations towards Matrix Independent Calibrations in Glow Discharge Mass Spectrometry; <u>Petr</u> <u>Smid</u>¹, Cristina Gonzalez-Gago², Volker Hoffmann³, Cornel Venzago¹, Thomas Hofmann¹; ¹AQura GmbH; ²University of Oviedo; ³IFW Dresden
- 2:40 (556) One Thing Leads to Another: Sixty Years of Spectroscopy Research; <u>Edward Steers</u>¹; ¹London 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;** <u>Francisco Calderon¹</u>, Andrew Margenot², Sanjai Parikh²; ¹USDA-ARS, Akron, Colorado; ²Department of Land, Air and Water Resources, University of California Davis
- 1:40 (558) Modeling the Time-Resolved Diffuse Reflectance; <u>Arnold Kim</u>¹; ¹University of California, Merced
- 2:00 (559) QCL-Standoff MIR Reflectance Spectroscopy Measurements of Hazardous Chemicals and Biological Threats; <u>Samuel P. Hernández-Rivera¹</u>, Leonardo C. Pacheco-Londoño¹, Amira Padilla-Jimenez¹, Nataly J. Galan-Freylr¹, Carlos Rios^{1,2}, John R. Castro-Suarez¹; ¹Department of Chemistry, University of Puerto Rico-Mayaguez

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

- 2:20 (560) Quantitative Infrared Directional/Hemispherical Reflectance Measurements; <u>Thomas Blake</u>¹, Carolyn Brauer¹, Yin-Fong Su¹, Russell Tonkyn¹, Tanya Myers¹, Brenda Kunkel¹, Bruce Bernacki¹, Timothy Johnson¹; ¹Pacific Northwest National Laboratory
- 2:40 (561) Detection Limits for Blood on Fabrics via IR Diffuse Reflection; <u>Michael Myrick¹</u>, Stephanie DeJong¹, Ray Belliveau¹, Stephen Morgan¹, Brianna Cassidy¹, Zhenyu Lu¹; ¹University 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 Jacobs³, Brendan Corey³; ¹Naval Medical Research Center; ²Uniformed Services University of Health Sciences; ³Walter Reed Army Institute of Research; ⁴Henry M. Jackson Foundation for the Advancement of Military Medicine
- 1:40 (563) **Direct Bacterial Analysis by Ambient Ionization Mass Spectrometry**; <u>Pu Wei</u>¹, Christopher Pulliam¹, Soumabha Bag¹, Alan K. Jamusch¹, Saerom Kim¹, Rafal M. Pielak², R. Graham Cooks¹; ¹Purdue University; ²L'Oréal California Research Center, San Francisco, CA
- 2:00 (564) An Analytical Approach to Designing Clinical MALDI-TOF Mass Spectrometer Instrumentation; James VanGordon¹; ¹bioMerieux, Inc.
- 2:20 (565) Surface Enhanced Raman Spectroscopy of Bacteria-Infected Wound Effluent of Combat Related Injuries; <u>Nicole Crane</u>^{1,2,3}, Shubha Yesupriya¹, Meron Ghebremedhin^{1,3}; ¹Naval Medical Research Center; ²Uniformed Services University of Health Sciences; ³Henry M. Jackson Foundation for the Advancement of Military Medicine
- 2:40 (566) Monitoring Bacterial Biofilm Growth and Removal using a Quartz Crystal Microbalance; <u>Hunter Sismaet</u>¹, Pegah Abadian¹, Edgar Goluch¹; ¹Northeastern 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**; <u>Alexandre Dazzi¹</u>, Jérémie Mathurin¹, Johanna Saunier², Najet Yagoubi², Ariane Deniset-Besseau¹, Kevin Kjoller³; ¹Laboratoire de Chimie Physique - Université Paris-Sud; ²Matériaux pour la santé, Faculté de Pharmacie, Chatenay-Malabry; ³Anasys Instruments
- 1:40 (568) Linear and Nonlinear Vibrational Mid-Infrared Photothermal Spectroscopy with a Compact Fiber Laser Probe; <u>Atcha Totachawattana^{1,3}</u>, Shyamsunder Erramilli^{2,3,4}, Michelle Sander^{1,3,4}; ¹Electrical and Computer Engineering, Boston University; ²Physics and Biomedical Engineering, Boston University; ³BU Photonics Center; ⁴Materials Science and Engineering, Boston University
- 2:00 (569) Laser Direct IR Imaging A New Paradigm for Mid-IR Spectroscopic Imaging; <u>Charles Hoke¹</u>, Yuri Beregovski¹, Andrew Ghetler¹, Yang Han¹, Christopher Moon¹, Richard Tella¹; ¹Agilent Technologies, Inc.
- 2:20 (570) Fast Time-resolved IR Measurements using EC-QCL; <u>Michael George</u>¹; ¹University of Nottingham
- 2:40 (571) EC-QC Laser Spectroscopy for mid-IR Transmission Measurements of Proteins in Aqueous Solution; <u>Bernhard Lendl</u>¹, Andreas Schwaighofer¹, Mirta R. Alcaraz¹; ¹Technische 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. <u>Gonzalez</u>^{1,2}, C. Derrick Quarles Jr.², Dayana D. Oropeza¹, Charles Sisson², Xianglei Mao¹, Vassilia Zorba¹, Rick Russo^{1,2}; ¹Lawrence Berkeley National Laboratory; ²Applied Spectra, Inc.
- 1:40 (573) **The Discrimination of Printing Inks using Laser Induced Breakdown Spectroscopy for Forensic Applications**; <u>Ruthmara Corzo¹</u>, Jose Almirall¹; ¹Florida International University
- 2:00 (574) Quantitative Evaluation of Spectral Interference in LIBS; Jessica Chappell^{1,3}, Brandon Seesahai², Martin Richardson², Michael Sigman^{1,3}, Matthieu Baudelet^{1,3}; ¹National Center for Forensic Science, University of Central Florida; ²Townes Laser Institute, CREOL-The College of Optics and Photonics, University of Central Florida; ³Chemistry Department, University of Central Florida
- 2:20 (575) Evaluation of a Handheld LIBS Instrument for First Responder and Forensic Applications; <u>Richard R. Hark</u>^{1,2,3}, David Day^{1,2,3}, Anthony H. Downey^{2,3}, Adam Miller², John Plumer²; ¹SciAps, Inc.; ²Synergos Global Security, LLC; ³Juniata College, Department of Chemistry
- 2:40 (576) Quantitative Elemental Composition Measurements of Plant Materials using LIBS; <u>Amy Bauer</u>¹, Markus Gaelli¹, Steven Buckley¹, Robert Robinsky¹; ¹TSI, 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; <u>Akos Vertes</u>¹, Hang Li¹, Pranav Balan¹, Linwen Zhang¹; ¹George Washington University
- 1:40 (578) Applications of Chemometrics to Ambient Ionization MS Analysis; Valentina Pirro¹, Alan K. Jarmusch¹, Christina R. Ferreira¹, R. Graham Cooks¹; ¹Chemistry Department, Purdue University
- 2:00 (579) Mass Spectrometry Imaging of Secondary Metabolites Directly on Fungal Cultures; <u>Nicholas</u> <u>Oberlies</u>¹; ¹University of North Carolina at Greensboro
- 2:20 (580) The Bioaccumulation of a Toxic Ionic Liquid in Zebrafish (Danio rerio) Analyzed by DESI-MS Imaging; <u>Consuelo Perez</u>¹, Alessandra Tata¹, Michel L. DeCampos³, Chun Peng², Demian R. Ifa¹; ¹Department of Chemistry, York University, Toronto, Ontario, Canada; ²Department of Biology, York University, Toronto, Ontario, Canada; ³UNICAMP, 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; <u>Tao Jiang</u>¹, Xiaohong Xiong¹, Wenhao Qi¹, Meilin Yang¹, Qiuju Liu¹, Lanfang Yi¹,Zhiqiang Zhu¹, Huanwen Chen¹; ¹Jiangxi 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**; <u>Steven Scheifers</u>¹; ¹Stepan Company
- 1:40 (583) Optimally Dividing Available Samples into Calibration and Validation Sets; <u>Bryan Bowie</u>¹; ¹ExxonMobil Research & Engineering
- 2:00 (584) Raman Spectroscopy for Lab Scale in situ Applications; <u>Xianghuai Wang</u>¹, John Roberts¹, Kevin Wier¹, Dimitris Katsoulis¹; ¹Dow Corning Corporation
- 2:20 (585) Moving Vibrational Spectroscopy from Chemical Process Monitoring to Bio-Process Monitoring; Jim Cronin¹; ¹DuPont
- 2:40 (586) **PAT Application in Lubricant Industry**; <u>Henry</u> <u>Xiao¹</u>; ¹Infineum

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; <u>Bhavya Sharma</u>¹, Richard Van Duyne¹; ¹Northwestern University
- 1:40 (588) Development of SORS for Nonchemical Subsurface Analysis; <u>Nick Stone</u>¹, Ben Gardner¹, Pavel Matousek²;
 ¹University of Exeter, UK; ²Central Laser Facility, STFC Rutherford Appleton Laboratory
- 2:00 (589) Development of Micro-SORS for Subsurface Analysis of Thin Layers in Art and other Areas; <u>Claudia</u> <u>Conti</u>¹, Chiara Colombo¹, Marco Realini¹, Pavel Matousek²; ¹Consiglio Nazionale delle Ricerche, Istituto per la Conservazione e la Valorizzazione dei Beni Culturali (ICVBC), Italy; ²Central Laser Facility, STFC Rutherford Appleton Laboratory
- 2:20 (590) *In vivo* Raman Spectroscopy for Assessing Tissues in Chronic Wounds; <u>Karen Esmonde-White¹</u>, Crystal Holmes¹, Michael Morris²; ¹University of Michigan Medical School; ²University of Michigan
- 2:40 (591) **Implementation of SORS for Three-dimensional Breast Margin Assessment**; <u>Anita Mahadevan-Jansen¹, T</u> Quyen Nguyen², Jennifer Giltnane¹, Brittany Caldwell¹, Melinda Sanders¹, Mark Kelley¹; ¹Vanderbilt University; ²Northwestern 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; <u>Michael</u> <u>Charlton¹</u>; ¹UCL Institute of Archaeology
- 1:40 (593) Classification and Geographic Origin of Garnets using Laser-Induced Breakdown Spectroscopy (LIBS); <u>Richard R. Hark</u>¹, Peter A. Defnet¹, Michael Wise², Russell S. Harmon³; ¹Department of Chemistry, Juniata College; ²Department of Mineral Sciences, National Museum of Natural History, Smithsonian Institution; ³Department 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; <u>Rachel Popelka-Filcoff¹</u>, Tiffany Reeves¹, Fabien Pottier², Claire Lenehan¹; ¹Flinders University; ²Museum National
- 2:20 (595) Archaeometry and Human Life Ways; <u>David</u> <u>George¹</u>; ¹Saint Anselm College
- 2:40 (596) Understanding the Materials and Techniques of Early Photographs through Non-Invasive Analysis and Reconstructions; <u>Silvia A. Centeno¹</u>, Anna Vila², Emmanuelle Marquis³, Yimeng Chen³, Julia Kohanek³, Yan Dong³, Alejandro Schrott⁴, Lisa Barro⁵, Nora W. Kennedy⁵; ¹The Metropolitan Museum of Art, Department of Scientific Research.; ²Statens Museum for Kunst, Center for Art Technological Studies and Conservation,; ³Department of Materials Science and Engineering, University of Michigan; ⁴IBM Research, Thomas J. Watson Center, NY; ⁵The 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**; <u>Emilie Ringe</u>¹; ¹Rice University
- 1:40 (598) Mapping Electric Fields Induced By Plasmons with Vibrational Stark Shifts; <u>Zachary Schultz</u>¹, Daniel Kwasnieski¹, Hao Wang¹, James Marr¹; ¹University of Notre Dame
- 2:00 (599) Reaching Beyond All-Metallic Plasmonics with Optoplasmonic Metallo-Dielectric Hybrid Materials; Bjoern Reinhard¹; ¹Boston University
- 2:40 (601) **One-Pot Synthesis of Silver Nanoparticles with an Ultra-Thin Silica Shell and Their Integration into SERS and LSPR Substrates**; <u>Daniel Willett</u>¹, George Chumanov¹; ¹Clemson University
- 2:20 (600) **Tuning Surface Plasmon Resonances on Gold Nanostars**; <u>Laura Fabris</u>¹, Theodoros Tsoulos¹, Roney Thomas^{1,3}, Swarnapali Indrasekara^{1,2}; ¹Rutgers University; ²Rice University; ³Wesleyan 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; <u>Kathleen Gough</u>¹, Catherine Findlay¹, Robert Johns², Hans Bechtel², Michael Martin², Susan Kaminskyj³, Tanya Dahms⁴; ¹University of Manitoba; ²Advanced Light Source Berkeley Lab; ³University of Saskatchewan; ⁴University of Regina
- 4:10 (603) Synchrotron Based Broadband IR Microspectroscopy and Spectromicrotomography; <u>Caol</u> <u>Hirschmugl</u>¹; ¹UW-Milwaukee
- 4:30 (604) Vibrational Spectroscopy: Disease Diagnostics and Beyond; <u>Hugh J. Byrne¹</u>; ¹Dublin Institute of Technology
- 4:50 (605) Infrared Spectral Imaging of Live Cells though Water; <u>Peter Gardner</u>¹, James Doherty¹, Michael Pilling¹, Zhe Zhang¹, Graeme Clemens¹, Alex Henderson¹, Gianfelice Cinque²; ¹Manchester Institute of Biotechnology, University of Manchester; ²Diamond Light Source, Diamond House

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

5:10 (606) Single Cell Analysis for Biological and Biomedical Applications Using Mid-IR Synchrotron Light and Laser Sources; <u>Ganesh D Sockalingum</u>¹, Valérie Untereiner¹, Abigail V Rutter², Marie Guilbert¹, Nick R Forsyth², Christophe Sandt⁴, Paul Dumas⁴, Katia Wehbe³, Gianfelice Cinque³, Josep Sule-Suso¹; ¹University of Reims Champagne -Ardenne, FR; ²University of Keele, UK; ³Diamond Synchrotron, UK; ⁴Soleil 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 Kasianowicz¹, Joseph Robertson¹, Arvind Balijepalli¹, Sina Bavari², Rekha Panchal², Jingyue Ju³, Minchien Chen³, Shiv Kumar³, Carl Fuller³, Joseph Reiner⁴; ¹NIST, Physical Measurement Laboratory, Gaithersburg, MD; ²US Army Medical Research Institute for Infectious Diseases, Ft. Detrick, MD; ³Dept. of Chemical Engineering, Columbia University, New York, NY; ⁴Department of Physics, Virginia Commonwealth University, Richmond, VA
- 4:10 (608) Engineered Protein Nanopores for Challenging Tasks in Molecular Diagnosis; <u>Liviu Movileanu</u>¹; ¹Syracuse University
- 4:30 (609) Molecular-Level Design of Nanoscale Tools for Enhanced Single-Molecule Sensing; Julie Whelan¹, Nuwan Bandara¹, Buddini Karawdeniya¹, Jason Dwyer¹; ¹University of Rhode Island
- 4:50 (610) Solid-state Single-Molecule Detection of DNA in Nanochannels; John Oliver¹; ¹Nabsys Inc
- 5:10 (611) **Deformation of Bacterial Morphology in Sub-**Micrometer Constrictions under Applied Pressure; <u>Nil</u> <u>Tandogan¹</u>, Edgar D. Goluch¹; ¹Northeastern University

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

Presider: Jorge Pisonero and Patrick Chapon; Presider: Jorge Pisonero

- 3:50 (612) A Study of Strategic Calibrations and Analyte Calculations; <u>Kim Marshall</u>¹; ¹Leco Corporation
- 4:10 (613) Applied Applications for GD OES in First Solar's Material Analysis Department; <u>Kristin Robison</u>¹; ¹First Solar
- 4:30 (614) Comparison of Two Analytical Techniques GD-MS and SIMS Applied in Depth Profile Analysis; <u>Piotr</u> Konarski¹; ¹Institute 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; <u>Edward Steers</u>¹, Sohail Mushtaq¹, Volker Hoffmann², Juliet Pickering³, Petr Smid^{1,4}, Zdenek Weiss⁴; ¹London Metropolitan University; ²Leibniz Institute for Solid State and Material Research Dresden; ³Imperial College, London; ⁴LECO
- 5:10 (616) Glow Discharge Optical Emission (GD-OES) Application for Thin Film Analysis of Metal Powders; Arne Bengtson¹, Mats Randelius¹; ¹Swerea 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**; <u>Alexander Scheeline</u>¹; ¹SpectroClick
- 4:10 (618) Ideas to Finance Your Spectroscopy Innovation; Roshan Shettty¹; ¹Anasys Instruments
- 4:30 (619) Finding a Niche Market in Busy Spectroscopy Field; <u>Rina Dukor</u>¹; ¹BioTools, Inc.
- 4:50 (620) When a Great Medical Device Isn't Great for the Company; <u>Bradford Clay</u>¹; ¹bioMerieux, 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**; <u>Michael F Roberto¹</u>, Randy Pell¹, L. Scott Ramos¹, Brian G. Rohrback¹; ¹Infometrix, Inc.
- 4:10 (622) SERS Detection of Foodborne Pathogens at 10 cfu/g Food in Less than 5 Hours; <u>Chetan Shende</u>¹, Katie Dana¹, Jay Sperry², Stuart Farquharson¹; ¹Real-Time Analyzers, Inc.; ²University of Rhode Island
- 4:30 (623) Data Transfer Between a FT-NIR Laboratory and a Miniaturized Hand-held NIR Spectrometer; <u>Heinz Siesler</u>¹, Uwe Hoffmann², Frank Pfeifer¹; ¹University of Duisburg-Essen; ²nir-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 Noda¹, Brian Sobieski¹, Liang Gong¹, C.J. McBrin¹, John Rabolt¹, Bruce Chase¹; ¹Department 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 Chang¹, Hoeil Chung¹;
 ¹Department 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; <u>Mark Phillips</u>¹; ¹Pacific Northwest National Laboratory
- 4:10 (627) Laser Ablation Molecular Isotopic Spectrometry (LAMIS): Factors Influencing Analytical Precision and Accuracy; <u>Xianglei Mao</u>¹, George Chan¹, Alexander Bol'shakov², Huaming Hou¹, Vassilia Zorba¹, Richard Russo¹; ¹Lawrence Berkeley National Laboratory; ²Applied Spectra, Inc.
- 4:30 (628) **Hybrid Interferometric/Dispersive Atomic Spectroscopy of Uranium**; <u>Phyllis Ko</u>¹, Jill Scott², Igor Jovanovic¹; ¹Penn State University; ²Idaho National Laboratory
- 4:50 (629) H and D Analysis Using Laser Induced Breakdown Spectroscopy in Helium Gas.; <u>Koo Hendrik Kurniawan</u>¹, Kiichiro Kagawa^{1,2}; ¹Maju Makmur Mandiri Research Center; ²Fukui University

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

5:10 (630) Detection of Isotopes in a Matrix with LIBS; <u>Alan</u> <u>Ford¹</u>, Charlemagne Akpovo², Staci Brown², Jorge Martinez², Lewis Johnson²; ¹Alakai Defense Systems; ²FAMU

> 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); <u>William D. Hoffmann¹</u>, Glen P. Jackson^{1, 2}; ¹West Virginia University, Department of Forensic and Investigative Science, WV; ²West 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**; <u>Xiaohong Xiong¹</u>, Tao Jiang¹, Meiling Yang¹, Wenhao Qi¹, Saijin Xiao¹, Zhiqiang Zhu¹,Huanwen Chen¹; ¹Jiangxi 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; <u>Andrew P. Storey¹</u>, Offer Zeiri^{1, 2}, Steven Ray¹, Allen White^{1,3}, Gary Hieftje¹; ¹Indiana University; ²Nuclear Research Center Negev; ³Rose-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. Zhang¹, R. Kenneth Marcus¹; ¹Clemson University
- 5:10 (635) Direct Analyte-Probed Nanoextraxtion (DAPNe) Coupled to Nanospray Ionization Mass Spectrometry Applied to Document Analysis; <u>Vivian Huynh</u>¹, Kristina Williams¹, Phillip Mach¹, Zachary Sasiene¹, Teresa Golden¹, Guido Verbeck¹; ¹University 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 Whiting¹, Pierre Puget², Eric Colinet², Philippe Andreucci², David Faulkner³, Philippe Coric³; ¹3 Degrees of Separation; ²APIX Analytics; ³EIF-Astute
- 4:10 (637) Fast GC Performance in the Real World: Multi Lab Studies for Repeatability & Reproducibility; John Crandall¹, Steve Bostic¹, Ned Roques¹; ¹Falcon Analytical
- 4:30 (638) FTIR & GC-FTIR Single Analyzer for Comprehensive Process Monitoring and Control; <u>Charles</u> <u>Phillips</u>¹, Martin Spartz¹, Anthony Bonanno¹, Stacey Larson¹, Alice Delia¹; ¹Prism Analytical Technologies, Inc.
- 4:50 (639) Application of Low Thermal Mass Column Technology to On-line Process Gas Chromatography; <u>Eric</u> <u>Schmidt</u>¹, Anna Sandlin¹, Linda Heinicke¹, Bill Winniford¹, Wilco Hoogerwerf², Jasper Van Noyen³, Dale Ashworth⁴, Chris Bishop⁴; ¹Analytical Sciences, The Dow Chemical Company, Freeport, TX; ²Analytical Sciences, The Dow Chemical Company, Terneuzen, The Netherlands; ³Hydrocarbons R&D, The Dow Chemical Company, Terneuzen, The Netherlands; ⁴Valco Instruments Company, Inc., Houston, TX

5:10 (640) **Portable Plant Performance Analyzer System**; <u>Matthew MacConnell¹</u>; ¹Air Products and Chemicals

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

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; <u>Douglas Minick¹</u>, Randy Rutkowske¹, Mark Hemling¹; ¹GlaxoSmithKline R&D
- 4:10 (642) Quantitation of Enantiomers by Vibrational Circular Dichroism (VCD); Laila Kott¹; ¹Takeda Pharmaceuticals International Company
- 4:30 (643) Pharmaceutical Applications of Vibrational Circular Dichroism (VCD); <u>Steven Wesolowski</u>¹; ¹AstraZeneca
- 4:50 (644) Advancing Supercritical Fluid Chromatography (SFC) Technology and its Applications in Drug Discovery; <u>Vingru Zhang¹</u>, Chunlei Wang¹, Jun Dai¹; ¹Bristol-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 Zhuang¹, Satish Kumar¹, Abu Rustum¹; ¹Merial, 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; <u>Christiaan van Swol¹</u>, Michelle Agenant^{1,2}, Trudy Jonges², Olivier Wegelin¹, Ruud Bosch², Harm van Melick¹, Matthijs Grimbergen¹; ¹St. Antonius Hospital Nieuwegein; ²University Medical Center Utrecht
- 4:10 (647) Raman Spectroscopic Techniques for the Identification of Ionizing Radiation Induced Damage in Tumour Cells; <u>Andrew Jirasek¹</u>, Quinn Matthews³, Samantha Harder², Martin Isabelle⁴, Julian Lum³, Alex Brolo²; ¹University of British Columbia; ²University of Victoria; ³BC Cancer Agency; ⁴Gloucester Royal Hospital
- 4:30 (648) Exploration of Wavelength Effects on Deep Tissue Detection in Transmission Raman Spectroscopy; <u>Adrian</u> <u>Ghita¹</u>, Pavel Matousek², Nick Stone¹; ¹University of Exeter, UK; ²STFC Rutherford Appleton
- 4:50 (649) Multiplexed Raman Micro-Spectroscopy using Spatial Light Modulators; <u>Faris Sinjab¹</u>, Graham Gibson², Miles Padgett², Ioan Notingher¹; ¹University of Nottingham; ²The University of Glasgow
- 5:10 (650) Rapid Fiber-Optic Raman Spectroscopy Enhances in vivo Diagnosis of Adenomatous Polyps at Colonoscopy; <u>Zhiwei Huang¹</u>; ¹National 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; <u>Celine Daher</u>¹, Ludovic Bellot-Gurlet², Francesca Casadio¹; ¹Art Institute of Chicago; ²MONARIS UMR 8233 UPMC/CNRS
- 4:30 (653) Identification of Copper Resinate in Artworks: in a Quest for the Optimal Raman Procedure; Jana Striova¹; ¹National 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; <u>Kristin Wustholz</u>¹, Kristen Frano¹, Shelley Svoboda²; ¹College of William and Mary; ²Colonial Williamsburg Foundation
- 5:10 (655) Raman Spectroscopy for Cultural Heritage: a Powerful Technique in the Conservation Scientist's Toolbox; <u>Federica Pozzi</u>¹; ¹Solomon 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; <u>Jonathan Sweedler</u>¹; ¹University of Illlinois



8:30 am – AES Mid Career Award (657) Microchip Electrophoresis: A Mid-Career Method?; <u>Adam Woolley</u>¹; ¹Brigham 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; <u>Elaine Zhu</u>¹; ¹University of Notre Dame
- 9:35 (659) Dielectrophoretic Monitoring of Alterations in C.difficile Colonization Due to Inter-Strain Antagonism; <u>Nathan Swami¹</u>, Yi-Hsuan Su¹, Ali Rohani¹, Cirle Warren²; ¹Electrical Engineering, University of Virginia; ²Infectious Diseases, University of Virginia
- 9:55 (660) XFEL Diffraction from Protein Nanocrystals Isolated using a Microfluidic Sorter; <u>Bahige Abdallah</u>¹, Nadia Zatsepin¹, Shatabdi Roy-Chowdhury¹, Jesse Coe¹, Katerina Dorner¹, Raymond Sierra², Hilary Stevenson³, Guillermo Calero³, Petra Fromme¹, Alexandra Ros¹; ¹Arizona State University; ²Stanford PULSE Institute; ³University of Pittsburgh
- 10:15 (661) Capturing Viruses using Dielectrophoretic Microdevice; Jie Ding¹, Robert Lawrence^{2, 3}, Brenda Hogue^{2,3}, Paul Jones¹, Mark Hayes^{1,4}; ¹Department of Chemistry and Biochemistry, Arizona State University; ²School of Life Sciences, Arizona State University; ³The Center for Infectious Diseases and Vaccinology, The Biodesign Institute, Arizona State University; ⁴Arizona State University
- 10:35 (662) Investigation of Spatial and Temporal Dynamics of Electrophoretic Exclusion on a Microdevice; <u>Fanyi Zhu</u>¹; ¹Arizona 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**; <u>Huanwen Chen</u>¹, Haidong Wang¹, Rui Su², Konstaintin Chingin¹; ¹Jiangxi Key Laboratory for Mass Spectrometry and Instrumentation, East China Institute of Technology, Nanchang, China; ²Changchun University of Chinese Medicine, Changchun, China
- 9:35 (664) Interpreting Geological Mineral Mixtures with Combined Raman-LIBS Spectroscopy (RLS); <u>Nina Lanza</u>¹, Samuel Clegg¹, Roger Wiens¹, Rhonda McInroy¹; ¹Los Alamos National Laboratory
- 9:55 (665) Atmospheric Microwave & Micro Plasmas for Ambient Desorption/Ionization Mass Spectrometry; <u>Yixiang Duan¹</u>; ¹Research Center of Analytical Instrumentation, College of Life Science, Sichuan University
- 10:15 (666) Analytical Instrumentation for Future Planetary Exploration Missions; <u>Peter Edwards¹</u>, Ian Hutchinson¹, Richard Ingley¹; ¹University of Leicester

10:35 (667) Advanced Experimental Design for Simultaneous Acquisition of Laser Induced Plasma and Raman Signals; <u>Soo-Jin Choi</u>¹, Jae-Jun Choi¹, Dae-Hyoung Kim¹, Dong-Woo Han¹, Jack J. Yoh¹; ¹Seoul 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; <u>Lingjun Li</u>¹; ¹University of Wisconsin
- 9:35 (669) **Pushing the Limits of Vibrational Spectroscopic Imaging with New Technology**; <u>Rohit Bhargava</u>¹; ¹University of Illinois at Urbana-Champaign
- 9:55 (670) Automating Epigenomics: Progress towards a Microfluidic Chromatin ImmunoCapture Device; <u>Ryan</u> <u>Bailey¹</u>, Yi Xu¹, Steven Doonan¹, Richard Graybill¹, Tamas Ordog²; ¹University of Illinois at Urbana-Champaign; ²Mayo Clinic
- 10:15 (671) Measuring Neurochemicals In Vivo using LC-MS; <u>Robert Kennedy</u>¹; ¹University of Michigan
- 10:35 (672) Single-cell Mass Spectrometry Tells of Asymmetry in the Body Plan of the Early Developing Embryo; Peter <u>Nemes¹</u>, Rosemary Onjiko¹, Sally Moody¹; ¹The George Washington University

Thursday Morning, *Room 555A* MUSCULOSKELETAL DISEASES Organizer and Presider: Nancy Pleshko

- 9:15 (673) A Portable Clinical Grade Raman Device for Pointof-Care Diagnosis of Gout and Pseudogout; <u>Ozan Akkus</u>¹, Bolan Li¹, Nora Singer², Donard Haggins³, Yener Yeni³; ¹Case Western Reserve University; ²Metro Health Hospital; ³Henry Ford Hospital
- 9:35 (674) Bone Tissue Composition and Heterogeneity at the Micro and Nano-scale; <u>Adele Boskey</u>¹, Eduardo Villareal¹, Lyudmila Spevak¹, Richard Mendelsohn²; ¹Hospital for Special Surgery; ²Rutgers University
- 9:55 (675) Emerging Magnetic Resonance Imaging and Spectroscopy Methods for the Assessment of Osteoporosis; Chamith Rajapakse¹; ¹University of Pennsylvania
- 10:15 (676) Developing Raman Spectroscopy for Clinical Detection of Peripheral Nerve Injury; <u>Katherine E.</u> <u>Cilwa</u>^{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}; ¹Regenerative Medicine, Naval Medical Research Center; ²Henry M. Jackson Foundation for the Advancement of Military Medicine; ³Uniformed Services University of Health Sciences; ⁴Walter Reed National Military Medical Center

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

10:35 (677) Mid Infrared Fiber Optic Evaluation of Ligament and Tendon Composition; <u>Mugdha Padalkar</u>¹, Cushla McGoverin¹, Arash Hanifi¹, Nicholas Caccese¹, Padraig Glenn¹, Scott Barbash²,Eric Kropf², Nancy Pleshko¹; ¹Dept. of Bioengineering, College of Engineering, Temple University, Philadelphia PA; ²Dept. 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; <u>Peter Gardner¹</u>, Michael Pilling¹, Alex Henderson¹, Ben Bird²; ¹Manchester Institute of Biotechnology, University of Manchester; ²Daylight Solutions
- 9:35 (679) The Role of High Resolution FTIR Spectrochemical Imaging in Resolving Clinical Issues; <u>Kathleen Gough</u>¹; ¹University of Manitoba
- 9:55 (680) Introducing Infrared Imaging Human of Blood Serum for High-throughput Biomedical Screening; <u>Caryn</u> <u>Hughes</u>^{1,2}, Graeme Clemens², Benjamin Bird³, Matthew Barre³, Jeremy Rowlette³, Matthew Baker²; ¹University of Manchester; ²University of Strathclyde; ³Daylight Solutions Inc.
- 10:15 (681) Infrared Spectroscopy in 3D and at Nano Scales; <u>Michael C. Martin¹</u>; ¹Advanced Light Source, Lawrence Berkeley National Laboratory
- 10:35 (682) *In situ* Attenuated Total Reflection Fourier Transform Infrared Analysis of Live Cells; <u>K. L. Andrew</u> <u>Chan¹</u>, Pedro L. Fale¹; ¹King

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**; <u>Leon Radziemski¹</u>; ¹Piezo Energy Technologies
- 9:55 (684) From the Calibration Curve to Machine Learning:; <u>Matthieu Baudelet</u>^{1,2}; ¹Townes Laser Institute, University of Central Florida; ²National Center for Forensic Science, University of Central Florida
- 10:15 (685) Calibration- and Calibration-Free LIBS: Past and Future; <u>Igor Gornushkin</u>¹, Wolfram Bremser¹, Andrey Demidov¹, Ulrich Panne^{1,2}; ¹Federal Institute for Materials Research and Testing (BAM); ²Humboldt-Universität zu Berlin, Department of Chemistry
- 10:35 (686) Calibration-Free LIBS, As It Was and As It Is; <u>Vincenzo Palleschi¹</u>, Emanuela Grifoni¹, Stefano Legnaioli¹, Giulia Lorenzetti¹, Stefano Pagnotta¹; ¹Applied 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 Coffey¹, Philip Martin¹, James Thomson¹; ¹Manchester University
- 9:35 (688) Inline Analysis for Rapid Optimization of Continuous Flow Processes; <u>Richard Bourne</u>¹, Nicholas Holmes¹; ¹University of Leeds

- 9:55 (689) Automated Stability Testing How *in-situ* Measurements Deliver Rapid Product Development; <u>Andy</u> <u>Brookes</u>¹, Faye Turner¹, Helen Williams¹; ¹Astrazeneca
- 10:15 (690) Mid-infrared Spectroscopy Based on a Supercontinuum Source and a MOEMS-based Fabry-Perot Microspectrometer; <u>Markus Brandstetter</u>¹, Jakob Kilgus¹, Petra Müller¹, Peter M. Moselund²; ¹RECENDT GmbH - Research Center for Non-Destructive Testing; ²NKT Photonics A/S
- 10:35 (691) Strategy to Improve Raman Multivariate Calibration Life-Cycle Model Performance: A Pharmaceutical Tablet Assay Example; Md. Nayeem Hossain¹, Md. Anik Alam¹, Benoît Igne³, Carl Anderson^{1,2,4}, James Drennen^{1,2}; ¹Graduate School of Pharmaceutical Sciences, Duquesne University; ²Duquesne University Center for Pharmaceutical Technology, Duquesne University; ³RD Platform Technology and Science, Glaxo SmithKline, King of Prussia; ⁴Duquesne 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 Nafie¹; ¹Syracuse University
- 9:35 (693) Role of Side-Chains and Environmental Variation in Forming Peptide Aggregates and Fibrils. IR and VCD Spectroscopic Studies; <u>Tim Keiderling¹</u>, Fernando Tobias¹, Ge Zhang¹, Heng Chi¹; ¹University of Illinois at Chicago
- 9:55 (694) UV Resonance Raman (UVRR) Structural Studies of Polyglutamine (polyQ) Side Chains and Fibrils; <u>David</u> <u>Punihaole¹</u>, Zhenmin Hong¹, Elizabeth Dahlburg¹, Ryan Jakubek¹, Riley Workman², Jeffry Madura², Sanford Asher¹; ¹University of Pittsburgh; ²Duquesne University
- 10:15 (695) Structure and Stability of Amyloid Fibrils Studied by Vibrational Spectroscopy and Surface Probe Microscopy; Maruda Shanmugasundaram¹, Dmitry Kurouski¹, Marketa Pazderkova², Tomas Pazderka², William Wan⁵, Gerald Stubbs⁵, Rina K. Dukor³, Laurence A. Nafie^{-3, 4}, Igor K. Lednev¹; ¹Department of Chemistry, University at Albany, State University of New York; ²Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic; ³BioTools Inc.; ⁴Department of Chemistry, Syracuse University; ⁵Department 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; <u>Patrik Johansson¹</u>, Patrick Koelsch^{1, 2}; ¹University of Washington; ²University 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.; <u>Catherine Kendall</u>¹, Oliver Old¹, Martin Isabelle¹, Gavin Lloyd¹, Katherine Lau², Neil Shepherd¹,Hugh Barr¹, Nick Stone³; ¹Gloucestershire Hospitals NHS Trust; ²Renishaw PLC; ³University of Exeter, UK
- 9:35 (698) Good Vibrations: Shining Light on Metabolism; <u>Roy</u> <u>Goodacre¹</u>, Katherine Hollywood¹, Lorna Ashton¹, David Cowcher¹; ¹University 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**; <u>Alison Hobro¹</u>, Nicolas Pavillon¹, Nicholas Smith¹; ¹Biophotonics Laboratory, Immunology Frontier Research Center, Osaka University
- 10:15 (700) Utility of Short-Wave Infrared Raman for SERS and SORS; <u>Neil Shand</u>¹; ¹Defence 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 Yamakoshi³, Kosuke Dodo^{1,3}, Katsumasa Fujita^{1,2}, Michio Murata^{2,4}, Mikiko Sodeoka^{1,3}; ¹AMED-CREST, AMED; ²Osaka University; ³RIKEN; ⁴Lipid 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; <u>Mark Peterman¹</u>, Merwan Benhabib¹, Samuel Kleinman¹; ¹OndaVia, Inc.
- 9:35 (703) **Drug Product Identification using 1064 nm Handheld Raman Spectroscopy**; <u>Joseph Stoltz</u>^{1,2}, Claire Dentinger^{1, 2}; ¹Pfizer, Inc; ²Rigaku Technologies
- 9:55 (704) Handheld Raman for Real-Life Chemical Detection and Identification; <u>Philip Zhou</u>¹, Katherine Bakeev¹; ¹B&W Tek, Inc.
- 10:15 (705) Novel Approaches to Overcoming Obstacles in Conducting Handheld Raman Measurements; <u>Thomas</u> <u>Tague</u>¹; ¹Bruker Corporation
- 10:35 (706) Advances & Applications of Handheld Raman & FTIR Spectrometers; <u>Michael Hargreaves</u>¹; ¹Thermo 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**; <u>Carolyn Hutchinson</u>¹, Rebecca Hansen¹, D. Paul Cole¹, Young Jin Lee¹; ¹Department of Chemistry, Iowa State University

Poster Board #2

(708) Identification of the Splicing Regulatory Factors using Mass Spectrometry; <u>Toru Takarada</u>¹, Ken-ichi Yoshino², Masafumi Matsuo³, Atsuko Takeuchi¹; ¹Kobe Pharmaceutical University; ²Kobe University; ³Kobe Gakuin University

Poster Board #3

(709) Analysis and Its Application of Urinary Prostaglandin D2/E2 Metabolites; <u>Atsuko Takeuchi¹</u>, Yoshihiro Urade², Masafumi Matsuo³; ¹Kobe Pharmaceutical University; ²Tsukuba University; ³Kobe Gakuin University

Poster Board #4

(710) High-sensitivity Capillary Electrophoresis Nanoelectrospray Ionization Mass Spectrometry using Tapered-tip Emitters: Toward Single-cell Proteomics; <u>Sam</u> (<u>Bok Dong</u>) <u>Choi</u>¹, Peter Nemes¹; ¹George 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; <u>Ross Carter</u>¹, Anjali Alving¹; ¹Bruker Daltonics *Poster Board* #6

(712) Development of a New Versatile Instrument for Complementary Analysis Combining Laser Ablation Mass Spectrometry and Laser Spectroscopy; <u>Andreas Bierstedt</u>¹, Knut Rurack¹, Jens Riedel¹; ¹BAM Federal Institute for Materials Research and Testing

Poster Board #7

(713) **Investigating Electrospray Ionization Using a Pulsed Nanospray Emitter**; <u>William P. McMahon¹</u>, Carina S. Minardi¹, Arjuna Subramanian¹, Kaveh Jorabchi¹; ¹Georgetown University

Poster Board #8

(7	(14) Plasma-Assisted Reaction Chemical Ionization Time of
F	light Mass Spectrometry for Identification and
Q	uantification of Halogenated Compounds; <u>Kunyu Zheng¹</u> ,
Р	eter Haferl ¹ , Haopeng Wang ¹ , Hamid Badiei ² , Feven
G	ezahegn ¹ , Kaveh Jorabchi ¹ ; ¹ Georgetown University; ² Perkin
E	lmer, Inc.
Poster	Board #9
(7	715) Soft µs Mid-IR Laser Desorption Ionization of
Α	coustically Levitated Liquids; Aleksandra Michalik-
<u>O</u>	nichimowska ^{1,2} , Carsten Warschat ¹ , Toralf Beitz ² , Ulrich
P	anne ¹ , Hans-Gerd Loehmannsroeben ² , Jens Riedel ¹ ; ¹ BAM
F	ederal Institute for Materials Research and Testing Division;
2 H	Physical Chemistry, University of Potsdam
Poster	Board #10
(7	716) Multistage Mass Spectrometry of Phospholipids Using
C	ollision-Induced Dissociation (CID) and Metastable Atom-
Α	ctivated Dissociation (MAD); Pengfei Li ¹ , William
Н	offmann ² , Glen P. Jackson ^{1,2} ; ¹ C. Eugene Bennett Department
0	f Chemistry, West Virginia University, Morgantown, WV;
2 I	Department of Forensic and Investigative Science, West
V	irginia University, Morgantown, WV
Poster	Board #11
(7	(17) Selective Separation of Metalloproteins using Aqueous
Т	wo-Phase System; Maria C. Hespanhol da Silva ¹ , Anna
D	onnell ² , Julio A. Landero ² , Joseph A. Caruso ² ; ¹ Universidade
F	ederal de Viçosa; ² University of Cincinnati
	Microfluidics Posters
Poster	Board #12
(7	(18) Moved to an oral
Poster	Board #13
(7	(19) Blood Sample Preparation using Gradient Insulator-
b	ased Dielectrophoresis (g-iDEP) Device; <u>Jie Ding</u> ¹ , Christine
W	/oolley ¹ , Mark Hayes ¹ ; ¹ Arizona State University
Poster	Board #14
(7	720) Developing New Trapping Efficient Designs for
G	radient Insulator-based Dielectrophoresis (g-iDEP)
	1 1 1

Devices; <u>Claire V. Crowther</u>¹, Mark A. Hayes¹; ¹Arizona State University

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

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Poster Board #15

(721) Electrophoretic Exclusion Based on a Microdevice; <u>Fanyi Zhu¹</u>, Mark Hayes¹, ¹Arizona State University

Poster Board #16

(722) Influence of Metal Cations on the EOF of Phospholipid Coated Capillaries; <u>Christopher Harrison</u>¹, Shane Wells¹, Eduardo de la Toba¹, Srilatha Vydha¹, Katherine Cortell¹; ¹San Diego State University

Poster Board #17

(723) **Biophysical Differentiation and Separation of Staphylococcus epidermidis Strains Based on Antibiotic Resistance**; <u>Shannon Huey Hilton</u>¹, Paul V. Jones¹, Mark A. Hayes¹; ¹Arizona State University

Poster Board #18

(724) **Gold Nanoporous Membranes for Tunable Protein and DNA Separations**; <u>John Orlet</u>¹, Daniel McCurry², Ryan Bailey²; ¹Truman State University; ²University 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; <u>Ute Schmidt¹</u>, Wei Liu², Thomas Dieing¹, Olaf Hollricher¹; ¹WITec GmbH; ²WITec Instruments

Poster Board #20

(726) **Multi-modal Molecular Imaging of Chemically Communicating Bacterial Communities**; <u>Nameera Baig</u>¹, Sage Dunham², Nydia Morales-Soto¹, Jonathan Sweedler², Joshua Shrout¹, Paul Bohn¹; ¹University of Notre Dame; ²University 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; <u>David Wetzel^{1,2}</u>, Mark Boatwright², Elieser Posner³; ¹Microbeam Molecular Spectroscopy Lab, Department of Grain Science, Kansas State University; ²Department of Biochemistry & Molecular Biophysics, Kansas State University; ³ESP 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 Wetzel¹, Mark Boatwright²; ¹Microbeam Molecular Spectroscopy Lab, Department of Grain Science, Kansas State University; ²Department of Biochemistry & Molecular Biophysics, Kansas State University

Poster Board #23

(729) New Applications Enabled by Ultra-miniaturized Hyperspectral Imagers; <u>Owen Wu¹</u>; ¹BaySpec, Inc.

Poster Board #24

(730) Fluorescence Imaging of Apurinic/Apyrimidinic Endonuclease 1 (APE1) Activity in Living Cells; <u>Meiping</u> <u>Zhao¹</u>, Junqiu Zhai¹, Simin Fang¹; ¹Peking University Poster Board #25

(731) A Surface Plasmon-Coupled Tunable Wavelength Filter for Wide-Field Hyperspectral Imaging.; <u>Ajaykumar</u> <u>Zalavadia</u>¹, John F. Turner II¹; ¹Cleveland State University Poster Board #26

(732) Combined NIR Imaging and Mapping Approach to Study Large Samples with High Spatial Resolution; <u>Patrick</u> <u>Wray¹</u>, John Gamble¹, Magnus Hoffmann¹, Gary McGeorge¹; ¹Bristol-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; <u>Anders Sparén¹</u> , 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 ; <u>Patrick Wray</u> 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
<u>Fang</u> 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; <u>Yan Zhang</u> ⁺ , Gary
McGeorge'; 'Bristol Myers Squibb
Poster Board #32
(738) Determination of Residence Time Distribution for a
Hot Melt Granulation Process using NIR and Raman
Probes; <u>Patrick S Wray</u> ⁴ , Keely Bergqvist ⁴ , John W Jones ⁴ ,
Martin Vernon', Gary McGeorge'; 'Bristol-Myers Squibb
Poster Board #33

(739) Structure of Biologics with Cutting Edge Vibrational Spectroscopy; <u>Carolina Carballo</u>, Rina Dukor; ¹BioTools Inc Raman-SERS Posters

Poster Board #34

(740) Surface Interaction of Nitrogen-Containing Aromatic Molecules with Gold Investigated with Surface Enhanced Raman Spectroscopy (SERS); <u>Ashish Tripathi</u>¹, Erik Emmons¹, Augustus Fountain², Jason Guicheteau², Martin Moskovits³, Steven Christesen²; ¹LEIDOS Inc.; ²U.S. Army Edgewood Chemical Biological Center; ³Department 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; <u>Erik Emmons</u>², Ashish Tripathi², Neal Kline³, Jerry Cabalo¹, Jason Guicheteau¹, Augustus Fountain¹, Steven Christesen¹; ¹Research and Technology Directorate, Edgewood Chemical Biological Center; ²LEIDOS Inc; ³Oak 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; <u>Buddini Karawdeniya</u>¹, Y. M. Nuwan Bandara¹, Caitlin Masterson¹, Julie Whelan¹, Brian Velleco¹, Jason Dwyer¹; ¹University of Rhode Island

Poster Board #37

(743) **Gold-based Multi-layered Probes for Enhanced SERS**; <u>Pietro Strobbia</u>¹, Alex Henegar¹, Theodosia Gougousi¹, Brian Cullum¹; ¹University 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**; <u>Heidi Fisk</u>¹, Jason Micklefield¹, Roy Goodacre¹; ¹The University of Manchester (UK)

Poster Board #39

(745) A Sheath-Flow Microfluidic Device for Combined Surface Enhanced Raman Scattering and Electrochemical Trace Detection; <u>Matthew R. Bailev</u>¹, Amber Pentecost², Asmira Selimovic², R. Scott Martin², Zachary D. Schultz¹; ¹University of Notre Dame; ²Saint Louis University

Poster Board #40

(746) **SERS Detection of Glucose Phosphate Isomers**; <u>Colleen</u> <u>Riordan¹</u>, Zachary Schultz¹; ¹University of Notre Dame *Poster Board #41*

(747) Development of a Stable, Gold Nanoparticle SERS

Substrate; <u>Md Shah Alam</u>¹, Mary M. J. Tecklenburg¹; ¹Central 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; <u>Aaron Crookes</u>¹, Casey Gallagher¹, Jonathan Scaffidi¹; ¹Miami University

Poster Board #43

(749) Evaluation of Sensitivity and Selectivity in Quantitative SERS-based Determination of Heavy Metal Concentrations; Jenny DeJesus¹, Ji Li¹, Audrey Hoffmann¹, Alyssa Meier¹, Jessica Krandel¹, Jonathan Scaffidi¹; ¹Miami University

Poster Board #44

(750) A Stable Nanostructured Substrate for Surface Enhanced Raman Scattering detection of Benzotriazole; <u>Brandon Russell</u>¹, Mary Tecklenburg¹; ¹Central Michigan University

Poster Board #45

(751) Multiplexed Homogenous SERS Immunoassay based on Antigen-Mediated Aggregation of Gold Nanoparticles; <u>Seth Filbrun¹</u>, Yen Lai¹, Arielle Lopez¹, Jeremy Driskell¹; ¹Illinois State University

Poster Board #46

(752) **Surface-Enhanced UV Fluorescence and Raman Scattering from Electrochemically Roughened Aluminum Substrates**; <u>Danielle Montanari</u>¹, Nathan Dean¹, Tyson Davis¹, Natascha Knowlton¹, Joel Harris¹; ¹University 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 Clark¹; ¹University of Exeter

Poster Board #48

(754) A Wet Synthetic Method Yielding Plasmonically Tunable Solid State SERS Substrates; <u>Seth Filbrun</u>², Jennifer Fasciano¹, Jonathan Scaffidi¹; ¹Miami University; ²Illinois State University

Poster Board #49

(755) Aluminum Substrates for UV-SERS; <u>Maria Fernanda</u> <u>Cardinal</u>¹, Bhavya Sharma¹, Michael B Ross¹, Alyssa Zrimsek¹, Sergei V. Bykov², David Punihao-le², Sanford A. Asher², George C. Schatz¹, Richard P. Van Duyne¹; ¹Department of Chemistry, Northwestern University; ²Department 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; <u>Richard Mathies</u>¹; ¹Chemistry Department, University of California at Berkeley
- 1:40 (757) Nanowires, Nanoelectronics and the Interface with Biological Systems; <u>Charles Lieber</u>¹; ¹Harvard University
- 2:00 (758) Extreme Separations-Cells: Antibiotic Resistance as a Differentiator in Staphylococcus epidermidis; <u>Mark</u> <u>Hayes</u>¹; ¹Arizona State University
- 2:20 (759) **Miniaturization of Liquid Chromatography**; <u>Milton</u> <u>Lee¹</u>, Sonika Sharma¹, Paul Farnsworth¹, Dennis Tolley¹, Alex Plistil², Hal Barnett², Stanley Stearns²; ¹Brigham Young University; ²VICI Valco
- 2:40 (760) Microfluidic Sample Preparation, Separation and Delivery for Ultrasensitive MS-Based Bioanalyses; <u>Ryan</u> <u>Kelly¹</u>, Yongzheng Cong¹, Tao Geng¹, Shanta Katipamula¹, Sachin Jambovane¹, Erin Baker¹, Keqi Tang¹; ¹Pacific 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; <u>Anita</u> <u>Mahadevan-Jansen¹</u>, John Nguyen¹, Zain Gowani¹, Margaret O'Connor¹, T. Quyen Nguyen¹, Xiaohong Bi², Ginger Holt¹; ¹Vanderbilt University; ²University of Houston; ³Northwestern University
- 1:40 (762) ALA-Induced Fluorescence Imaging of Breast Cancer Margins Detects Tumors Otherwise Occult to the Surgeon; <u>Ralph DaCosta</u>^{1,2,2}, Kristina Blackmore¹, Kathryn Ottolino-Perry¹, Stephanie DeLuca¹, Susan Done¹, Alexandra Easson¹, Wey-Liang Leong¹; ¹University Health Network; ²University of Toronto; ³Techna Institute
- 2:00 (763) Tethered Capsule Endomicroscopy for Barrett's Esophagus Screening: <u>Rohith Reddy</u>^{1,2}, Michalina Gora^{1, 2}, Robert Carruth², Tim Ford^{1,2}, Jing Dong^{1,2}, Guillermo Tearney^{1,2}; ¹Harvard Medical School; ²Massachusetts General Hospital
- 2:20 (764) **Developing Infrared Biofluid Diagnostics**; <u>Matthew</u> <u>Baker¹</u>, James Hands¹, Lila Lovergne¹, Caryn Hughes¹, Graeme Clemens¹, Ganesh Sockalingum², Benjamin Bird³; ¹University of Strathclyde; ²Universite de Reims; ³Daylight Solutions
- 2:40 (765) Multiplexed Detection of Breast Tumor Antigen with Nanprobe-Amplified Spectro-Immunoassay; Ishan Barman¹, Ming Li¹; ¹Johns 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; <u>Stephanie DeJong</u>¹, Zhenyu Lu¹, Brianna Cassidy¹, Stephen Morgan¹, Michael Myrick¹; ¹University of South Carolina
- 1:40 (767) **Optimal Preprocessing and Similarity for Automatic Whole-Spectrum Matching**; <u>CJ Carey</u>¹, M. Darby Dyar², Thomas Boucher¹, Stephen Giguere¹, Sridhar Mahadevan¹; ¹College of Information and Computer Sciences, University of Massachusetts - Amherst; ²Department of Astronomy, Mount Holyoke College
- 2:00 (768) Hotelling Trace Criterion as a Figure of Merit for the Optimization of Chromatogram Alignment; Edward Soares¹, Gopal Yalla¹, John O'Connor¹, Kevin Walsh¹, Amber Hupp¹; ¹College of the Holy Cross
- 2:20 (769) Design of Experiments in Spectral Space for Efficient Development of Near-Infrared Methods in Tablet Analysis; <u>Md Anik Alam</u>^{1,2}, James Drennen III^{1,2}, Carl Anderson^{1,2,3}; ¹Graduate School of Pharmaceutical Science, Duquesne University; ²Duquesne University Center for Pharmaceutical Technology; ³Duquesne University
- 2:40 (770) Development of Multiple Merit Ranking Methods for Automatic Selection of Multiple Tuning Parameters in Multivariate Calibration and Maintenance; <u>Alister</u> <u>Tencate¹</u>, John Kalivas¹, Alexander White²; ¹Department of Chemistry, Idaho State University; ²Department 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; <u>Facundo Fernandez</u>¹, Xiaoling Zang¹, Maria Eugenia Monge², Nael McCarty^{3,4}, Arlene Stecenko^{3,4}; ¹Georgia Institute of Technology; ²Centro de Investigaciones en Bionanociencias (CIBION); ³Emory+Children; ⁴Emory University School of Medicine and Children
- 1:40 (772) Ultrasensitive and Accurate Quantification of Oncogenic microRNAs using Nanoplasmonic Sensors; <u>Rajesh Sardar¹</u>, Gayatri Joshu¹, Samantha Deitz-McElyea^{2,3}, Sonali Mali¹, Murray Korc^{2,3}; ¹Indiana University-Purdue University Indianapolis; ²Indiana University School of Medicine
- 2:00 (773) **Plastic Antibodies for SERS Detection**; <u>Amanda</u> <u>Haes</u>¹, Wenjing Xi¹, Anna Volkert¹; ¹University of Iowa
- 2:20 (774) **SERS on Core-Shell Substrates**; <u>Christy Haynes</u>¹, Zhe Gao¹, Antonio Campos¹; ¹University of Minnesota
- 2:40 (775) Single Hotspot Raman Spectroscopy of a Self-Assembled Monolayer using Scanning Near-Field Optical Microscopy Excitation; <u>Camiel van Hoorn</u>¹, Freek Ariese¹, Arjan J.G. Mank²; ¹Faculty of Sciences and LaserLaB, VU University, Amsterdam, The Netherlands; ²Philips 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; <u>Christian</u> Parigger¹; ¹University of Tennessee Space Institute
- 2:00 (777) **Issues and Advances of Calibration Transfer in LIBS**; <u>Jean-Baptiste Sirven</u>^{1,2}, Jessica Picard^{1, 2}, Cécile Maury^{1,2}, Maria El Rakwe^{1,2}; ¹CEA; ²DEN, DANS, DPC, SEARS, LANIE
- 2:20 (778) Understanding the Complex Mechanisms Leading to Signal Enhancement in Double Pulse LIBS; <u>Prasoon</u> <u>Diwakar¹</u>, Patrick Skrodzki¹, Jason Becker¹, Tatyana Sizyuk¹, Ahmed Hassanein¹; ¹Center for Materials Under eXtreme Environment, School of Nuclear Engineering Purdue University
- 2:40 (779) **Standoff LIBS using a Spatial Heterodyne Spectrometer**; <u>Patrick Barnett</u>¹, Nirmal Lamsal¹, S. Michael Angel¹; ¹University 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 Nuceloprotein Complexes by Surface Induced Dissociation Coupled to Ion Mobility; <u>Vicki Wysocki¹</u>; ¹Ohio State University
- 1:40 (781) Structural Biology in the Gas Phase: New Approaches for Conformationally-selective Inhibitor Screening and Multiprotein Topology Mapping; <u>Brandon</u> <u>Ruotolo¹</u>; ¹University 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; <u>Matthew F Bush</u>¹; ¹University of Washington
- 2:20 (783) What Multiplexing Can Do for Your Experiment: Tangible Enhancements for Ion Mobility Spectrometry; <u>Brian</u> <u>Clowers¹</u>, Austen Davis¹, Kelsey Morrison¹; ¹Washington State University
- 2:40 (784) **Developing IMS-HDX-MS/MS Techniques for Structural Proteomics Investigations**; <u>Mahdiar</u> <u>Khakinejad</u>¹, Samaneh Ghassabi-Kondalaji¹, Gregory Donohoe¹, James Arndt¹, Stephen Valentine¹; ¹West 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; <u>Sergey Arzhantsev</u>¹, Justin Bueno¹, John Kauffman¹; ¹US FDA
- 1:40 (786) In in Formulation: Developability and Predictive Stability Techniques; <u>Deniz Temel</u>¹; ¹Biogen
- 2:00 (787) Design of Pharmaceutical Formulations: ATR-FTIR Spectroscopic Imaging to Study Drug Release and Tablet Dissolution; <u>Andrew Ewing</u>¹, Graham Clarke², Sergei Kazarian¹; ¹Imperial College London; ²Bristol-Myers Squibb
- 2:20 (788) Using Spectroscopic Methods to Probe the Effects of Formulation Excipients on Protein Aggregation and Structure; Julie Wei¹; ¹Biogen Inc.
- 2:40 (789) Introduction of Raman to Raw Materials Testing; Sanjeev Johar¹; ¹Genzyme

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; <u>Kathryn Dana¹</u>, Chetan Shende¹, Stuart Farquharson¹, Albert Arias²; ¹Real-Time Analyzers, Inc.; ²Veterans Affairs Hospital of Connecticut
- 1:40 (791) **Hyperspectral Imaging of Crystalline Domains in Biopolymers**; <u>Venkata N K Rao Bobba</u>¹, John F. Turner II¹; ¹Cleveland State University
- 2:00 (792) Statistical Developments for In-Line Sensitivity and Selectivity Improvement in Single Molecule Dynamic-SERS; <u>Thibault Brulé</u>^{1,2}, Alexandre Bouhelier², Hélène Yockell-Lelièvre^{1,2}, Aymeric Leray², Alain Dereux², Jean-Francois Masson¹, Eric Finot²; ¹Département de Chimie, Université de Montréal; ²Laboratoire Interdisciplinaire Carnot de Bourgogne, Université de Bourgogne, Dijon, France
- 2:20 (793) **Towards Quantitative Lipid Characterization in** Cellular Matrices using Raman Microspectoscopy; <u>Nils</u> <u>Kristian Afseth</u>¹, Ingrid Måge¹, Zdenek Pilat², Ulrike Böcker¹, Jens Petter Wold¹, Volha Shapaval¹,Silvie Bernatova², Ota Samek²; ¹Nofima - Norwegian Institute of Food, Fisheries and Aquaculture Research; ²Institute 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; <u>Kelly Curtis</u>¹, Julian Moger¹, Catherine Kendall², Hugh Barr², Oliver Old², Nick Stone¹; ¹University of Exeter, UK; ²Gloucestershire 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 Gordon¹; ¹University of Otago, Dunedin, New Zealand
- 1:40 (796) Raman Spectroscopy of Low Energy Phonons; <u>David</u> <u>Tuschel¹</u>; ¹HORIBA Scientific
- 2:00 (797) Novel Brillouin-Raman Microspectroscopy of Hydrated Connective Tissue; <u>Francesca Palombo¹</u>, Ryan S. Edginton¹, Ellen Green¹, Nick Stone¹, C. Peter Winlove¹, Daniele Fioretto²; ¹University of Exeter, UK; ²University of Perugia, Italy
- 2:20 (798) Ligand Chemistry and the Low-Frequency Vibrations of Semiconductor Nanocrystals; <u>Anna Jolene</u> <u>Mork¹</u>, Elizabeth Lee¹, Nabeel Dahod¹, William Tisdale¹; ¹Massachusetts Institute of Technology
- 2:40 (799) Low Frequency Raman Spectroscopy for the Structural Analysis of Polycyclic Aromatic Hydrocarbons; <u>Anjan Roy</u>¹, James Carriere¹, Randy Heyler¹, Peter Larkin², Eric Chan³; ¹Ondax Inc; ²CytecIndustries; ³Bristol-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 Caruso¹, Anna Daigle Donnell¹, Aleksey Porollo², Julio Landero-Figueroa¹, Kavitha Subramanian¹, George Deepe¹; ¹University of Cincinnati; ²Cincinnati 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; <u>Steven</u> <u>Soper¹</u>; ¹University of North Carolina, Chapel Hill
- 4:30 (802) SERS in Live 3D Cell Cultures as a New Tool for Drug Discovery; <u>Colin Campbell</u>¹, Lauren Jamieson¹, Pierre Bagnaninchi¹, David Harrison²; ¹University of Edinburgh; ²University of St Andrews
- 4:50 (803) **Five-dimensional Single Particle Tracking in Live Cells**; <u>Ning Fang</u>^{1,2,3}; ¹Georgia State University; ²Iowa State University; ³Ames 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

- (806) Raman spectroscopy as a Versatile Tool for Fundamental Research and Practical Applications; Igor Lednev¹; ¹University at 9:15 Albany, SUNY
- (807) Shedding Light on Terahertz Radiation; <u>Richard Temkin</u>¹; ¹MIT 9:45

10:15 Preview of 2016 Conference

⁽⁸⁰⁴⁾ Mid- and Near-Infrared Spectroscopy; <u>Peter Griffiths</u>¹; ¹Griffiths Consulting LLC
(805) X-ray Spectroscopy with Compact X-Ray Sources; <u>Christoph Rose-Petruck</u>^{1,3}, Petr Bruza⁴, Bernhard Adams², Yishuo Jiao¹; ¹Brown University; ²Argonne Natl. Laboratory; ³Research Instruments Corporation; ⁴Czech Technical University 8:45

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...our joint-symposia with the ACS, coinciding with the International Year of Light

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