

FACSS Presents

SCIX2016

National Meeting of:
Society for Applied Spectroscopy (SAS)

Co-Meeting with: 23rd International
Symposium on Electro and Liquid
Phase-Separation Techniques
(ITP2016)



FINAL PROGRAM

SEPTEMBER 18 - 23

Hyatt Regency Hotel - Minneapolis, MN

scixconference.org

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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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WELCOME TO SciX 2016

On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) it is our pleasure to welcome you to Minneapolis for SciX 2016. We are excited to be in such a vibrant, beautiful, and cultural city! With the numerous restaurants and city attractions within a short walk of the conference hotel, attendees will surely be talking about this year's conference as one of the best.

Our 12 FACSS sponsoring societies are a reflection of the diversity within the analytical sciences. These organizations have worked diligently to produce an equally diverse and strong conference. As in the past, the focus of SciX 2016 is the technical program organized under the leadership of the Program Chair, Alexandra Ros. The Sunday Keynote speaker is Dr. Aydogan Ozcan, Chancellor's Professor at UCLA and Professor with the Howard Hughes Medical Institute. The program also has a special focus this year on Easing World Poverty and special sessions on Women and Diversity in Analytical Sciences, Mass Cytometry, and Art and Archaeology. We are co-meeting this year with the International Symposium on Electro- and Liquid-Phase Separations Techniques (ITP) which further broadens our programming within the separation sciences.

A prominent feature of the SciX program each year is the honoring of our colleagues for their superlative contributions to their fields. Awards addresses and sessions include the *Spectroscopy* Magazine's Emerging Leader in Molecular Spectroscopy Award (Matthew Baker), FACSS Charles Mann Award (Brian Marquardt), the ANACHEM Award (Paul Cremer), the Lester W. Strock Award (Raymond Arvidson), the Applied Spectroscopy William F. Meggers Award (Mike George), the Coblentz Society Craver Award (Karen Faulds), and the AES Mid-Career Award (Amy E. Herr).

Starting Sunday evening and continuing through Friday morning, you will find quality presentations by students, early-career professionals and seasoned scientists. Poster sessions at SciX provide a more relaxed environment to discuss cutting edge scientific results and include daily poster awards for student presenters. Under the guidance of the Program Chair, the Section Chairs and Session Chairs have worked extremely hard over the past year to organize symposia across the many exciting topics and applications within the analytical sciences. The chairs also secure financial support from our sponsoring industrial partners. These funds go directly into the program to help bring in the best and brightest as our presenters. We also are pleased to honor the four finalists in the competitive FACSS Innovation Award session on Thursday afternoon. We close out the diverse technical program with a session addressing Science Beyond Borders; speakers from academics, journalism, and the chemical industry will inspire us to extend our science beyond the laboratory.

SciX 2016 is the National Meeting for the Society for Applied Spectroscopy and a co-meeting with ITP. Supportive, friendly, well-attended networking opportunities are spread throughout the conference, 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 on Tuesday, and the Wednesday night fun and casual "Welcome to the Great Outdoors" all-inclusive event. For smart phone or tablet users, please take advantage of the free SciX app to plan your week's schedule and navigate the conference. We know you leave SciX 2016 with many new research ideas and new friends. We learn a lot and have fun doing it!

On a closing note, remember that SciX and FACSS are run by the consensus of 12 non-profit member societies – by scientists, for scientists. The planning for each conference starts years in advance, takes thousands of emails and conversations, and requires an immeasurable number of volunteered hours. Each year, we depend on dozens of experienced colleagues to help judge posters and select award winners. We rely on people like you to get involved. So consider what you can do to contribute to future meetings – then find a FACSS or SciX Chair and volunteer! The volunteer SciX 2016 team and the FACSS Executive Committee are grateful for the unwavering support of Marin Walker at the FACSS / SciX International Office. Her support brings about our success.

We know you will enjoy SciX 2016 and all its exceptional offerings - program, plenary lectures, awards symposia, poster sessions, workshops, networking events, and an extensive exhibition. The cutting edge science at the conference will no doubt be enhanced by the beauty and culture of Minneapolis.

Mary Kate Donais, Saint Anselm College - SciX General Chair 2016
Alexandra Ros, Arizona State University – SciX Program Chair 2016
Mike Carrabba, Hach – SciX Exhibits Chair 2015 - 2020
Mark Henson, Shire Pharmaceuticals – SciX Workshops Chair
Heather Brooke, CAMO Software, Inc. – SciX Workshops Chair
John Wasylyk, Bristol-Myers Squibb – SciX / FACSS Marketing Chair 2014-2019
Steven J. Ray, SUNY Buffalo, Governing Board Chair, 2016-2017

SciX Conference and FACSS International Office

2019 Galisteo Street, Building I-1, Santa Fe, NM 87505

(505) 820-1653 ○ (505) 820-1648 ○ facss@facss.org ○ www.scixconference.org ○ www.facss.org

GENERAL INFORMATION

LOCATION. All plenaries, symposia, workshops and the exhibits are located at the Hyatt Regency Minneapolis.

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, Nicollet A
7:00–9:00 pm SAS Poster Session & SciX Welcome Mixer

Monday Poster Session – Nicollet A

Set up posters between 9:00 – 10:00 am and remove by 5:00 pm

11:00 am – 12:00 noon – Poster Session

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

Tuesday and Wednesday Poster Sessions – Exhibit Hall

Posters remain up all day on their designated day. Set up posters between 9:00 – 10:00 am and remove Tuesday posters by 4:30 pm and Wednesday posters by 3:50 pm.

11:00 am – 12:00 noon – Poster Session

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

Thursday Poster Session – Nicollet A

Posters remain up all day. Set up posters between 9:00 – 10:00 am and remove at 3:50 pm

11:00 am – 12:00 noon – Poster Session

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

WORKSHOPS. A list of workshop, descriptions, and the locations begins on page 41. You must register for a SciX workshop at the conference registration desk

EMPLOYMENT BUREAU/ INTERNET CAFE. Available in the Nicollet Promenade conference registration area. See page 4

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

Monday (Opening Reception) 5:30 pm – 7:30 pm

Tuesday 10:00 am – 4:30 pm

Wednesday 10:00 am – 4:00 pm

WHAT'S HOT VENDOR PRESENTATIONS.

Sunday, 4:20 – 6:00 pm, *Nicollet B/C*

Tuesday, 11:30 am – 1:20 pm, *Exhibit Hall*

Wednesday, 11:30 am – 1:20 pm, *Exhibit Hall*

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 – *Nicollet A*

Tuesday and Wednesday morning and afternoon break.

11:00 am – 12:00 pm & 3:00 – 3:50 pm – *Exhibit Hall*

INTERNET ACCESS. Free Wi-Fi is available in all meeting space. Connect to *Hyatt Meeting Space* network. Password is *scix2016*.

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

SPECIAL EVENTS.

SUNDAY

6:15 pm **SciX 2016 Welcome.** Mary Kate Donais

Keynote Lecture. Democratization of Next-Generation Imaging, Sensing and Diagnostics Tools through Computational Photonics; **Aydogan Ozcan**, UCLA and Howard Hughes Medical Institute, *Nicollet B/C*

7:00 – 9:00 pm **Welcome Mixer and SAS Sponsored Student Poster Session.** SAS, Coblenz, and FACSS Student Award Presentations, *Nicollet A*

MONDAY

7:45 am **Opening Address.** Alexandra Ros Nicollet *B/C*

8:00 am **Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award.** Serum Spectroscopic Diagnostics: The Future for Clinical Diagnostics?; **Matthew Baker**, University of Strathclyde, *Nicollet B/C*

8:30 am **ITP Plenary Lecture.** Capillary Electrophoresis for Bottom-up Proteomic Analysis of Complex Mixtures; **Norman Dovichi**, University of Notre Dame, *Nicollet B/C*

Noon **Coblenz Speed Mentoring, Great Lakes A1**

5:30 – 7:30 pm **Reception for Exhibit Opening** (wine, beer, light hors d'ouvres) *Exhibit Hall*

TUESDAY

8:00 am **FACSS Charles Mann Award for Applied Raman Spectroscopy.** Process Raman: Reproducibility Drove Capability; **Brian Marquardt**, University of Washington, *Nicollet B/C*

8:30 am **Coblenz Society Craver Award.** Multiplexed and Quantitative Bioanalysis using Surface Enhanced Raman Spectroscopy (SERS); **Karen Faulds**, University of Strathclyde, *Nicollet B/C*

12:00 - 12:45 pm **Complimentary lunch in the Exhibit Hall.** Ticket required

12:45 pm **Coblenz Challenge, Isles**

6:00 pm **Raman Reception** Invitation Only. *Great Lakes A*

7:00 pm **ITP Dinner Reception** (ticket required), *Greenway H/I*

7:30 pm **Society for Applied Spectroscopy Wine and Cheese Awards Reception.** *Great Lakes B/C*

WEDNESDAY

8:00 am **ANACHEM Award.** Metallomembranes: Exploring the Interactions of Transition Metal Ions with Lipid Bilayers; **Paul Cremer**, Pennsylvania State University, *Nicollet B/C*

8:30 am **Applied Spectroscopy William F. Meggers Award.** Probing Reactions using Time-Resolved Infrared Spectroscopy in Solution and in the Solid State Using Quantum Cascade Lasers; **Mike George**, Nottingham Univ, *Nicollet B/C*

12:00 - 12:45 pm **Complimentary lunch in the Exhibit Hall.** Ticket required

3:00 pm **Diversity Networking Coffee Break.** *Greenway F*

3:05 pm **ITP Closing Plenary Lecture.** **Daniel Armstrong**, University of Texas at Arlington, *Nicollet B/C*

6:00 pm **Wednesday Evening All Inclusive Event,** Conference badge required. *Great Lakes Ballroom*

THURSDAY

8:00 am **Lester W. Strock Award.** Spectroscopy as an Important Key for Understanding Martian Paleoclimates; **Raymond Arvidson**, Washington University in Saint Louis, *Nicollet B/C*

8:30 am **AES Mid Career Award.** Electrophoretic Cytometry: Targeted Proteomics in Single Cells; **Amy E. Herr**, UC Berkeley, *Nicollet B/C*

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

FRIDAY

8:00 am **Closing Session.** *Lakeshore Ballroom*
Announcement of Innovation Award

8:15 am **Science Beyond Borders**

10:15 am **Preview of 2017 Conference**

EVENTS OF SPECIAL INTEREST TO STUDENTS

SUNDAY EVENING, *Nicollet A*

- Welcome Mixer: 7:00 – 9:00 pm
- SAS Sponsored Poster Session: 7:00 – 9:00 pm
 - SAS and Coblenz 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

TUESDAY WORKSHOP

- 2:00 – 3:30 pm. **How to Get Published**
 No Charge (Register at the SciX registration desk)
 This workshop will cover the fundamentals of preparing a manuscript for publication in an academic journal with direct reference to the Society of Applied Spectroscopy's own journal *Applied Spectroscopy*. The workshop will include an overview of the publishing landscape; how the publishing landscape is evolving; how to select a relevant publication; preparing your manuscript for submission to a journal; an overview of the peer review process; publication ethics and author rights and how to promote your article once published.
 Instructors: Louisa Strain, Naomi Blumson, *SAGE Publishing* and Kristin MacDonald, *Applied Spectroscopy*

EMPLOYMENT BUREAU / INTERNET CAFÉ

The Employment Bureau is located in the Registration Area in conjunction with the internet café Monday through Thursday. Computers and printers will be available in the Nicollet Promenade

EMPLOYERS: Bring either hard copy or print an 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 prospective employers to review.

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

CONFERENCE REGULATIONS AND CODE OF CONDUCT

The following regulations are in the best interest of the conference. FACSS/SciX reserves the right to revoke anyone's conference badge and attendance to the meeting.

General:

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 areas.
4. Only official exhibitors may display in the Exhibit Hall.
5. No demonstration of instrumentation or distribution of any type of literature is allowed outside the Exhibit Hall.

While in Sessions:

1. All devices including cell phones must be silenced.
2. No talking during oral presentations and awards ceremonies.
3. No Photography of PowerPoint presentations or Posters.
4. No distribution of product/meeting literature.

Expected Behavior throughout the Conference:

1. Be respectful and considerate of others and the facilities.
2. Be mindful of your surroundings and of your fellow participants.
3. Alert a SciX volunteer if you notice a dangerous situation or someone in distress.

Unacceptable Behavior:

1. Harassment, intimidation or discrimination in any form will not be tolerated.
2. Physical or verbal abuse of anyone attending or involved with the conference is not tolerated.
3. Alert a SciX volunteer if you witness or are the subject of unacceptable behavior.

FACSS and SciX CONFERENCE ORGANIZATION

MEMBER ORGANIZATIONS OF FACSS

AES Electrophoresis Society
 American Chemical Society, Division of Analytical Chemistry
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 ANACHEM
 The Coblenz Society
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 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

Co-Meeting with:

The 23rd International Symposium on Electro- and Liquid Phase-Separation Techniques

2016 SciX Conference Chair Persons

General Chair	Mary Kate Donais , <i>Saint Anselm College</i> Email: mdonais@anselm.edu
Program Chair	Alexandra Ros , <i>Arizona State University</i> Email: alexandra.ros@asu.edu
Exhibit Chair	Mike Carrabba , <i>Hach Company</i> Email: mcarrabba@hach.com
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Marketing Chair	John Wasyluk , <i>Bristol-Myers Squibb</i>
Social Media Chair	Richard Osibanjo , <i>Intel</i>

2016 Program Section Chairs

Atomic Spectroscopy	Jorge Pisonero , <i>Universidad de Oviedo</i>
Awards	Matthieu Baudelet , <i>University of Central Florida</i>
Biomedical and Bioanalytical	Karen Esmonde-White , <i>Kaiser Optical Systems, Inc.</i>
Chemometrics	Peter Harrington , <i>Ohio University</i>
Electrophoresis	Jason Dwyer , <i>University of Rhode Island</i> and Ryan Kelly , <i>PNNL</i>
ITP	Ziad El Rassi , <i>Oklahoma State University</i> and Blanca Lapizco-Encinas , <i>Rochester Institute of Technology</i>
Laser-Induced Breakdown Spectroscopy	Matthieu Baudelett , <i>University of Central Florida</i>
Mass Spectrometry	Glen P. Jackson , <i>West Virginia University</i> and Yu Xia , <i>Purdue University</i>
Molecular Spectroscopy	Curt Marcott , <i>Light Light Solutions and University of Delaware</i>
Nanotechnology	Wei Zhao , <i>University of Arkansas at Little Rock</i>
Pharmaceutical Analysis	John Wasyluk , <i>Bristol-Myers Squibb</i>
Process Analytical Technology	James Rydzak , <i>Specere Consulting</i>
Raman Spectroscopy	Duncan Graham , <i>University of Strathclyde</i> ; Ian R. Lewis , <i>Kaiser Optical Systems</i> ; and Pavel Matousek , <i>Rutherford Appleton Laboratory</i>
Security and Forensics	Greg Klunder , <i>Lawrence Livermore National Laboratory</i> and Edita Botonjic-Sehic , <i>Implant Sciences Corporation</i>
Surface Plasmon Resonance	Jean-Francois Masson , <i>Université de Montreal</i>
Surface Science	Kateryna Artyushkova , <i>University of New Mexico</i>

2016 FACSS Executive Committee

Governing Board Chair	Steven Ray , <i>SUNY Buffalo</i> Email: sjray2@buffalo.edu
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GENERAL CHAIR, SciX



Mary Kate Donais
Saint Anselm College

Mary Kate Donais received her B.S. in chemistry from Bucknell University in 1991 and her Ph.D. in analytical chemistry from the University of Massachusetts, Amherst in 1996. After early career positions in both government (National Institute of Standards and Technology) and the instrument industry (VG Elemental), she joined the Saint Anselm College Chemistry Department in 1999 where she holds the position of Professor. The current focus of Dr. Donais' research is in applications of spectroscopy for cultural heritage analysis with a particular interest in portable instrumentation. She is a member of the American Chemical Society, Royal Society of Chemistry, Society for Archaeological Sciences, and the Society for Applied Spectroscopy. She has held many positions within the Society for Applied Spectroscopy including President and was named a Fellow in 2014.

PROGRAM CHAIR, SciX



Alexandra Ros
Arizona State University

Dr. Alexandra Ros is Associate Professor in the School of Molecular Sciences and faculty member of the Center for Applied Structural Discovery (CASD) at the Biodesign Institute. She received her Diploma in Chemistry from the Ruprecht-Karls University in Heidelberg, Germany, and her PhD from the Swiss Federal Institute of Technology, Lausanne, Switzerland. Since her PhD, Dr. Ros has been interested in microfluidic platforms and their analytical applications. Dr. Ros joined the Biophysics and Nanoscience Group at Bielefeld University, Germany, in 2000 where she followed her interests in microfluidics and biophysics during her post doctoral training. Since 2001, she served as principle investigator at Bielefeld University, Germany, on several projects investigating migration mechanisms and single cell analysis in the microfluidic format. In 2007, she finished her Habilitation and received the *Venia Legendi* in Experimental Physics from Bielefeld University. Dr. Ros joined Arizona State University in 2008 as Assistant Professor where she was promoted to Associate Professor in 2014. In the same year she was appointed faculty member of the Center for Applied Structural Discovery (CASD) at the Biodesign Institute. In 2015-16, Dr. Ros was appointed visiting scientist at the Georg-August University Goettingen, Germany. She received a NSF Career Award in 2012 as well as a Fellowship for Experienced Researchers from the Alexander-von-Humboldt Foundation, Germany, in 2015. Dr. Ros' current research interests include migration mechanisms in the micro- and nanoenvironment, single cell analysis, surface design and developing microfluidic tools for crystallography.

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 ultra-cooled gas phase molecules in a supersonic jet molecular beam. After graduate school, he 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. patents. After leaving EIC, he joined Chromex, Inc, a 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 the 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 member of the Governing Board. He has been serving as the FACSS/SciX Exhibits Chair since 2006. Dr. Carrabba has also been a member of the Society for Applied Spectroscopy (SAS) for almost 30 years and has served on several SAS committees including Awards (Chairperson), Membership and By-Laws. He has also been honored with the Distinguished Service Award in 2011 and was named a Fellow of the Society in 2012.

Dr. Carrabba has also received numerous awards for his service to the spectroscopic community. In 2003 he received the ASTM Award of Merit and became an ASTM Fellow 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 Award from FACSS in 2009. Dr. Carrabba is also a lifetime member of the Coblentz Society.

GOVERNING BOARD CHAIR, FACSS



Steven J. Ray
SUNY Buffalo

Steven Ray, Ph.D. is currently the Winkler Assistant Professor of Chemistry in the Department of Chemistry, State University of New York at Buffalo. Prior to serving as the FACSS governing board chairman for 2016-2017, Steven served as the SciX Program Chair, Atomic Section Chair, and Session organizer. He has published more than 100 manuscripts, book chapters, and patents. Steven serves on the Editorial Board of the *Journal of Analytical Atomic Spectrometry*, and the advisory boards of *Applied Spectroscopy*, *Analytical and Bioanalytical Chemistry*, *Spectrochimica Acta, Part B*, and *Spectroscopy* magazine. He was the recipient of a 2011 R&D100 Award, the 2013 Ron Hites Award for the best manuscript in *Journal of the American Society for Mass Spectrometry*, the 2014 SAS Lester Strock Medal, the 2015 *Analytical and Bioanalytical Chemistry* 'Best Paper' Award, and the 2016 Young Plasma Spectrochemist Award. His research interests involve novel aspects of analytical instrumentation, including distance-of-flight mass spectrometry, atomic spectroscopy, ambient mass spectrometry, plasma spectrochemistry, and metallomics methodologies. Steven lives in Buffalo, NY with his wife Jill, and sons Nico and Tim, where he enjoys snow.

PROGRAM and CONFERENCE SPONSORS

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DISTINGUISHED SERVICE AWARDS

*Awarded to an individual(s) for recognition of exceptional, long-term service to the FACSS organization.
The 2016 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, Nicollet B/C



John Chalmers
ICI plc, retired

John spent most of his career in industry. He was employed by ICI plc in the UK for 34 years working within the chemical company's research departments in the application and development of vibrational spectroscopy in support mainly of the company's research, production and development activities. He 'early retired' as a Business Research Associate at the end of 1999, thereafter setting himself up as a self-employed consultant specialising in vibrational spectroscopy. Additionally, he held part-time posts within the Department of Chemistry in the University of Nottingham from 2000-2010. John is a Fellow of The Royal Society of Chemistry, CChem FRSC. In 1994, he was the recipient of the Williams-Wright Award presented by The Coblenz Society for outstanding contributions in the 'Field of Industrial Infrared Spectroscopy', and in 2015 was made an honorary member of The Coblenz Society. John has served as President (2008) of the Society for Applied Spectroscopy (SAS) and was a founding member of the SAS UK regional Section, formed in 2010. For many years he served in various committee roles for the Royal Society of Chemistry Analytical Division (RSC AD) Molecular Spectroscopy Subject Group. From 2008-2015, he served as the RSC AD representative to FACSS. He has been an active member for many years of the U.K. Infrared and Raman Discussion Group (IRDG) for which he served as its Chair for a period of nine years. He has published over 50 peer-reviewed papers in scientific journals, and over 30 technical papers in conference proceedings or other specialised publications. He has co-authored one book, and additionally, he has edited or co-edited another 10 books/reference works, and, also, co-edited with Professor Peter Griffiths the highly acclaimed reference work the 5-volume *Handbook of Vibrational Spectroscopy* published in 2002; he has authored or co-authored 24 book chapters/reference works. Since 2000, he has been the Article Editor for the publication *Spectroscopy Europe*. As full retirement has increasingly loomed, John has become more focused on gardening and walking the beautiful UK Yorkshire dales and moors.



John Graham
INVISTA

Technical Director with experience in directing the operation and setting the strategic direction for the R&D support services groups (Analytical, bioanalytical, Engineering, and IT), and their application to methods development, product characterization, problem solving, and customer support. Management experience includes, budgeting, capital expense planning, liaison with product development teams, plant liaison, technical reporting, and LIMS. Management skills include well-developed communication, interpersonal and leadership skills. Results oriented team player who leads by example. Technical abilities consist of strong analytical and problem solving skills. Skills in analytical chemistry are current and specialize in

chromatography and molecular spectroscopy; GC, GC-MS, FT-IR, NIR, Raman, GC, HPLC, IC, fluorescence, UV-VIS, and color spectroscopy. Working knowledge of wet chemistry methods including: acid no., moisture, and Hach methods. Computer proficiency includes MS office, LIMS, OpenLab, Chromeleon, Omnic, VB programming, and selected lab instrument software.



James Rydzak
Specere Consulting

Jim is an independent consultant and founder of Specere Consulting. Jim was previously a Team Leader and Sr. Investigator who was responsible for the formation of the Process Analytical Technology (PAT) group at GSK. Jim joined the spectroscopy group at SmithKlineBeecham, now GlaxoSmithKline, in 1999 and became the PAT Team Leader in 2004. Jim also started the PAT group at Colgate-Palmolive, where he worked for 16 years, first as molecular spectroscopist, then starting the Process Analytical Group and later as a Group Leader and Analytical & Package Testing lab manager at the Mennen Consumer Product facility, a subsidiary of Colgate Palmolive. Jim's background in FT-IR, Raman and NIR spectroscopy and interest in real time analysis led him into the field of Process Analytical. Jim received his B.S. in Chemistry from Mount Union College in Alliance, Ohio and his M.S. in Analytical Chemistry working for Dr. Peter Griffiths at Ohio University. Jim has taught short courses in molecular spectroscopy for the Center for Professional Advancement for eight years in Amsterdam and New Jersey. Jim has also taught a short course entitled "Process Analytical Chemistry: Out of the Lab and into the Pipes" on PAT at the Federation of Applied Chemistry and Spectroscopy Societies (FACSS/SciX) Conference for ten years. Jim is active in presenting at and organizing sessions at SciX Conferences and has served as chair of the SciX program, FACSS Governing Board, Long range planning, sight selection, workshops and employment committee. He is a long time governing board member first serving on the board in 1996 representing the Coblenz Society. Jim was responsible for re-establishing the Process Analysis presence at the conference in the early 90's. Jim has been a long term SAS member and he is currently the past President of the Coblenz Society. Jim is a founding member of the ASTM E55 Committee for the Manufacture of Pharmaceuticals and has served as Executive Secretary and led a working group that wrote a Guidance standard for the Validation of PAT Applications and also is a member of the E13 Committee on Analytical Instrumentation. Jim has also authored a number of technical papers and presented many at the FACSS/SciX conferences over the years. Jim has founded a consulting company, Specere Consulting. His background in spectroscopy coupled with his extensive experience in Pharmaceutical, Consumer Health, Biopharmaceutical, Polymer and Chemical industries provides unique expertise to his consulting clients.

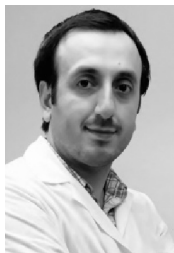
PREVIOUS AWARDEES

1993	Edward Brame and Syd Fleming	2010	Scott McGeorge and Alexander Scheeline	2015	Michael Blades, Gary Brewer and Keith L. Olson
1994	L. Felix Schneider	2011	Jon W. Carnahan and Patricia B. Coleman		
2001	David Coleman	2012	Bruce Chase and O. Karmie Galle		
2003	Jeanette Grasselli Brown	2013	Mark A. Hayes and Cynthia M. Lilly		
2009	Paul Bourassa and Mike Carrabba	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 AWARD



Mustafa Unal

Case Western Reserve University

Oral Presentation: Monday, 4:10 pm, Room Greenway G

Mustafa Unal earned his B.Sc. degree in mechanical engineering from Selcuk University in Turkey. His success in B.Sc. was recognized with M.Sc. and PhD fellowships from Turkish Government. In 2012, he received his M.Sc. degree from the University of Texas at San Antonio (UTSA), where he has been involved in musculoskeletal research for the first time. He is currently a PhD candidate under the supervision of Prof. Ozan Akkus at Case Western Reserve University (CWRU). During his first year at CWRU, he discovered the power of vibrational spectroscopy to assess the changes in the molecular constituents of musculoskeletal tissues due to diseases and aging which led him to focus his doctoral research efforts in the development of novel spectroscopic techniques as tools for assessment of bone and cartilage quality. His current research includes Raman spectroscopic analysis of the changes in composition of bone and cartilage with diseases and aging. More specifically, he has focused on developing novel Raman spectroscopic techniques to assess the involvement of water and collagen in bone and cartilage quality. He has recently developed Raman spectroscopy-based a novel nondestructive modality to assess

the hydration status in bone and cartilage. It was the first time in the literature that OH-stretching band region was characterized for bone and cartilage to identify different water compartments as a novel tool to assess bone and cartilage quality. He has further worked on several side projects including the novel use of Raman spectroscopic techniques for point of care testing devices such as diagnosis of microcrystals in urine for early detection of kidney stone and diagnosis of crystals-induced arthropathies. Up to now, he has published 6 peer-reviewed papers and 1 book chapter, and presented 14 poster/oral presentations in scientific conferences. He has been recognized as a promising young investigator in the field of biomedical vibrational spectroscopy and musculoskeletal research, as evidenced by several national and international prestigious awards, including Coblenz Student Award, SAS Barbara Stull Graduate Student Award, ORS Osteoarthritis Young Investigator Award, Baxter Young Investigator Award, The Victor M. Goldberg Award, and The George W. Codrington Charitable Foundation Student Research Award. He has also been selected as one of the ten finalists of 2016 CIMIT Student Technology Prize for Primary Healthcare.

FACSS AWARDS

FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS – Call for Applications for 2017

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 2017 conference in Reno, Nevada (October 8 - 13). In 2016 one FACSS Student Award 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 abstracts 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

- the form, available on the SciX website
- a 250 word abstract of the work to be reported
- 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
- a copy of the candidate's resumé
- a copy of the candidate's graduate transcript
- 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 2017. Go to www.scixconference.org to submit an application.

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



Kyle C. Doty
University at Albany

Oral Presentation: Wednesday, 4:50 pm, Room Greenway D

Kyle C. Doty completed a dual degree program at Buffalo State College (Buffalo, NY) in 2009 where he received a B.A. degree in Chemistry and a B.S. degree in Forensic Chemistry, with a minor in Criminal Justice. During his undergraduate studies Kyle performed research under the mentorship of Dr. Zeki Al-Saigh on projects involving the synthesis and analysis of biodegradable polymers. In the summer of 2008 Kyle participated in an American Chemical Society IREU (International Research Experience for Undergraduates) program where he performed organic synthesis research for a project dealing with supramolecular polymers. For this IREU program he worked with Professor Bruno Andrioletti at the Université Claude Bernard Lyon 1 in Lyon, France. Before entering graduate school Kyle worked for two years as a formulation scientist at Bausch + Lomb, Inc. (Rochester, NY). He is about to enter into his fifth year of the Chemistry doctoral program at the University at Albany where he is currently a Ph.D. candidate. He has recently received a prestigious National Institute of Justice STEM (Science, Technology, Engineering, and Mathematics) fellowship for carrying out novel research, under the mentorship of Dr. Igor K. Lednev, which will help to solve forensically-relevant problems related to bloodstains. Specifically, his graduate research projects utilize Raman spectroscopy and multivariate statistical analyses to analyze bloodstains to: determine the (a) time since deposition and (b) age of the blood donor, as well as differentiate human blood from that of (c) a variety of animal species' blood and (d) potential false positive substances. Kyle is also a 2016 recipient of the New York Society for Applied Spectroscopy graduate student award and the University at Albany Graduate Student Award for Excellence in Research.



Mario Saucedo-Espinosa
Rochester Institute of Technology

Oral Presentation: Tuesday, 4:40 pm, Room Nicollet B/C

Mario A. Saucedo-Espinosa received his B.Sc. in Chemical Engineering from the Autonomous University of Nuevo León (UANL), Mexico, in 2008. As an undergraduate student, he received the Academic Merit Award for the highest GPA in his class. His interest in computational modeling and optimization attracted him to obtain a M.Sc. in Systems Engineering from the same institution in 2012. His work, focused on the development of learning algorithms by means of Bayesian statistics and machine learning, was recognized nationwide with the Award to the Best Master Thesis on Artificial Intelligence, granted by the Mexican Society for Artificial Intelligence. As part of his graduate education, he was a visiting researcher at the Laboratory of Physics of Complex Systems at the University of Florence, Italy. Currently, Mario is a Ph.D. Candidate in Microsystems Engineering at Rochester Institute of Technology, where he joined the Microscale Bioseparations Laboratory under the supervision of Prof. Blanca Lapizco-Encinas. His current work, funded by both the National Science Foundation and the National Council for Science and Technology (CONACyT) of Mexico, focuses in the development of electrokinetic devices, with particular focus on insulator-based dielectrophoresis (iDEP), for the analysis of complex biological mixtures. His recent achievements include the design of optimal iDEP devices that reduce up to 84% the electric potential requirements without sacrificing performance, the design of a novel iDEP device that allows larger and more fragile particles/cells to be isolated promptly, and the development of a hybrid device that combines the advantages of iDEP with those of electrode-based dielectrophoresis. During his academic path, Mario has been the recipient of multiple awards, including a Fulbright-García Robles Scholarship, and First Places in the 2015 AES Electrophoresis Society Graduate Student Poster Competition and the 2016 AES/BioMicrofluidics Art in Science Competition.

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.

2015 INNOVATION AWARD WINNERS:

- SERS in Live 3D Cell Cultures as a New Tool for Drug Discovery; **Colin Campbell**, *University of Edinburgh*
- Five-dimensional Single Particle Tracking in Live Cells; **Ning Fang**, *Georgia State University*;

Thursday Afternoon, Nicollet B/C 2016 FACSS INNOVATION AWARD SYMPOSIUM

Organizer and Presider: Matthieu Baudelet

- | | |
|------|--|
| 3:50 | (944) Nanowell Sample Preparation Combined with Ultrasensitive LC- and CE-MS towards Single Cell Omics ; <u>Ryan Kelly</u> ¹ , Ying Zhu ¹ , Yongzheng Cong ¹ , Richard Smith ¹ ; ¹ Pacific Northwest National Laboratory |
| 4:10 | (945) An Inexpensive Medical Device for Barrett's Esophagus Screening ; <u>Rohith Reddy</u> ^{1,2} , Michalina Gora ^{1,2} , Jing Dong ^{1,2} , Matthew Beatty ² , Wolfgang Trasischker ^{1,2} , Kanwarpal Singh ^{1,2} , Amna Soomro ² , Catriona Grant ² , Mireille Rosenberg ² , Guillermo Tearney ^{1,2} ; ¹ Harvard Medical School; ² Massachusetts General Hospital |
| 4:30 | (946) Innovative Environmental Monitoring of Inorganic Compounds by means of 'Microalgae Sensors' ; <u>Frank Vogt</u> ¹ , Zachary Ogburn ¹ ; ¹ University of Tennessee |
| 4:50 | (947) Combining Functionalised Nanoparticles and SERS for the Detection of miRNA Biomarkers Related to Type 2 Diabetes ; <u>Laila Al Maqbali</u> ¹ , Karen Faulds ¹ , Duncan Graham ¹ ; ¹ University of Strathclyde |

FACSS CHARLES MANN AWARD

For Achievements in the Field of Applied Raman Spectroscopy

Brian J. Marquardt
University of Washington

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



Brian J. Marquardt, Director of the Center for Process Analysis and Control (CPAC) and Senior Principal Engineer at the Applied Physics Laboratory, University of Washington. Co-founder of MarqMetrix Inc., an optical sensor and instrumentation company focused on industrial process measurement and control. Research interests include the development and application of spectroscopic instrumentation, primarily Raman and LIBS, for continuous real-time chemical, biological and environmental analysis. Commercial technical motivation involves the design and implementation of novel fiber-optic Raman probes/sensors for real-time monitoring of industrial and environmental processes. Primary research focus is to understand the optical sampling characteristics of various spectroscopic techniques to improve measurement precision, accuracy and stability for improved process understanding and control.

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.

2016 Award Recipient
Patrick D. Barnett

Implementation of a Cell Phone Camera as a Detector for a Miniature Spatial Heterodyne Raman Spectrometer;
Patrick D. Barnett¹, S. Michael Angel¹; ¹University of South Carolina

Presentation Monday 2:00, Lakeshore A



Patrick D. Barnett is a Ph.D. candidate in analytical chemistry at the University of South Carolina working with Professor S. Michael Angel, and is expected to graduate in December 2016. Patrick earned his B.S. in Chemistry at the University of Central Missouri in 2011. As an undergraduate, Patrick's research focused on the development of a coulometric-based method to investigate the ability of several varieties of switchgrass (*Panicum virgatum*) to sequester atmospheric carbon dioxide into soil. Currently, Patrick's research is focused on developing a miniature, millimeter-scale, spatial heterodyne Raman spectrometer (SHRS), a dispersive interferometer, for use in Raman experiments for extreme environments, including planetary exploration. Patrick has demonstrated the first use of a standard cell phone camera as a detector for a miniature SHRS for Raman measurements of a variety of samples. He demonstrated the first measurements of standoff laser-induced breakdown spectroscopy (LIBS) with a miniature SHRS. Additionally, he developed a new method of applying the Fourier transform to the interference pattern generated by the SHRS to correct optical alignment errors. Patrick received the North American Society for Laser-Induced Breakdown Spectroscopy Student Presentation Award for a paper presented at SciX 2015. He also received the Dr. James R. Durig Graduate Student Travel Award twice, 2015 and 2016.

2016 CASSS STUDENT AWARDS

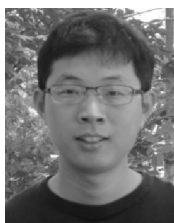
CASSS and FACSS have teamed up to provide a limited number of travel grants to help students attend the SciX/ITP conference in 2016. Award Winners receive \$500 in travel support from CASSS, plus a discounted hotel rate and a complimentary conference registration. CASSS is a global community of industry, academic and regulatory professionals who work together to resolve scientific challenges in the field of biopharmaceutical development and regulation.



Pranav Agrawal,
University of Minnesota



Sarah Alharthi,
Oklahoma State
University



Pengfei Niu,
NIST



Amar Oedit,
Leiden University



**Rosilene Cristina
Rossetto Burgos,**
Leiden University



DISTINGUISHED SERVICE AWARD

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



James A. de Haseth

LLS Instruments

James de Haseth received his B.S. in Chemistry from the University of Illinois at Chicago in 1972 and his Ph.D. in Analytical Chemistry from the University of North Carolina at Chapel Hill in 1977. Jim studied with Thomas L. Isenhour and his main interest of study was computerized information retrieval from spectrometric data. It was in graduate school that Jim became interested in Fourier transform infrared (FT-IR) spectrometry and decided to pursue further studies in vibrational spectrometry. This led to an eighteen-month postdoctoral research position with Gleb Mamantov at the University of Tennessee where Jim studied time-resolved FT-IR spectrometry involving fluorine-based reaction chemistry.

In 1979 Jim accepted a position as an Assistant Professor of Chemistry at the University of Alabama. He moved to the University of Georgia in 1983, where he was later promoted to Professor of Chemistry. Research interests have involved numerous projects in vibrational spectrometry, and include gas and liquid chromatographic interfaces as well as capillary electrophoretic interfaces to FT-IR spectrometers, vibrational circular dichroism, protein structure by infrared spectrometry, and the use of infrared fibers for the study of reaction kinetics. Research interests also focused on the design and development of field deployable spectrometers in the ultraviolet through mid-infrared spectral regions.

In 2009 Jim retired from the University of Georgia and co-founded a consulting group, Light Light Solutions, LLC, with three scientists from the Agricultural Research Service of the USDA (Franklin Barton, David Himmelsbach, and Dan Akin) as well as with Curt Marcott from Proctor and Gamble. In 2011 Jim and Franklin Barton spun off an instrument company, LLS Instruments, Inc., to develop a field-portable NIR spectrometer. The unit is designed to measure large areas to provide more accurate analyses of sample components. Commodities measured include living plants, bales, products on conveyor belts, and materials in vehicles, such as trucks, railroad cars, and ship holds. Work with the instrument has been in the fiber, rubber, and sugar industries to name a few, in the US, Canada, and Australia.

Jim became a member of SAS in 1978 and has held several positions within the Society. He has been a member of the Coblentz Society since 1980 and was named an Honorary Member in 2011. Since 1974 Jim has been a member of the American Chemical Society and is also a member of the Council on Near Infrared Spectroscopy.

Jim remains active in teaching and is an instructor for IR Courses, Inc. That organization regularly conducts courses for the interpretation of infrared and Raman spectra. Three such courses were taught in 2016 in Texas, the United Kingdom and Maine. In addition, since 1982 Jim has taught numerous vibrational spectroscopy short courses for the Society for Applied Spectroscopy, FACSS, the Pittsburgh Conference, and for several overseas organizations. Jim is co-author with Peter R. Griffiths for the treatise "Fourier Transform Infrared Spectrometry," John Wiley & Sons, New York, 1986, and the second edition, 2007.

HONORARY MEMBERSHIP AWARD

Recognizing those individuals who have made exceptional contributions to spectroscopy.



Sanford A. Asher

University of Pittsburgh

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, and 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 2016 SAS Honorary Membership Award, 2016 Society of Analytical Chemists of Pittsburgh (SACP) Award in Analytical Chemistry, 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 Coblenz 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 an 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 295 publications and is the inventor in over 29 patents in the area of photonic crystals.

Future SciX Meeting: October 8 – 13, 2017, Reno, Nevada



Jaan Laane

Jaan Laane was born in Estonia in 1942 but fled with his family from the Soviets in 1944, winding up in a displaced persons camp in Germany. In 1949 the family immigrated to the USA, settling in the small town of Polo, Illinois. Jaan graduated high school as class valedictorian and then attended the University of Illinois as a Sloan Scholar and James Scholar. He graduated with Highest Distinction in Chemistry in 1964 receiving the Kendall Award as the top chemistry major. He then carried out graduate work at MIT with Richard C. Lord as a National Science Foundation and Woodrow Wilson Fellow, receiving his Ph.D. and the Kodak Award as the top graduate student in 1967.

Following a year at Tufts University, Jaan moved to Texas A&M University where he soon was promoted to Full Professor (1976). His research focused on the determination of vibrational potential energy surfaces in both ground and excited electronic states. He has contributed to the theoretical understanding of molecular vibrations and structures and to the experimental methodology in these areas. He has more than 300 publications and three books. He has been in the forefront of writing computer programs for analyzing potential energy surfaces. These have been widely distributed and utilized. Laane has supervised the research of more than 40 Ph.D. students, 60 undergraduates, and dozens of post-docs and visiting professors. He has received the Humboldt Award, a Texas A&M teaching award and the Lippincott Award among others. He was Chair of the Physical and Nuclear Chemistry Division for many years and Associate Dean of Science and Speaker of the Faculty Senate. Since 1994 Laane has been Editor for the Journal of Molecular Structure.

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

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.



S. Roy Koirtyohann

S. Roy Koirtyohann was born Sept 11, 1930, the seventh of nine children by Earl and Carrie Koirtyohann. He was raised on their farm near Washington MO and graduated from Washington High School in 1949. He enrolled in the University of Missouri (MU) that fall, majoring in Agricultural Chemistry and became like the bad penny that could not be thrown away for MU. After graduation in 1953 he was on active duty in the army for two years before returning to MU for a Master's Degree under E. E. Pickett. He then worked at Oak Ridge National Laboratory for four years before returning to MU once more for the PhD and a faculty position.

His research activities resulted in nearly 100 publications in journals such as Applied Spectroscopy, Analytical Chemistry, and Spectro Chimica Acta as well many oral presentations at national and international conferences. Accomplishments include measurement of the free atom fraction for analytes in flames, identification of the cause for background problems in flames used for AA, and invention of continuum source background correction in AA.

He became active in the St. Louis SAS section while in graduate school. As his career progressed he became a very active participant and organizer for conferences such as FACSS which included SAS as a sponsor. He was SAS President in 1990.

He retired in 1995 after 32 years on the MU faculty. Roy and his wife, Laura, then moved to their 165 acre farm (Roy's playground) and started collecting, restoring, and showing antique agricultural equipment. Caring for the farm eventually got to be too much and they moved to a modest house on 5 acres a few miles North of Columbia, MO. Roy still tinkers with the remnants of his collection and does some gardening. Both he and Laura remain in good health for their age. On March 7th, 2016 they celebrated their 64th wedding anniversary.

LESTER W. STROCK AWARD

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



Raymond Arvidson

Washington University in Saint Louis

Presentation: Thursday, 8:00 am, Nicollet B/C

Raymond Arvidson received a Ph.D. from Brown University in 1974. He is presently the James S. McDonnell Distinguished University Professor Washington University in St. Louis, where he focuses on teaching and research about current and past environments on the Earth, Mars, and Venus. He is a fellow of the McDonnell Center for the Space Sciences. He has been instrumental in development and implementation of both orbital and landed missions to the planets, including participation in the Magellan Radar Orbiter Mission to Venus, Team Leader for the Viking Lander Imaging System on Mars, member of the Project Science Group for the Mars Global Surveyor Mission, Deputy Principal Investigator for the highly successful Mars Rover Missions (Spirit and Opportunity), the Robotic Arm Investigator for the Mars Phoenix Lander Mission, Co-Investigator for the hyper-spectral mappers OMEGA (Mars Express orbiter) and CRISM (Mars Reconnaissance Orbiter), and a Science Team Member for the Mars Science Laboratory Curiosity Rover that landed on Mars in August 2012. He is the Director of the NASA Planetary Data System Geosciences Node, making available ~300 terabytes of NASA data to the worldwide research community. He is a Fellow of the Geological Society of America and the American Geophysical Union (AGU), received the AGU Whipple Award, has been honored as the Missouri Teacher of the Year, has been honored with three NASA Public Service Medals, and several dozen NASA citations for excellence. He has received several awards from Washington University in Saint Louis for research and teaching excellence.

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

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



Mustafa Unal

Case Western Reserve University

Mustafa Unal received his B.Sc. in mechanical engineering at Selcuk University in Turkey. He is currently a PhD candidate under the supervision of Prof. Ozan Akkus at Case Western Reserve University (CWRU). His current research focuses on Raman spectroscopic analysis of the changes in composition of bone and cartilage with diseases and aging. More specifically, he has focused on developing novel Raman spectroscopic techniques to assess the involvement of water and collagen matrix in bone and cartilage quality. He has recently developed Raman spectroscopy-based a novel nondestructive modality to assess the hydration status in bone and cartilage by developing a customized short wave infrared spectrometry system that is optimized to probe the water region in biological tissues. He was the first person to characterize OH-stretching bands of bone and cartilage to identify different water compartments as a novel tool to assess bone and cartilage quality. He has further worked on several side projects, including the novel use of Raman spectroscopic techniques for point of care testing such as diagnosis of microcrystals in urine for early detection of kidney stone and diagnosis of crystals-induced arthropathies. Since 2014, he has published 6 peer-reviewed articles, 1 book chapter, and presented 14 poster/oral presentations in scientific conferences. He has received several national and international prestigious awards, including FACSS Student Award, Coblenz Student Award, Baxter Young Investigator Award, ORS Osteoarthritis Young Investigator Award, The Victor M. Goldberg Award, and The George W. Codrington Charitable Foundation Student Research Award. He has also been selected as one of the ten finalists of 2016 CIMIT Student Technology Prize for Primary Healthcare.



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 18, 2016, 7-9 p.m. *(during the SciX mixer)*

Sponsored by
The Society for Applied Spectroscopy and SciX

WILLIAM F. MEGGERS AWARD

*Recognizing the author(s) of an outstanding paper appearing in
Applied Spectroscopy
Presented for "Probing Organometallic Reactions by Time-
Resolved Infrared Spectroscopy in Solution and in the Solid State
Using Quantum Cascade Lasers" Volume 69, Issue 5, (May 2015),
pp 519-524.*



Mike George

Nottingham University

Presentation: Wednesday, 8:30 am, Room Nicollet B/C

Mike George received a PhD from the University of Nottingham under the supervision of Professor Martyn Poliakoff FRS and remained at Nottingham for 18 months where he began a very fruitful collaboration with Professor Jim Turner FRS in the area of using fast infrared spectroscopy for monitoring electron transfer in inorganic excited states. Fast infrared spectroscopy has continued to be a central feature of his research. He was awarded a Royal Society/STA of Japan postdoctoral fellowship to probe organic excited states with Professor Hiro-o Hamaguchi. He returned to Nottingham as an Experimental Officer (1993) and was promoted to Research Officer (1996), lecture (1998), reader (2001) and professor (2003). Over the past two years he has taken a 50% secondment to be Vice-Provost for Research and Knowledge Exchange at the University of Nottingham Ningbo China. Many of his research interests combine photochemistry, fast time-resolved infrared spectroscopy (TRIR) and instrument development particularly focused at elucidating inorganic, organic and biological reaction mechanisms. He is particularly interested in the coordination and reactivity of small molecules such as CO₂ and alkanes and noble gases including studies focusing on the factors affecting C-H activation. He is currently working in a consortium applying time-resolved X-ray measurements at the Research Complex at Harwell. He was involved in the development of two national facilities (PIRATE and ULTRA) at the Rutherford Appleton laboratory, Oxford and the latter facility is currently underpinning a range of ultrafast science in the UK. He also works in a range of other areas of analytical chemistry particularly combining using vibrational spectroscopic studies with supercritical fluids ranging from phase measurements associated with Carbon Capture and Storage (CSS) to new ways synthesizing antimalarial drugs for the developing world. His work has been recognised by several awards including Royal Society of Chemistry Sir Edward Frankland Fellowship (2002/3); Corday-Morgan medal (2003), Photochemistry Award (2005) and Inorganic Reaction Mechanisms Award (2013) together with Horiba award (2005); Seaborg Lectureship UC Berkeley (2010) and the Craver award (2011) from The Coblenz Society. He was Programme Chair for SciX in Milwaukee (2013) and ICAVS-8 (2015). He is on the Editorial Board of Applied Spectroscopy and he has also served on the committee of the Infrared and Raman Discussion Group (IRDG) since 1999.

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*



Keshav Kumar

Umea University

Award Session: Wednesday 3:50, Nicollet D2/D3

Keshav Kumar obtained his M.Sc. and Ph.D. from Department of Chemistry, Indian Institute of Technology-Madras, India, in year of 2008 and 2014, respectively. His PhD research work was focused on integrating the chemometric methods with Total Synchronous Fluorescence Spectroscopy (TSFS). He showed that TSFS data structure is intrinsically different and a better understanding is required for its integration with different chemometric techniques. One of his most significant contributions in this area is to prove that TSFS data set lacks the trilinear structure and must not be subjected to the parallel factor (PARAFAC) analysis. He has also successfully proposed a scheme that provides a computationally economical way of achieving trilinear decomposition of TSFS data sets using PARAFAC analysis. He has been successful in studying various aspects of performing Multivariate Curve Resolution Alternating Least Square (MCR-ALS) analysis of TSFS data sets. In a comparative study, he found that combination of chemometrics and TSFS provide quite a few significant analytical advantages over combination of excitation-emission matrix fluorescence (EEMF)-chemometrics for the analyses of dilute aqueous multifluorophoric mixtures.

He received the Best PhD and MSc Thesis award, from Department of Chemistry, Indian Institute of Technology-Madras. He received KBC postdoctoral fellowship from Kempe Foundation, Sweden in 2015 and since then he is working as a postdoctoral researcher at the Department of Molecular biology, Umea University, Sweden. His current research mainly deals with the application of advanced chemometric methods on the chromatographic and mass spectrometry data sets to identify the novel bacterial cell wall targets.

SAS FELLOWS AWARD

Recognizes individual members for their outstanding service to the field of spectroscopy and the Society for Applied Spectroscopy.



Mike Angel is a Professor of Chemistry at the University of South Carolina where he has held the Fred M. Weissman Palmetto Chair in Chemical Ecology since 2005. He received his PhD from North Carolina State University in 1985 and carried out Postdoctoral work with Tomas Hirschfeld at Lawrence Livermore National Laboratory. Angel's research group works mainly in the areas of remote and in-situ laser spectroscopy with a focus on deep-ocean, planetary, and homeland security applications of Raman and LIBS. Recent work includes developing the spatial heterodyne Raman spectrometer (SHRS) and exploring its use for deep UV Raman, standoff Raman and for use on future planetary landers and SmallSats.

Angel is a member of the Mars 2020 SuperCam science team and is an elected Fellow of AAAS. He has been a SAS Tour speaker, an A-Page Advisory Panel member for Analytical Chemistry and on the editorial advisory boards of Talanta and the International Journal of Spectroscopy, and a member of the scientific committee of NASLIBS and the International LIBS conference. Other honors include the 2015 Southern Chemist Award, 2012 Applied Spectroscopy William F. Meggers Award, 2012 ACS South Carolina Chemist of the Year Award, 2011 Federation of Analytical Chemistry & Spectroscopy Societies (FACSS) Innovation Technology Award, and 2006 Lawrence Livermore National Laboratory Physics and Advanced Technologies Directorate Award



Jaan Laane was born in Estonia in 1942 but fled with his family from the Soviets in 1944, winding up in a displaced persons camp in Germany. In 1949 the family immigrated to the USA, settling in the small town of Polo, Illinois. Jaan graduated high school as class valedictorian and then attended the University of Illinois as a Sloan Scholar and James Scholar. He graduated with Highest Distinction in Chemistry in 1964 receiving the Kendall Award as the top chemistry major. He then carried out graduate work at MIT with Richard C. Lord as a National Science Foundation and Woodrow Wilson Fellow, receiving his Ph.D. and the Kodak Award as the top graduate student in 1967.

Following a year at Tufts University, Jaan moved to Texas A&M University where he soon was promoted to Full Professor (1976). His research focused on the determination of vibrational potential energy surfaces in both ground and excited electronic states. He has contributed to the theoretical understanding of molecular vibrations and structures and to the experimental methodology in these areas. He has more than 300 publications and three books. He has been in the forefront of writing computer programs for analyzing potential energy surfaces. These have been widely distributed and utilized. Laane has supervised the research of more than 40 Ph.D. students, 60 undergraduates, and dozens of post-docs and visiting professors. He has received the Humboldt Award, a Texas A&M teaching award and the Lippincott Award among others. He was Chair of the Physical and Nuclear Chemistry Division for many years and Associate Dean of Science and Speaker of the Faculty Senate. Since 1994 Laane has been Editor for the Journal of Molecular Structure.



Barry K. Lavine is a Professor of Chemistry at Oklahoma State University where he both teaches and performs research in analytical and forensic chemistry. Lavine's research interests encompass many aspects of chemical analysis including vibrational spectroscopy (both infrared and Raman), infrared imaging, and the applications of pattern recognition, multivariate curve resolution, and multivariate calibration using genetic algorithms and other evolutionary optimization techniques to chemical analysis. Currently, Lavine's research activities are focused on the development of search algorithms for samples with similar IR spectra under sparse sample and data conditions. Lavine is also investigating the decantation of infrared image data of cross sectioned layers (prepared using a microtome) to obtain a pure IR spectrum of each layer. This methodology is currently being evaluated using automotive paints, which are well-suited to the exploration and application of concatenation-decantation methods because a large database of pure IR spectra from automotive paint systems exists.

Lavine has published more than 100 research papers, 20 book chapters, 16 review articles, and editor for 3 ACS monographs, is on the editorial board of several journals including the Journal of Chemometrics, Microchemical Journal, Chemoinformatics and Analytical Letters and has served as Chair of the Northern New York (1997-2004) and the Oklahoma (2006-2008) sections of the American Chemical Society. Lavine has been Program Chair and General Chair for several scientific meetings including Program Chair of FACSS (1992), Northeast Regional ACS Meeting (1999), and the Pentasectional Meeting of the local Oklahoma Sections of the American Chemical Society (2005).



R. Kenneth (Ken) Marcus, Ph.D., is Professor of Analytical Chemistry at Clemson University, beginning his tenure in 1986. 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 a dozen 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 34 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 also been honored as a Fellow of the Royal Society of Chemistry and the American Association for the Advancement of Science.

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 Cleveland Regional Section

The SAS Cleveland Section is being recognized as this year's outstanding section for maintaining a consistently high level of activity throughout the year and completing a large number of projects which furthered the mission and goals of SAS. These projects included the 59th annual May Conference, which included a full day of programming with three parallel sessions and several plenary/invited talks and award presentations. The conference fostered communications between members, students, and equipment vendors. The Section organized the event in conjunction with the local ACS and AVS sections and the Microscopy Society, and was able to obtain 28 (!) industrial sponsors. The latter achievement, in particular, is a strong example of the success that regional sections can have in finding financial support for projects.

Other Cleveland Section activities included seven monthly meetings, several of which featured speakers from outside the Section's boundaries, and a number of educational outreach presentations. Of the latter, one activity of note was the "Spectroscopy for Kids" program, which reached a total of ~1800 students (elementary to high school) at 10 different events, and included a teacher training workshop.



*The Society for Applied Spectroscopy
Cordially Invites All SAsS Members
to Join Us at Our Annual
Wine and Cheese Awards Reception
Tuesday, September 20, 2016 7:30 p.m.
Hyatt Regency Hotel
Great Lakes Ballroom B/C*

This is a member's only event.

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 Coblenz 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 Coblenz 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 Coblenz Society Craver Award.



Karen Faulds

University of Strathclyde

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



Karen Faulds' research involves the development of surface enhanced Raman scattering (SERS) for novel analytical detection strategies and in particular multiplexed bioanalytical applications. SERS is a spectroscopic technique that offers significant advantages over other established techniques such as fluorescence and her research has highlighted these advantages by creating new examples of increased capability predominantly in healthcare applications. Karen Faulds received her PhD from the University of Strathclyde under the supervision of Prof Ewen Smith in 2003 on the detection of drugs of abuse using SERS. She was appointed as a full time lecturer in Chemistry at the University of Strathclyde in 2006 and due to her sustained research achievements promoted to Senior Lecturer in 2010, Reader in 2012 and full Professor in 2015. She is currently training 8 PhD students and 2 PDRA as principal supervisor and, as part of the large team ethos she embraces, she is also co-supervisor to another 16 PhD students and 6 PDRAs. She currently holds research funding of £9M

as both Principal Investigator and Co-Investigator. She has published over 100 peer reviewed primary publications, 20 peer reviewed conference proceedings, 7 invited book chapters, 3 editorials and 5 patents. In 2009 she was presented with the *Nexxus Young Life Scientist of the Year award* and in 2011 was elected to the *Royal Society of Edinburgh Young Academy of Scotland*, the first such Academy amongst the national academies in the UK and was elected *Fellow of the Royal Society of Chemistry* in 2012. She was awarded the *2013 RSC Joseph Black Award* for her '*outstanding contributions focused on the quantitative analysis of biomolecules using surface enhanced Raman scattering (SERS)*'. The Joseph Black Award is awarded to a young scientist, within 10 years of PhD award, in any field covering the practice and teaching of analytical science. Due to her contributions to the vibrational spectroscopic community she has recently been elected as the first female and youngest Chair of the Infrared and Raman Discussion Group (IRDG) which is the oldest spectroscopic discussion society in the UK. She is also the Strathclyde Director of the Centre for Doctoral Training (CDT) in Optical Medical Imaging (Optima) where she is responsible for the Strathclyde leadership of the Centre, with a support team of an administrator and an outreach officer, as well as an intake of 60 PhD students between the Universities of Strathclyde and Edinburgh over a 5-year period. She currently serves as an editorial advisory board member for the RSC journal *Analyst*.

As a result of her outputs, she has received a number of invitations to speak at prestigious international conferences. This includes over 70 national and international conferences with over 50 as an invited speaker including Thailand, Japan, China, Russia and the USA. As part of her contribution to the subject area, she has also been on the organising committee for several conferences such as the RSCs Analytical Research Forum, Nano Meets Spectroscopy, regularly organises IRDG meetings and Martin and Willis student meetings as well as organising the IRDG Raman Symposium at SciX.

The Coblentz Society call for Award Nominations.

Visit www.coblentz.org 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 3rd - July 15th**.

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 1st**

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 1st - May 1st**

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 contribution to the field of vibrational spectroscopy or any other field related to the purposes of the Society. Nominations close on February 1st each year, with the awards announced at the Annual Members Meeting at Pittcon and presented at SciX. Please send your nominations to Mark Drury, Coblentz Society President at madrury@gmail.com

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 Coblenz 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 Coblenz 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.



2016 Coblenz Society's William G. Fateley Student Awardee and Student Award – Mustafa Unal



Mustafa Unal received his B.Sc. degree in Mechanical Engineering from Selcuk University in Turkey. His success in B.Sc. was recognized with M.Sc. and PhD fellowships from Turkish Government. He is currently a PhD candidate under the supervision of Prof. Ozan Akkus at Case Western Reserve University. His current research includes Raman spectroscopic analysis of bone and cartilage with diseases and aging. He has recently developed Raman spectroscopy-based a novel nondestructive modality to assess hydration status in bone and cartilage. It was the first time in the literature that OH-stretching band region was characterized for bone and cartilage to identify different water compartments as a novel tool to assess bone and cartilage quality. He further works on several side projects including the novel use of Raman spectroscopic techniques for point of care testing devices such as diagnosis of crystals in urine for early detection of kidney stone formation and diagnosis of crystals-induced arthropathies. Since 2014, he has published 6 peer-reviewed articles, 1 book chapter, and presented 13 poster/oral presentations in scientific conferences. He has been recognized as a promising young investigator in the field of biomedical vibrational spectroscopy and musculoskeletal biomechanics, as evidenced by several national and international prestigious awards, including FACSS Student Award, ORS Osteoarthritis Young Investigator Award, Baxter Young Investigator Award, The Victor M. Goldberg Award, and The George W. Codrington Charitable Foundation Student Research Award. He has been also selected as one of the ten finalists of 2016 CIMIT Student Technology Prize for Primary Healthcare.

The Coblenz Society call for Award Nominations.

Visit www.coblenz.org for more information



- Fateley Student Award
- Coblenz Student Awards

In addition to Awards for professionals in industry, academia and government laboratories, the Coblenz Society encourage young scientists to pursue studies in all areas of vibrational spectroscopy through the presentation of Student Awards. The Coblenz Student Award recognizes excellence in research involving vibration spectroscopy and/or coursework including vibration spectroscopy. The three leading graduate students selected by the Coblenz 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.

Coblenz and William G. Fateley Awards – The Coblenz Society seeks nomination of outstanding students for the Coblenz student awards. Nominations by e-mail are preferred and may be sent to the Chair of the Coblenz Student Affairs Committee, Prof. Christian Pellerin, at c.pellerin@umontreal.ca. Graduate or undergraduate students who have shown excellence in vibrational spectroscopy research and/or coursework including vibrational spectroscopy may be nominated. The nominations window for Coblenz 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.coblenz.org/awards>.

COBLENTZ SOCIETY 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*.



Alyssa Cassabaum received her B.S. in Chemistry in 2011 from Hope College in Holland, MI. Before attending graduate school, she worked as a visiting scientist under Dr. JoAnn Buscaglia in the Counterterrorism and Forensic Science Research Unit at the Federal Bureau of Investigation. While at the FBI her research was focused on differentiating copper samples by their trace element signatures using

ICP-MS. Alyssa is currently a chemistry PhD student in Dr. Renee Frontiera's research group at the University of Minnesota. She is interested in studying charge-transfer mechanisms and structural dynamics of organic photovoltaics by femtosecond stimulated Raman spectroscopy.



Emily L. Keller received her B.S. in Chemistry with Honors from the University of Texas at Austin in 2013. As an undergraduate, she studied how the composition of dendrimer-encapsulated metal nanoparticles affected their ability to catalyze the reduction of p-nitrophenol with sodium borohydride. She then continued her studies in Chemistry at the University of Minnesota's Chemistry Ph.D. program with Prof. Renee Frontiera. Her current work

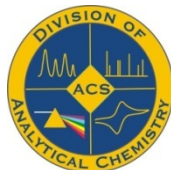
examines how plasmon excitation can affect ultrafast transient surface-enhanced Raman scattering signal and how it relates to hot electron generation from the plasmonic substrate. She wrote a review in *Analyst* on ultrafast surface-enhanced Raman spectroscopy as the first author in 2015 and received an Honorable Mention from NSF's Graduate Research Fellowship Program in 2014.



Aashish Tuladhar earned his B.S. in Chemical Engineering (with Mathematics and Chemistry minors) in 2010 at Villanova University and was invited to be a member of TAU BETA PI (an engineering honor society) in recognition his academic accomplishments. During his junior year, he joined his first research group led by Prof. Robert Giuliano where he was introduced to the field of spectroscopy while investigating

the properties of carbohydrate-functionalized graphite nano-fibers using FLOSS (fluorescent labelling of surface species). This led to him changing his field and joining the graduate program at Temple University, where is pursuing a Ph.D. in Chemistry under the supervision of Professor Eric Borguet.

Aashish is currently the team leader of the non-linear optics group where they use surface sensitive techniques to investigate the interfacial environment. His graduate research has been focused on understanding the structure and dynamics of water at mineral surfaces (mainly silica and alumina) using non-linear spectroscopy techniques, e.g., steady-state and time-resolved vibrational sum frequency generation (vSFG). He has also been involved in the construction of ultra-broadband, ultra-short mid infrared sources by employing non-collinear optical parametric amplification (NOPA) technology in bulk non-linear crystals. The goal here is to have two independent mid IR sources in order to perform two-color narrowband IR pump – broadband vSFG probe experiments, which is close to completion. Additionally, Aashish has detected interfacial OH stretch overtones from silica/water interface using novel vibrationally resonant near IR second harmonic generation spectroscopy. As of now, Aashish has 2 peer-reviewed articles published, one more recently submitted, and few more in preparation. He has presented his work at the Gordon Research Conference/Seminar (GRC/GRS) and the Time-Resolved Vibrational Spectroscopy (TRVS) conference. Aashish has also been invited to give guest lectures on non-linear optics in undergraduate and graduate classes in the Chemistry and Physics Departments at Temple University. Aashish has also undertaken the responsibility of mentoring new graduate and undergraduate students in the field of interfacial laser spectroscopy.



Call for Nominations
ACS Division of Analytical Chemistry Awards 2017
 Deadline: November 1, 2016

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 2017 Awards, nominations shall be sent by email or postal mail no later than November 1, 2016 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.**

IRDG CHALMERS AND DENT STUDENT AWARD

The Chalmers and Dent Student Travel Award has been established to recognise and support an outstanding PhD student through financial support to present their research to an international audience at the annual SciX meeting. The award is named after two previous chairs of the IRDG, John Chalmers and Geoff Dent, in recognition of their continuing support for the IRDG and in particular for their support of students and early career researchers. Throughout their careers, both John and Geoff have been highly active in the development and promotion of the vibrational spectroscopists of the future in both academia and industry through mentoring, encouragement and inspiration.

**2016 IRDG Chalmers and Dent Student Award Recipient**

Carl Mensch, *University of Antwerp*



Carl Mensch obtained his Master's degree in Chemistry from the University of Antwerp in June 2013. During his undergraduate studies, Carl's passion for science was further developed throughout his summer jobs at the Molecular Spectroscopy Group in Antwerp, where he was introduced to the world of vibrational optical activity. Particularly, the symbiosis of theoretical and experimental approaches in physical chemistry sparked his interest.

In his Master thesis work under the supervision of Prof. dr. Christian Johannessen, Carl became submerged in the world of Raman optical activity (ROA) and the application of this spectroscopic technique to the structural studies of proteins and other biomolecules. This initial work paved the way to a PhD in the Molecular Spectroscopy Group, where Carl currently is investigating the detailed relations between the ROA spectral patterns of proteins and how these can be informative about the solution structure of proteins. Ultimately, making detailed spectral assignments might aid in the comprehension of the poorly understood intrinsically disordered proteins that play central roles in the pathogenesis of Alzheimer's and Parkinson's disease, which is the key goal of Carl's PhD.

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.



Paul Cremer
Pennsylvania State University



Presentation: Wednesday, 8:00 am; Nicollet B/C

Paul Cremer received his Ph.D. in Chemistry in 1996 at the University of California – Berkeley. He then spent two years as the Irving S. Sigal Postdoctoral Fellow at Stanford University before beginning his own independent research career in 1998 at Texas A&M University, where he became a distinguished professor and Arthur E. Martell Chair of Chemistry. In 2013, he moved to Penn State University as the J. Lloyd Huck Chair in Natural Sciences where he currently holds appointments in the Department of Chemistry and the Department of Biochemistry and Molecular Biology. His research is at the cross roads of physical chemistry, analytical chemistry, biochemistry, materials science and engineering. His group has exploited linear and non-linear vibrational spectroscopies to follow the interactions of ions with peptides, proteins, and macromolecules. This has helped unravel the molecular level mechanisms of the Hofmeister series, a rank ordering of how salt ions affect the physical behavior in mixtures of water, organics, and salts. His group has also invented a wide variety of high throughput, low sample volume microfluidic techniques. For example, he is the inventor of temperature gradient microfluidics as well as pH modulation sensing for the label free detection of peptide, small molecule, ion, and protein binding at lipid membrane interfaces. Most recently, his laboratory has pioneered studies of the metallomembrane, including the tight binding of Cu^{2+} and other first row transition metal ions to lipids in bilayer membranes containing amine groups such as phosphatidylserine and phosphatidylethanolamine.

Cremer has written over 125 papers and given over 250 invited lectures. He is the recipient of numerous awards including the Beckman Young Investigator Award, the Pittsburgh Conference Achievement Award, a Sloan Fellowship, a Dreyfus Fellowship, the Norman Hackerman Award in Chemical Research, and the Edith and Peter O'Donnell Award in Science. He is currently an associate editor for *J. Am. Chem. Soc.* as well as a fellow of the American Chemical Society and the American Association for the Advancement of Science.

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.



Amy E. Herr
University of California, Berkeley



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

Amy E. Herr is the Lester John & Lynne Dewar Lloyd Distinguished Professor of Bioengineering at the University of California, Berkeley. Prof. Herr joined UC Berkeley as Assistant Professor of Bioengineering in 2007, was promoted to Associate Professor with tenure in 2012, and promoted to Full Professor in 2015. Prior to joining UC Berkeley, she was a staff member in the Biosystems Research Group at Sandia National Laboratories (Livermore, CA; 2002-2007). She earned her PhD in Mechanical Engineering at Stanford with Profs. Tom Kenny & Juan Santiago as an NSF Graduate Research Fellow, an MS in Mechanical Engineering also from Stanford, and a BS in Engineering & Applied Science from Caltech.

Professor Herr is an elected Fellow of the American Institute of Medical and Biological Engineering (AIMBE), a Board Member of the Chemical & Biological Microsystems Society (CBMS) which oversees the microTAS conferences, is a standing member of the NIH Nanotechnology Study Section, and is an Advisory Board Member for the UCSF Rosenman Institute and the journals Analytical Chemistry and ACS Sensors. She has served as a Co-Director of the Cold Spring Harbor Laboratory's Single Cell Analysis summer course (2015 & 2016), both Chair (2009) and Vice-chair (2007) of the Gordon Research Conference (GRC) on the Physics & Chemistry of Microfluidics. She is faculty advisor to the UC Berkeley chapter of the Society of Women Engineers (SWE) and the Graduate Women in Engineering (GWE).

Professor Herr's research has been recognized by: the 2015 Georges Guiochon Faculty Fellow from HPLC, the 2012 Young Innovator Award from Analytical Chemistry/CBMS, the 2012 Ellen Weaver Award from the Association for Women in Science (AWIS, for mentoring), a 2011 NSF CAREER award, a 2010 NIH New Innovator Award, a 2010 Alfred P. Sloan Research Fellowship in chemistry, a 2010 New Investigator Award in Analytical Chemistry from Eli Lilly & Co., a 2009 Defense Advanced Research Projects Agency (DARPA) Young Faculty Award, a 2009 Hellman Family Faculty Fund Award from UC Berkeley, a 2008 Regents' Junior Faculty Fellowship from the University of California. Professor Herr has also been recognized by the 2012 Outstanding Instructor Award in Bioengineering (Bioengineering Honor Society student vote) and a 2007 Outstanding Mentor Award from Sandia National Laboratories.



ANALYST EMERGING INVESTIGATOR LECTURESHIP

This lectureship was launched as a platform for an early career analytical scientist to raise the profile of the analytical sciences to the wider scientific community and general public. The candidates were asked to submit an original essay of no more than 1000 words highlighting the significant and wide-reaching impact on scientific and societal issues related to this year's theme of health in the analytical sciences. Their essay will also be published as a Perspective article in Analyst.



2016 Lectureship Recipient
Patrick Hayes, Université de Montréal

Patrick Hayes is Assistant Professor of the Atmospheric and Analytical Chemistry Group at the Université de Montréal since Summer 2013. He obtained his PhD in Analytical Chemistry at Northwestern University, USA. His postdoctoral CIRES fellowship was performed at the University of Colorado. His research group focusses on the chemistry of atmospheric aerosols and the study of fundamental chemical and physical interactions occurring at solid/liquid interfaces important to the environment. He has more than 30 peer-reviewed publications, and has given more than 20 oral presentations, including 7 invited lectures. He has also served as a Member of the Board of Directors for the Environmental Division of the Chemical Institute of Canada.

ROYAL SOCIETY OF CHEMISTRY THEOPHILUS REDWOOD AWARD

The Theophilus Redwood Award is given to a leading analytical scientist who is also an outstanding communicator. This year's winner is Duncan Graham from the University of Strathclyde for innovation and leadership in exploiting surface enhanced Raman spectroscopy in the analytical community.



2016 Redwood Recipient
Duncan Graham, University of Strathclyde

Duncan Graham is Research Professor of Chemistry and Deputy Head of Department for Pure and Applied Chemistry at the University of Strathclyde in Glasgow having being appointed there as a lecturer in 2002 and then to a chair in 2004.

He is currently Chair of the Editorial Board of Analyst and president elect of the Analytical Division of the Royal Society of Chemistry. He serves on the advisory boards of Chemical Society Reviews, Chemical Science, Journal of Raman Spectroscopy, the Journal of Biomedical Spectroscopy and Imaging and the new Cell Press journal, Chem. He has been a co-chair of the Raman program for SciX since 2013 and in 2016 took over as the RSC representative for FACSS from John Chalmers. He has been awarded numerous awards for his research including the RSCs SAC Silver medal (2004), Nexxus Young Life Scientist of the year (2005), Corday Morgan prize (2009), a Royal Society Wolfson Research Merit award (2010), the Craver Award from the Coblentz Society (2012), Fellows Award from the Society for Applied spectroscopy (2012) and was elected to the fellowship of the Royal Society of Edinburgh (2008). He has published over 200 papers and graduated over 50 PhD students. He is a cofounder and director of Renishaw Diagnostics Ltd (2007) which now has 42 FTE and has a CE marked SERS based diagnostic now available for use in European hospitals. He completed a PhD in organic chemistry at the University of Edinburgh (1996) and his interests are in developing new diagnostic assays based on nanoparticles and spectroscopy with target molecules including DNA, RNA, proteins and small molecule biomarkers.

PREVIOUS FACSS BOARD AND MEETING CHAIRS

1973			1984 - Philadelphia	
Jeannette Grasselli	Governing Board Chair		Theodore Rains	Governing Board Chair
1974 – Atlantic City			D. Bruce Chase	General
James White	Governing Board Chair		Patricia Rouse Coleman	Program
George Heinz	General		Fred Corcoran	Arrangements
James White	Program		Peter Keliher	Exhibit
Edward Ruffing	Exhibit		1985 - Philadelphia	
1975 - Indianapolis			Robert Barford	Governing Board Chair
James Holcombe	Governing Board Chair		Fred Corcoran	General
Gerald Wallace	General		Matthew Klee	Program
James Holcomb	Program		Marshall Fishman	Arrangements
Edward Ruffing	Exhibit		Peter Keliher	Exhibit
1976 - Philadelphia			1986 - St. Louis	
Edward Brame	Governing Board Chair		Ronald Schroeder	Governing Board Chair
Edward Brame	General		Marshall Fishman	General
Edward Dunlap	Program		Alexander Scheeline	Program
Douglas Robinson	Arrangements		Terry Hunter	Arrangements
Edward Ruffing	Exhibit		Edward Brame	Exhibit
1977 - Detroit			1987 - Detroit	
Edgar Peck	Governing Board Chair		Patricia Rouse Coleman	Governing Board Chair
Mitch Kapron and James Burns	General		David Coleman and L. Felix Schneider	General
Jeannette Grasselli	Program		John S. Beaty	Program
L. Felix Schneider	Arrangements		Edward Brame	Exhibit
Edward Ruffing	Exhibit		1988 - Boston	
1978 - Boston			James Cavanaugh	Governing Board Chair
James Williamson	Governing Board Chair		Frank Plankey and John S. Beaty	General
Paul Lublin	General		Roger Gilpin	Program
James Cosgrove	Program		Edward Brame	Exhibit
James Cornwell	Arrangements		1989 - Chicago	
Edward Ruffing	Exhibit		Alexander Scheeline	Governing Board Chair
1979 - Philadelphia			Paul Bourassa	General
Peter Keliher	Governing Board Chair		Robert G. Michel	Program
Douglas Robinson	General		Edward Brame	Exhibit
Philip LeFleur	Program		1990 - Cleveland	
Sydney Fleming	Arrangements		Nancy Miller-Ihli	Governing Board Chair
Edward Ruffing	Exhibit		Charles Belle	General
1980 - Philadelphia			Steven Hughes	Program
L. Felix Schneider	Governing Board Chair		Edward Brame	Exhibit
Sydney Fleming	General		1991 - Anaheim	
Theodore Rains	Program		David Coleman	Governing Board Chair
Robert Barford	Arrangements		Richard Deming and Constance Sobel	General
Edward Ruffing	Exhibit		James Holcombe	Program
1981 - Philadelphia			Edward Brame	Exhibit
Jack Katon	Governing Board Chair		1992 - Philadelphia	
Robert Barford	General		Karmie Galle	Governing Board Chair
Mary Kaiser	Program		Matthew Klee	General
James Cavanaugh	Arrangements		Barry Lavine	Program
Peter Keliher	Exhibit		Edward Brame	Exhibit
1982 – Philadelphia			1993 - Detroit	
Sydney Fleming	Governing Board Chair		Robert Watters	Governing Board Chair
James Cavanaugh	General		L. Felix Schneider and David Coleman	General
Andrew Zander	Program		Julian Tyson	Program
Matthew O'Brien	Arrangements		Mildred Barber	Exhibit
Peter Keliher	Exhibit		1994 - St. Louis	
1983 - Philadelphia			Paul Bourassa	Governing Board Chair
Mary Kaiser	Governing Board Chair		Terry Hunter	General
Matthew O'Brien	General		John Koropchak	Program
John Lephardt	Program		Mildred Barber	Exhibit
D. Bruce Chase	Arrangements			
Peter Keliher	Exhibit			

PREVIOUS FACSS BOARD AND MEETING CHAIRS

1995 – Cincinnati		2006 – Orlando	
Jon W. Carnahan	Governing Board Chair	Diane Parry	Governing Board Chair
Joseph A. Caruso	General	Christine Wehlburg	General
Richard F. Browner and R. Kenneth Marcus	Program	S. Douglass Gilman	Program
Mildred Barber	Exhibit	Mike Carrabba	Exhibit
1996 – Kansas City		2007 – Memphis	
Rachael Barbour	Governing Board Chair	James Rydzak	Governing Board Chair
O. Karmie Galle	General	Paul Bourassa	General
William Fateley	Program	Ian R Lewis	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
1997 - Providence		2008 – Reno	
Mildred Barber	Governing Board Chair	Gary Brewer	Governing Board Chair
Chris Brown	General	John Hellgeth	General
John Olesik	Program	Greg Klunder	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
1998 - Austin		2009 – Louisville	
John Graham	Governing Board Chair	Becky Dittmar	Governing Board Chair
David Laude	General	Jessica Jarman	General
Isiah Warner and Linda McGown	Program	Curtis Marcott	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
1999 - Vancouver		2010 – Raleigh	
Robert G. Michel	Governing Board Chair	S. Douglass Gilman	Governing Board Chair
Michael Blades	General	David J. Butcher	General
Ronald Williams	Program	André J. Sommer	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
2000 - Nashville		2011 – Reno	
John Koropchak	Governing Board Chair	S. Douglass Gilman	Governing Board Chair
Arlene Garrison	General	Greg Klunder	General
Michael Carrabba	Program	Pavel Matousek	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
2001 – Detroit		2012 – Kansas City	
David A. Laude	Governing Board Chair	Ian R. Lewis	Governing Board Chair
David Coleman and L. Felix Schneider	General Co-Chairs	Brandye Smith-Goettler	SciX General
David J. Butcher	Program	Steven Ray	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibits
2002 – Providence		2013 – Milwaukee, WI	
Michael Carrabba	Governing Board Chair	Ian R. Lewis	Governing Board Chair
Robert G. Michel	General Chair	Fred LaPlant	SciX General
Mark A. Hayes	Program Chair	Mike George	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit
2003 – Fort Lauderdale		2014 – Reno, NV	
Ronald Williams	Governing Board Chair	Greg Klunder	Governing Board Chair
Rina Dukor	General	Luisa T. M. Profeta	SciX General
James Rydzak	Program	José R. Almirall	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit
2004 – Portland		2015 – Providence, RI	
Michael Blades	Governing Board Chair	Greg Klunder	Governing Board Chair
David Trimble	General	Edita Botonjic-Sehic	SciX General
George Agnes	Program	Glen P. Jackson	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit
2005- Quebec City, Canada			
Mark Hayes	Governing Board Chair		
Denis Boudreau	General		
Paul Farnsworth	Program		
Scott McGeorge	Exhibit		

SOCIETY AND COMMITTEE MEETINGS AND EVENTS

FACSS/SciX ORGANIZATION

Sunday, September 18, Room: Lake Minnetonka, 4th Floor

1:00 – 3:00 pm SciX Long Range Planning Meeting (Conference)
 4:00 – 6:00 pm FACSS Long Range Planning Meeting (Federation)
 7:15 – 7:45 pm Program Committee

Monday, September 19, Room: Minnetonka, 4th Level

12:15 – 1:15 pm SciX 2017 Reno Meetings: Budget and Planning
 3:20 – 3:50 pm Budget and Finance Committee

Wednesday, September 21, Minnetonka, 4th Level

12:15 – 1:15 pm SciX 2017 Reno Meetings: Program
 3:20 – 3:50 pm SciX 2018 Atlanta Meetings: Budget, Program and Planning

Thursday, September 22

Noon Executive Committee Meeting (*for the Executive Committee only*), Room: Minnetonka
 6:00 pm Governing Board Meeting (light dinner will be provided), Room: Minnetonka, 4th Floor
 9:00 pm Governing Board Chair Reception (delegates and invitees), Room: Calhoun, 4th Floor

COBLENTZ SOCIETY

Monday, September 19

Noon – 1:00 pm Coblentz and SAS Speed Mentoring Session, Room: Great Lakes A1, 4th Level. 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 setting to meet other scientists, expand professional networks, and potentially form a mentoring relationship. Registration is free and lunch will be provided.
 1:00 - 3:00 pm Coblentz Board Meeting, Room: Harriet, 4th Level

Tuesday, September 20

12:45 – 1:30 pm Coblentz Challenge, Room: Isles, 4th Level. 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 which prospective mentors may choose. The objective is to find vibrational spectroscopists who have 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.

SOCIETY FOR APPLIED SPECTROSCOPY

Saturday, September 17

3:00 – 9:00 pm SAS Executive Committee, Room: Lake Minnetonka, 4th Level

Sunday, September 18

12:00 – 4:00 pm SAS Members Only Event, Brit's Pub
 7:00 pm SAS Student Poster Session Room: Nicollet A

Monday, September 19

12:00 – 2:00 pm SAS Publications Committee Room: Calhoun, 4th Level
 8:00 - 11:00 pm SAS Student Event, O'Donovan's Pub

Tuesday, September 20

12:00 – 2:00 pm SAS Editorial Board Meeting Room: Calhoun, 4th Level
 1:00 – 1:20 pm SAS PAT Technical Section Business Meeting Room: Greenway D
 4:00 – 7:00 pm SAS Governing Board Meeting Calhoun, 4th Level
 7:30 pm SAS Wine and Cheese Awards Reception, Room: Great Lakes B/C

Wednesday, September 21

9:00 – 11:00 am SAS Membership/Publicity Committee Room: Minnetonka, 4th Level

NASLIBS

Monday, September 19

12:00 – 2:00 pm NASLIBS Board Meeting, Room: Isles, 4th Level

ITP

Monday, September 19

6:00 – 9:00 pm VIP Dinner (invitation only), Room: Great Lakes A2

Tuesday, September 20

11:00 am – 12:30 pm Wiley/ ELECTROPHORESIS Board Meeting, Room: Minnetonka, 4th Level

Tuesday, September 20

7:00 – 9:00 pm ITP Dinner Reception (ticket required), Room: Greenway H/I

SciX EXHIBITORS and EXHIBIT HALL ACTIVITIES

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, September 18

4:20 pm What's Hot Exhibitor Presentations, *Nicollet B/C*

Monday, September 19

5:30 pm Exhibit Hall Opening Reception, *Exhibit Hall*

Tuesday, September 20 and Wednesday, September 21

10:30 am Pick up your Exhibitor Discovery Raffle Card
for a chance to win an iPad Mini at Exhibit Hall Entrance
(chance to win each day)

11:00 am – 12:00 pm Poster Session and Coffee Break in Exhibit Hall

11:40 am What's Hot Exhibitor Presentations in Exhibit Hall

12:00 noon Complimentary lunch for all attendees in Exhibit Hall

3:00 – 3:50 pm Poster Viewing and Break

Exhibit Hours:

Monday 5:30 pm – 7:30 pm

Tuesday 10:00 am – 4:30 pm

Wednesday 10:00 am – 4:00 pm

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EXHIBITOR DESCRIPTIONS

ACS Division of Analytical Chemistry

2019 Galisteo St., Bldg 1-1
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.

AES Electrophoresis Society

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.

Agilent Technologies, Inc.

2850 Centerville Rd.
Wilmington, DE 19808

www.agilent.com

Agilent Technologies leads the industry with robust, reliable instruments that provide the ability to analyze, confirm and quantify substances of interest. Our workflow solutions enable you to maintain stringent practices from sample preparation, through analysis, to final report. When combined with our informatics architecture, large quantities of data can be managed while preserving the integrity and security of the results. Agilent offers a complete line of GC, LC, MS and Spectroscopy instruments and technologies, as well as the related consumables, support and services. For more information visit our website.

Analytik Jena US, Inc.

500 W Cumming Park, Ste 1800
Woburn, MA 01801

www.analytik-jena.com

Analytik Jena is a leading provider of high-end analytical measuring technology, of instruments and products in the fields of biotechnology and molecular diagnostics, as well as of high quality liquid handling and automation technologies. Its portfolio includes traditional analytical technology, particularly to measure concentrations of elements and molecules, as well as systems for bioanalytical applications in the Life Science area spanning the highly complex analytic cycle of a sample from sample preparation to detection. Automated high-throughput screening systems for the pharmaceutical sector are also part of this segment's extensive portfolio. Analytik Jena's products are focused to offer customers and users a quality and the reproducibility of their laboratory results. Comprehensive laboratory software management and information systems (LIMS), services, as well as device-specific consumables and disposables, such as reagents or plastic articles, complete the Group's

Booth #109

extensive range of products. Analytik Jena is part of the Swiss Endress+Hauser Group.

Anasys Instruments

325 Chapala St
Santa Barbara, CA 93101

www.anasysinstruments.com

Anasys pioneered the field of AFM based analytical property measurements with our multiple award winning technologies. We offer the only full-featured AFM that offers true nanoscale chemical analysis via nanoscale IR Spectroscopy. We achieve this breakthrough by using the AFM probe as the IR absorbance detector. We also offer AFM probe based nanoscale IR sSNOM, nanoscale thermal analysis (via our breakthrough thermal probes) and AFM based wideband mechanical spectroscopy. For those with an AFM, we offer a nanoscale thermal analysis module that interfaces with most commercially available AFMs.

Booth #24

Andor Technology

300 Baker Avenue, Suite 150
Concord, MA 01742

www.andor.com

Andor Technology is a global leader in the pioneering and manufacturing of high performance scientific imaging cameras, spectroscopy solutions and microscopy systems for research and OEM markets. Andor has been innovating the photonics industry for over 20 years and aims to continue to set the standard for high performance light measuring solutions that allow consumers to perform light measurements previously considered impossible. Through continuous dialogue with customers and strong teamwork, Andor continues to innovate ground-breaking products that improve the world in which we live. Andor Technology is part of Oxford Instruments plc, a leading provider of high technology tools and systems for industry and research.

Booth #96

Applied Spectra, Inc.

46665 Fremont Blvd
Fremont, CA 94538

www.appliedspectra.com

We are a leading supplier of analytical instruments based on laser ablation technology. We offer a comprehensive suite of innovative LIBS (Laser Induced Breakdown Spectroscopy), LA (Laser Ablation) and tandem LIBS/LA instruments for rapid elemental and isotopic analysis without sample prep. Our analytical products are helping our customers perform effective and efficient forensic analysis, QC work during solar and battery manufacturing, and hazardous substance detection in the environment. We are world class LIBS/LA experts ready to support our customers with measurement method and application development.

Booth #87

Booth #70

EXHIBITOR DESCRIPTIONS

art photonics GmbH

Rudower Chaussee 46
Berlin, Germany 12489
www.artphotonics.com

Booth #79

art photonics GmbH was founded in Berlin in 1998 to develop and produce specialty fiber cables, bundles and spectroscopy probes for a broad spectral range of 0.2-16µm. FlexiSpec® fiber probes are produced for all methods of remote process-spectroscopy used in lab, industry and clinical diagnostics. The robust industrial fiber probes can withstand aggressive or toxic media under high or low pressure and temperature to analyze process with fluorescence, FT-IR-absorption, Raman-scattering and UV-Vis-NIR-reflection or transmission spectroscopy. The tiny medical fiber probes help to define tumor margins in oncology using all these methods with Multi-Spectral Fiber systems – which enable optimal selection of the most sensitive, specific and accurate methods for any tumor and development of spectral fiber sensor customized for its type.

Avantes

9769 W. 119th Dr., Ste 4
Broomfield, CO 80021-2560
www.avantes.com

Booth #74

Avantes is a leader in field of fiber optic spectroscopy offering a complete range of spectroscopy instrumentation to support measurements in the range from 160-2500 nm. With an installed base of over 25,000 instruments worldwide and 22 years serving the needs of scientists and engineers, Avantes is equipped to meet the challenges presented by applications of our customers. Avantes' ISO certified, 35,000 square foot engineering and manufacturing facilities are located in Apeldoorn, the Netherlands. Avantes instrument and system configurations support fluorescence, UV/VIS absorbance, reflectometry/thin film metrology, LIBS, Raman, spectroelectrochemistry, optical emission spectroscopy and many other spectroscopic techniques. Avantes will be featuring the new AvaSpec-HERO higher resolution and high sensitivity back-thinned, TE cooled instrument at SCiX 2017.

AXSUN Technologies

1 Fortune Drive
Billerica, MA 01821
www.axsun.com

Booth #14

B&W Tek

19 Shea Way, Ste 301
Newark, DE 19713
www.bwtek.com

Booth #85

B&W Tek is an advanced instrumentation company that delivers lab quality Raman, LIBS and NIR spectroscopy solutions through user-friendly mobile platforms. Our commitment to innovative solutions has made B&W Tek the leading provider in Raman spectroscopy solutions worldwide for the pharmaceutical, biomedical, physical, chemical and research communities. Further, we offer cutting-edge handheld or portable LIBS and NIR analyzers that can be developed according to specific needs in both industrial and laboratory applications. With a strong vertical integration capability, B&W Tek also provides custom product development, design and manufacturing, utilizing our array of high performance, low-cost UV/VIS/NIR spectrometers and diode, DPSS and fiber lasers.

Barnett Technical Services

55050 Laguna Blvd, Ste 112-620
Elk Grove, CA 95758
www.barnett-technical.com

Booth #91

Barnett Technical Services is a distribution company specializing in the spectroscopy field. Products of interest to SciX attendees include: Micro Support Micromanipulators – Computer-based micromanipulators for fine material processing including particle

isolation, sample cutting, milling off a surface, and liquid delivery to/from a surface. Systems consist of free-standing microscopes and arms that can be added to existing microscopes (including Raman microscopes). Tokyo Instruments Raman Imaging – Provides rapid, high-resolution Raman micro-imaging systems. Micro Emission Elemental Analyzers – Simple systems for the elemental analysis of small volumes of liquids to the ppm level. Ideal for simple lab use or field operation.

BaySpec, Inc.

1101 McKay Drive
San Jose, CA 95131
www.bayspec.com

Booth #50

BaySpec, Inc., founded in 1999 with 100% manufacturing in the USA (San Jose, California), is a vertically integrated spectroscopy company. The company designs, manufactures and markets advanced spectral instruments, from UV-VIS-NIR and Raman spectrometers to handheld and portable NIR and Raman analyzers, to bench-top in-line process and Raman microscopes for the biomedical, pharmaceuticals, chemical, food, semiconductor, and homeland security industries. BaySpec's core technologies include: ultra-high throughput Volume Phase Gratings (VPGTM), optimized deep-cooled detector/cameras, and high power narrowband lasers, which allow for cost effective customized solutions without the custom expenses. Designs are optimized for performance and long-term reliability featuring no moving parts. The company has experience shipping over 35,000 spectral engines of all types. For more information visit us at www.bayspec.com.

Bio-Rad Laboratories, Informatics Division

2000 Market Street, Ste 1460
Philadelphia, PA 19103
www.knowitall.com

Booth #69

Bio-Rad Laboratories specializes in Spectroscopy Databases & Software Solutions (IR, Raman, NMR, MS, UV-Vis). They are a leading producer of spectral databases with over 1.5 million spectra including Sadtler™ Data. Their KnowItAll® Spectroscopy Software offers a range of solutions including: spectral search, spectral data management, spectral identification, quality control, mixture analysis, polymer analysis, chemometrics, etc. This unique combination of spectral software with a vast collection high-quality spectral reference data gives KnowItAll users a distinct advantage when it comes to spectral analysis.

BioTools, Inc.

17546 Bee Line Highway
Jupiter, FL 33458
www.btools.com

Booth #22

BioTools is pleased to announce several disruptive new products: 1) the first portable Raman microscope - □-BioRAMAN - combining the capabilities of a portable Raman microscope with resolution and specifications of a bench-top Raman systems. 2) MANTIS – a DualPEM VCD accessory for Thermo FT-IR spectrometers and 3) a RAMAN spectrometer that provides measurements of four forms of ROA, Raman microscopy / imaging and AFM. With these introductions, BioTools continues its tradition developing state-of-the-art innovative and unique vibrational spectroscopy products. BioTools was the first company to introduce spectrometers for the measurement of VCD & ROA– the ChiralIR-2XTM and the ChiralRAMAN-2XTM. Our PROTA-3S system for measurements and analysis of FT-IR spectra of proteins, viruses, sugars and nucleotides is the number one choice of biopharmaceutical scientists. We also offer software for calculations and modeling, databases and unique sampling cells and accessories for temperature controlled studies.

EXHIBITOR DESCRIPTIONS

BrightSpec, Inc. 770 Harris St, Suite104-6 Charlottesville, VA 22903 www.brightspec.com	Booth #17	Czitek 6 Finance Dr Danbury, CT 06810 www.czitek.com	Booth #82
Bruker Corporation 19 Fortune Dr. Billerica, MA 01821 www.bruker.com	Booth #34	Daylight Solutions 15378 Avenue of Science, Ste 200 San Diego, CA 92128 www.daylightsolutions.com	Booth #62
<p>Bruker Optics, part of Bruker Corporation, is a leader in FTIR, NIR, Raman and Terahertz Spectrometers and Imaging Spectrographs for various markets and applications. Whether it's a high-end research system, a life sciences tool, a routine quality control instrument or process analyzer, Bruker Optics offers a wide variety of innovative analytical tools for all of your demanding needs. Visit us at FACSS booth #34 and our website at www.bruker.com/optics</p>		<p>A mid-IR technology leader, Daylight Solutions has delivered more mid-IR lasers & systems worldwide than anyone else. Whether your application is molecular spectroscopy, life sciences, remote sensing, defense and security, or process control, we have a laser system that will meet your needs. If you need CW output, pulsed output, broad tuning, line widths</p>	
CAMO Smart Software, Inc. One Woodbridge Ctr, Suite 319 Woodbridge, NJ 07095 www.camo.com	Booth #100	Eigenvector Research, Inc. 3905 West Eaglerock Dr Wenatchee, WA 98801 www.eigenvector.com	Booth #72
<p>CAMO Software's analytical modeling, prediction and optimization solutions are the preferred choice for over 25,000 data analysts worldwide across a wide range of industries. CAMO Software's flagship simulation and prediction software product is The Unscrambler® X, which is recognized for its ease of use, exceptional data visualization and advanced multivariate methods. CAMO also offer a range of software products which can be integrated directly into scientific instruments, process monitoring solutions, as well as optimization software. Headquartered in Oslo, CAMO's passion is the comprehension and simplification of complex data, resulting in efficient identification, cost, research and design as well as faster analytical results. This allows our clients to benefit from an accelerated return on investment in product development and manufacturing and improved business analytics capabilities.</p>		<p>Eigenvector Research, Inc. (EVRI) is a full-service Chemometrics company, offering software, training and consulting. EVRI provides advanced chemometrics support for a wide variety of industries and academia. Our chemometric software products include our flagship MATLAB-based PLS_Toolbox and stand-alone Solo. We also offer MIA_Toolbox and Solo+MIA for Multivariate Image Analysis. Automated application of our chemometric models is simple with our Solo_Predictor and Model_Exporter. EVRI offers chemometrics training, such as our short courses here at SCIX, plus our renowned Eigenvector University (EigenU) held each spring in Seattle. We also do in-house training for many Fortune 500 companies and government agencies. Our consulting services have been an important part of projects in both start-up and large established companies. Our consulting staff has over 100 years of combined chemometric experience. Make EVRI your complete source of chemometric tools and know-how!</p>	
Cobalt Light Systems Inc. Suite 1319, 11951 Freedom Dr Reston, VA 20190 www.cobaltlight.com	Booth #25	ELEMISSION 108-4030 Cote Vertu Montreal, QC H4R1V4 Canada www.elemission.ca	Booth #68
<p>Coblentz Society www.coblentz.org Professional organization that fosters the understanding and application of vibrational spectroscopy. Through the voluntary efforts of its members, the society sponsors scientific conferences, creates 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 www.coblentz.org.</p>	Booth #107	<p>We are the leading manufacturer of automated on-line atomic emission spectrometry. We provide real-time innovative solution for elementary analysis from ore to final product on process stream using Laser-Induced Breakdown Spectroscopy (LIBS). Our products identify and monitor critical-to-quality parameters to ensure quality, productivity and accuracy of product specifications during manufacturing. ELEMISSION also provides innovative and affordable research and development to solve your persistent production problems.</p>	
Cobolt AB Vretenvägen 13 Solna, 171 54 www.cobolt.se	Booth #65	Energetiq Technology, Inc. 7 Constitution Way Woburn, MA 01801 www.energetiq.com	Booth #20
Continuum, Amplitude Laser Group 3150 Central Expressway Santa Clara, CA 95051 www.continuumlasers.com	Booth #84	<p>Energetiq is a developer and manufacturer of advanced light sources that enable the manufacture and analysis of nano-scale structures and products. Used in complex scientific and engineering applications, Energetiq's light products are based on new technology that generates high brightness and high power light in the 1nm to 1000nm range with high reliability, high stability, and long life, all in a compact package.</p>	

EXHIBITOR DESCRIPTIONS

FACSS/SciX

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

www.facss.org; www.scixconference.org

SciX 2017 presented by FACSS will be held October 8-13 in Reno, NV at the Grand Sierra Resort. 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.

Booth TBD

FiberTech Optica, Inc.

330 Gage Avenue, Ste 1
Kitchener, ON, N2M 5C6 CANADA

www.fibertech-optica.com

Fibertech Optica (FTO) is a leader in the manufacture of specialty fiber optic solutions providing outstanding technical support, quality and competitive pricing on both custom and standard products.

Offering process control cables to 500 meters, fiber bundles, assemblies, spot to line converters, low FRD cables, reflectance probes, RAMAN probes, v-groove arrays, micro-lens assemblies and high power laser cables with multimode, singlemode and borosilicate fibers. Fiber options available for applications with wavelengths from the deep UV to the MIR, with NA's from 0.12 to 0.66. FTO also produces fiber coupled LED multi-emitter light sources and vacuum feedthroughs. From prototype through production quantities, FTO supports applications in industrial process control, biomedical, spectroscopy, astronomy, scientific instrumentation, laser delivery, research and academics.

Booth #98

Fiveash Data Management (FDM)

211 Vista Road
Madison, WI 53726

www.fdm spectra.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.

Booth #12

Hamamatsu Corporation

360 Foothill Rd.
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.

Booth #15

Harrick Scientific

141 Tompkins Ave
Pleasantville, NY 10570

www.harricksci.com

Harrick Scientific produces an extensive array of spectroscopic sampling devices and reaction cells for FTIR, UV-Vis, and Raman. Sampling technologies include ATR, diffuse reflection, specular reflection, and transmission. The new ConcentratIR2 multiple-reflection ATR provides capabilities for highly sensitive measurements of microliter volumes of samples such as aqueous protein solutions. Temperature-controlled accessories include heated and cooled chambers for in-situ Operando catalysis and photochemistry research, adaptable to FTIR, UV-Vis, and X-ray spectroscopic techniques. We work in partnership with researchers to develop effective and novel solutions for challenging research studies. Harrick Scientific---for over 40 years the leading innovator in molecular spectroscopy sampling technologies.

Booth #71

Hellma USA, Inc.

80 Skyline Drive
Plainview, NY 11803

www.LearnRaman.com

Hellma has been serving the US research and educational market with the highest precision sample analysis components since 1963. Here at SciX 2016, we are giving one of our first showings of our latest initiative to advance chemistry education. Visit Booth #103 to learn about how we can enable the widespread understanding of the hottest analytical principle to industry.

Booth #103

HORIBA Scientific

Attn: Raman Spectroscopy
3880 Park Avenue

Edison, NJ 08820

www.horiba.com/scientific

This year's SCIX theme is, 'The Great Outdoors.' It should come as no surprise, then, that HORIBA takes it a bit farther.....to the very outdoorsy era of the Vikings (the Nordic ones, not the football ones.) HORIBA Vikings will be sailing our dragon ship full of spectroscopy products into SciX, and docking at booth 26. In our booth, we will show 'tis very important to have the right tools for the job. Our Viking warriors and warrior maidens will show you the latest tools of our trade. You can check out our Raman, Fluorescence, GD-OES, SPRi and XRF instruments. Find out about the latest developments in Raman microscopy, AFM/Raman, transmission Raman, microsecond and millisecond Raman imaging, along with combined CL/PL/Raman accessories for SEM. We will have our XploRA Raman microscope that incorporates unique and powerful functions in a reliable, fast, high performance system, ideally suited to the research and analytical lab. We'll also have information on our instruments for elemental analysis offering advanced ICP/GD-OES systems like C/S/O/N/H analyzers, and our latest Surface Plasmon Resonance imaging (SPRi) instruments that make Multiplex Label-free molecular interaction fast and easy. And, we'll have the MESA-50, our smallest spot EDXRF instrument, for screening samples containing hazardous elements for RoHS, End of Life compliance, and chlorine for halogen-free As and Sb applications. Finally, we offer the highest sensitivity Fluorescence systems on the market - including TCSPC and EEM/UV-VIS analysis. So, stop-eth by. Put on your horned helmet, grab an oar and join us for a photo op, good cheer, beer and spectroscopy to be sure you get into the Valhalla of spectroscopy.

Booth #26

EXHIBITOR DESCRIPTIONS

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: Very high efficiency/throughput (low optical loss), High thermal stability and robustness. Our spectrometer products include: ROCK for high throughput, FREEDOM for ultra-compact size and low cost, EAGLE for high resolution, I-MON wavelength interrogation monitor for FBG sensing systems in the 850, 1310, and 1550 nm wavelength ranges and Custom built OEM spectrometers to match our customer's exact needs. Our grating products include: Phase Masks for Fiber Bragg Grating manufacturing, Pulse Compression Gratings for high power lasers, Polarization insensitive gratings (PING) for Telecom WSS, OCM and tunable filters and High efficiency spectrometer gratings. Ibsen Photonics is a privately held company with headquarter in Farum, Denmark. For more information please visit www.ibsen.com

Booth #101

ICP Information Newsletter, Inc.

PO Box 666
Hadley, MA 01035-0666
www.icpinformation.org

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 2018 Winter Conference is planned for January 7 - 13, 2018 on Amelia Island, Florida. The ICP Information Newsletter now in its 42nd year of publication is distributed to subscribers in computer – readable format on CD-ROM. Visit icpinformation.org for subscription and conference details.

Booth #78

Innovative Photonic Solutions

4250 U. S. Highway 1, Ste 1
Monmouth Junction, NJ 08852
www.innovativephotonics.com

IPS specializes in the manufacture of high performance wavelength stabilized lasers for use in Raman spectroscopy, illumination and homeland security applications. Our proprietary technology enables us to lock the laser to a specific wavelength without complex feedback mechanisms. The technology is applicable to both single and multi-mode lasers and enables the manufacture of both high power multi-mode and narrow linewidth (less than 100 KHz) single frequency lasers. Standard wavelengths include 532 nm, 633 nm, 638 nm, 785 nm, 808 nm, 830 nm, 976 nm and 1064 nm. Our products are available in TO-56 or 14-Pin BF packages, OEM Modules, or in turn-key UL/CE/IEC certified modules with integral control electronics. New products include ultra-high throughput integrated Raman probes which offer 2 - 5X higher throughput than traditional modular Raman setups and a dual wavelength laser package that can be used for Raman stitching.

Booth #52

Kaiser Optical Systems, Inc.

371 Parkland Plaza
Ann Arbor, MI 48103
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 Systems™ 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.

Booth #56

Keit Spectrometers

Rutherford Appleton Laboratory, R71
Didcot, Oxfordshire, OX11 0QX UK
www.keit.co.uk

Keit developed a rugged Fourier Transform Infrared (FTIR) spectrometer designed to take on the rigours of the manufacturing environment with simple, fixed components. Extremely stable, and low maintenance, this compact spectrometer is an easy-to-use tool for process monitoring of liquids and slurries either indoors or out. The Keit FTIR spectrometer was originally developed for the space program making it inherently tough and vibration tolerant. Now the power of FTIR spectroscopy is available for use in industrial environments. With no moving parts, the FTIR spectrometer is able to work directly on the manufacturing floor to help chemical engineering and production staff make process-optimising decisions in real time both for batch and in-line process monitoring without the hassle of long fibre-optic cables.

Booth #73

LabSmith

6111 Southfront Rd, Suite E
Livermore, CA 94551
www.labsmith.com

LabSmith excels at making microfluidics work for researchers, startups, and industry. LabSmith's products run the gamut from multichannel high-voltage sequencers, compact motorized epifluorescence microscopes, miniature pumps, valves, pressure sensors, fittings, microfluidic chips, breadboards, and much more. Our software makes automation and coordination of these devices fast and painless. Look to LabSmith for everything to make your lab hum with invention. Visit our booth to meet with LabSmith personnel and to see live demonstrations of our equipment - including our new 8000 V high voltage sequencer and our thermal control and sensing products.

Booth #95

EXHIBITOR DESCRIPTIONS

LC-GC Magazine / Spectroscopy Magazine (Advanstar) Booth #1
485F US Highway 1 South, Ste 100
Iselin, NJ 08830

www.spectroscopyonline.com; www.chromatographyonline.com
Spectroscopy's mission is to enhance productivity, efficiency, and the overall value of spectroscopic instruments and methods as a practical analytical technology across a variety of fields. Scientists, technicians, and laboratory managers gain proficiency and competitive advantage for the real-world issues they face through unbiased, peer-reviewed technical articles, trusted troubleshooting advice, and best-practice application solutions. We serve subscribers by using print and digital media to disseminate highly focused editorial content that combines peer-reviewed scientific articles with practical, solutions-based information, helping readers to become better spectroscopists whether they work in the laboratory, on the process line, or in the field.

LECO Corporation
3000 Lakeview Avenue
St. Joseph, MI 49085
www.leco.com

Booth #35

For more than 75 years, industries around the world have trusted LECO to deliver technologically advanced products and solutions. Today, that commitment continues with innovative products such as our Glow Discharge Atomic Emission Spectrometers, which offer state-of-the-art technology designed for routine elemental determination. Other LECO product lines include high-quality analytical and mass spectrometry instrumentation, metallography and optical equipment, and consumables. LECO has over 30 subsidiaries worldwide, with additional distributors authorized to sell or service LECO products to the rest of the world. A family-owned company, LECO designs and manufactures most instrument components at our headquarters in St. Joseph, Michigan. Our products are also backed by exceptional service and support long after the sale is complete. For more information, visit www.leco.com.

Metrohm USA
6555 Pelican Creek Circle
Riverview, FL 33578
www.metrohmusa.com

Booth #60

Metrohm offers a complete line of analytical laboratory and process systems for titration, ion chromatography, electrochemistry and spectroscopy. From routine moisture analysis to sophisticated anion and cation quantification, we are ready to help you develop your method and configure the optimum system. Move your analysis from the lab to the production line with our custom process analyzers. At Metrohm we provide systems that find solutions, stop by our booth and meet Metrohm.

Middleton Spectral Vision
8505 University Glen
Middleton, WI 53562
www.middletonspectral.com

Booth #103A

Middleton Spectral Vision is an innovative company specializing in hyperspectral imaging and spectroscopy. We are the US distributor of SPECIM Ltd hyperspectral imaging cameras, spectrographs, and systems. We have a dedicated design team that can help customers develop hyperspectral-based solutions to solve complex problems for research or industry. We serve a variety of markets including Aerospace, Agriculture, Research, Plant Science, Pharmaceutical and Mining.

Molecular Vista
6840 Via Del Oro, Suite 110
San Jose, CA 95119
www.molecularvista.com

Booth #16

Molecular Vista provides a tool for nanochemical spatial mapping – routinely, and on a wide variety of system archetypes. VistaScope provides a flexible hybrid atomic force microscopy (AFM) and optical spectroscopy platform for studying material & biological systems with chemical specificity at the nanometer scale, through the patented photo-induced force microscopy (PiFM) where the photo-induced polarization of the sample is measured directly in the near-field by detecting the time-integrated force between the tip and the sample. Imaging infrared wavelengths specific to different chemical entities, PiFM can resolve the nanometer-scale distribution of each chemical species in diverse multi-phase and multi-component systems, thereby revealing an unprecedented and spectacular molecular vista to the researcher. MVI was founded by Drs. Sung Park and Kumar Wickramasinghe.

MONTFORT Laser GmbH
Im Holderlob 6A
Goetzix, VA 6840, Austria
www.montfortlaser.com

Booth #104

MONTFORT Laser – “Uniquely Compact Laser Sources” - develop and produce compact, robust pulsed laser sources based on its unique diode-pumped solid-state laser technology. Applications include laser analytics, microscopy, research, industry, and defense. The M-NANO product achieves >50 mJ / 10 ns / 0-100 Hz from a small foot print laser system including driver, with dimensions of 139mm x 132mm x 64mm (l x w x h) and a weight of 1.7kg (pure laser head 0.65kg only), suitable for integration in compact instrumentation and for battery-powered operation. The M-FEMTO and M-PICO products are diode-pumped modelocked oscillators generating up to >3W pulse trains (ca. 80MHz) with superbly clean optical spectra due to the soliton modelocking technique employed.

Neaspec GmbH
Bunsenstrasse 5
Martinsried, Bava, Germany 82152
www.neaspec.com

Booth #19

Neaspec is dedicated to delivering innovative solutions for nanoscale optical imaging & spectroscopy for research laboratories in industry and academic institutions. Neaspec's engineers developed the 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).

EXHIBITOR DESCRIPTIONS

Ocean Optics, Inc.
830 Douglas Avenue
Dunedin, FL 34698
www.oceanoptics.com

Booth #38

Ocean Optics is the inventor of the world's first miniature spectrometer and a global leader in optical sensing technologies for research, education, industry and quality. Ocean Optics also provides a full range of complementary technologies such as optical fibers, probes, sensors and sampling accessories. From UV through NIR, from modular components to full LIBS and Raman systems, Ocean Optics has a solution for virtually every application need and every budget.

Ondax, Inc.
850 E. Duarte Rd.
Monrovia, CA 91016
www.ondax.com

Booth #46

Ondax Inc. is a world leading manufacturer of low frequency/THz-Raman® systems and wavelength stabilized lasers to enable best-in-class 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.
2233 Faraday Avenue,
Suite E
Carlsbad, CA 92008
www.opotek.com

Booth #92

OPOTEK manufactures compact, widely tunable laser systems based on patented OPO technology. Systems are used in fields, such as photochemistry/biology, photoacoustics, mass spectrometry and hyperspectral imaging. Products range from OPO modules to fully automated, turn-key systems. End-users select a wavelength or scan over a range from 190 to 2500 nm in 1 nm increments or less. OPOTEK offers the only portable and transportable OPO systems commercially available and caters to custom requests.

Optigrate Corp
562 S Econ Cir.
Oviedo, FL 32765
www.optigrate.com

Booth #4

BragGrate™ Raman Filters from OptiGrate are unmatched in the industry for narrow linewidth, optical density, and optical transmission. BragGrate notch filters enable measurements of ultra-low wavenumber Raman bands in the THz frequency range down to 4 cm⁻¹, while at the same time, provide a broad transmission band that covers the complete frequency range +/- 4000 cm⁻¹. This new generation of BragGrate Raman filters are available in 2016 at standard wavelengths such as 488, 514, 532, 633, 785, and 1064 nm as well as any custom wavelength from 355 nm to 2.5 microns. Our laser line cleaning filters (BragGrate™ Bandpass Filter), with a linewidth narrower than 5 cm⁻¹ at FWHM, condition beams from laser diodes, solid state, or gas lasers, which are used for ultra-low frequency Raman measurements. OptiGrate Corp is a pioneer and world leader in commercial volume Bragg gratings (VBGs) and VBG-based ultra-narrow band optical filters.

Optokey Inc.
3944 Trust Way
Hayward, CA 94545
www.optokey.com

Booth #3

PD-LD, Inc.
30-B Pennington-Hopewell Rd
Pennington, NJ 08534
www.pd-ld.com

Booth #89

Since 1993, PD-LD Inc. is focused on volume production of high performance photonic components for high performance spectroscopic systems. PD-LD developed and patented Volume Bragg Grating (VBG®) technology which is incorporated in many standard wavelength stabilized laser products used for Raman and SERDS system solutions. These stabilized lasers are available as full turnkey, enclosed modules.. Standard wavelengths available include: 405nm, 488nm, 515nm, 520nm, 647nm, 785nm, 1064nm and many others in the NIR. New products for SciX 2015 include SLM-632.8nm Single Frequency/Single-Mode series HeNe laser alternative and the power stabilized PLM-Series blue and green laser modules. PD-LD is also demonstrating the Prism Award winning LS-2 LabSource Dual Laser System for research innovators of Shifted Excitation Raman Difference Spectroscopy, SERDS. The LS-2 provides the two closely matched wavelengths required to greatly reduce or completely eliminate fluorescence from low Raman sample emissions. From component to bench-top, PD-LD has the right laser for your spectroscopic performance requirements.

PerkinElmer
940 Winter St.
Waltham, MA 02451
www.perkinelmer.com

Booth #99

PerkinElmer is a global company focused on improving the health and safety of people and their environment. From earlier medical insights and more effective therapies to cleaner water and safer homes, PerkinElmer touches the lives of millions of people every day. Our Environmental Health business develops analytical instrumentation, illumination and detection technologies and support services to protect the quality and sustainability of our environment and the security of people within their surroundings.

Pike Technologies
6125 CottonWood Drive
Madison, WI 53719
www.piketech.com

Booth #10

Pittcon 2017
300 Penn Center Blvd., Ste 332
Pittsburgh, PA 15235
www.pittcon.org

Booth #33

Pittcon, a leading conference and exposition for laboratory science, shines light on new technology and scientific research. Pittcon offers a dynamic, innovative exposition showcasing the latest products used in spectroscopy and other methodologies. Discover new applications for spectroscopy in fields such as biomedical, homeland security, industrial processes and more. Network with others on topics including NMR, UV/Vis, Raman and infrared spectroscopy. Learn about recent advances from world-renowned members of the scientific community at Pittcon's robust, multi-discipline Technical Program and skill-building Short Courses. Pittcon 2017 is March 5-9 in Chicago, IL.

EXHIBITOR DESCRIPTIONS

Princeton Instruments, Inc.

3660 Quakerbridge Rd.
Trenton, NJ 08619

www.princetoninstruments.com

Princeton Instruments is a premier designer and manufacturer of high-performance spectrographs, CCD, ICCD, EMCCD, emICCD and InGaAs cameras for the scientific research and OEM communities. We take pride in partnering with our customers to solve challenging problems in unique, innovative ways. We are excited to feature the new, small footprint IsoPlane 160 imaging spectrograph. Similar to the award-winning IsoPlane SCT-320, it includes an exclusive, state-of-the-art optical design which produces sharply focused images across the entire focal plane. With the IsoPlane more photons end up in the peak, increasing the height and effective signal-to-background ratio, rather than in the wings, where they contribute to the background noise. IsoPlane spectrographs are compatible with a wide variety of Princeton Instruments cameras and accessories. They are used in a variety of applications including Raman, microspectroscopy, TERS, LIBS, multi-channel spectroscopy and biomedical imaging. Stop by the Princeton Instruments booth for a demonstration. Visit www.princetoninstruments.com for more information.

Booth #7

Prism Analytical Technologies

2625 Denison Dr
Mt. Pleasant, MI 48858
www.pati-air.com

Prism Analytical Technologies, Inc. is a recognized leader in the development and deployment of ambient air testing methodologies for Fortune 100 companies and environmental consultants. Prism employs science-based technologies and wide range of air testing support to help clients solve indoor air quality, process control, industrial, and environmental challenges. Prism has developed a new GC-FTIR technology called MAX™. Our MAX systems have numerous advantages over today's GCs and GC/MS systems including a constant calibration, instrument-to-instrument calibration, a large dynamic range (9 orders), operates with N2 carrier gas and is ideal for Thermal Desorption Tubes. The MAX system comes functionally complete, so you are running immediately. MAX is an ideal analyzer for environmental, chemical process, gas supplier and petroleum samples.

Booth #93

Quantel USA

601 Haggerty Lane
Bozeman, MT 59715
www.quantel-laser.com

Quantel, founded in 1970, is a global leader in the design and manufacture of high-power, solid-state lasers. With design centers in Paris and the USA (Bozeman, MT), Quantel lasers are used in applications ranging from spectroscopy to atom cooling; PIV to combustion research. Uniquely, Quantel offers customers very flexible scientific lasers with user configurable wavelengths and performance parameters as well as "designed for purpose" ruggedized lasers for industrial applications.

Booth #37

Renishaw, Inc.

5277 Trillium Blvd.
Hoffman Estates, IL 60192
www.renishaw.com

Renishaw is a global company with core skills in measurement, motion control, spectroscopy and precision machining. We develop innovative products that significantly advance our customers' operational performance - from improving manufacturing efficiencies and raising product quality, to maximizing research capabilities and improving the efficacy of medical procedures. Renishaw Raman spectrometers are configurable to include: multiple excitation sources from the UV through NIR with automated laser switching and

Booth #44

alignment; quick-launch fiber-optic probes; AFM/NSOM/Raman interfaces, SEM-Raman interfaces, microscope accessories including hot/cold cells, macro-sampling; global Raman imaging, near the excitation line analysis

Royal Society of Chemistry

Thomas Graham House
Science Park, Milton Road
Cambridge, UK CB4 0WF
www.rsc.org

The Royal Society of Chemistry is the world's leading chemistry community, advancing excellence in the chemical sciences. With over 50,000 members and a knowledge business that spans the globe, we are the UK's professional body for chemical scientists; a not-for-profit organisation with 175 years of history and an international vision for the future. We promote, support and celebrate chemistry. We work to shape the future of the chemical sciences – for the benefit of science and humanity.

Booth #108

RPMC Lasers, Inc.

203 Joseph Street
Ofallon, MO 63366
www.rpmclasers.com

RPMC Lasers, Inc. offers innovative Diode Pumped Solid-State Lasers and Laser Diode Modules in wavelengths in the IR, visible, and near-UV spectrums with market-leading output power. The DPSS lasers feature a monolithic resonator technology that ensures true single-frequency emission along with excellent power, wavelength, and pointing stability.

Booth #67

SciAps Inc.

2 Constitution Way
Woburn, MA 01801
www.sciaps.com

SciAps, Inc., is a Boston based instrumentation company specializing in handheld analyzers to identify compounds, minerals, and elements, both on-site and in real time. Visit us at booth 21 to see the world's most advanced handheld LIBS analyzer family, the Z-series, and handheld Raman instruments. Our LIBS analyzers feature SciAps leading PULSAR laser technology, offering high pulse energy (5-6 mJ/pulse) and 10-20 Hz rep rate. The Z combines the laser with our patent-pending spectrometer that ranges from 185 nm out to 850 nm or optionally 930 nm (model dependent). SciAps is a fully ISO-accredited Company.

Booth #21

Society for Applied Spectroscopy

168 West Main Street #300
New Market, MD 21774
www.s-a-s.org

The Society for Applied Spectroscopy is a non-profit membership organization representing scientists in all areas of spectroscopy. Members receive numerous benefits including a subscription to the internationally recognized, peer reviewed journal Applied Spectroscopy. Visit our booth for more information and to join!

Booth #105

EXHIBITOR DESCRIPTIONS

SpectroClick, Inc.

904 Mayfair Rd
Campaign, IL 61821
www.spectroclick.com

Booth #97

SpectroClick's booth features SpectroClick spectrometers and SpectroClick Kit teaching materials. SpectroClick makes visible absorbance and reflectance spectrometers for easy and reliable field use anywhere. The exponential cost savings of SpectroBurst™ technology can be used to generate spectra or, in combination with YouTube style multi-language video instructions, go directly to actionable information. SpectroClick Kit teaching materials introduce spectrometry and its applications to students from primary to college level. By constructing a rudimentary spectrometer, students build their intuition of dispersion, diffraction, absorption, and fluorescence. And everyone can have fun with the SpectroBurst™ Viewer! Contact SpectroBurst@spectroclick.com for K-12 information.

tec5usa

80 Skyline Dr
Plainview, NY 11803
www.tec5usa.com

Booth #102

tec5usa offers high quality products for optical spectroscopy. Our UV-VIS-NIR spectrometer systems are based on high quality spectrometer modules with spectral ranges from 190-2200 nm and permanent wavelength calibration. The electronics have fast readout rates and high signal-to-noise. Fiber-optic immersion probes or measuring heads can be included. All hardware is designed for process control environments, including versions where high-temperature or explosion-proof protection is necessary. Our in-depth knowledge of the components within the modular system allows us to tailor a system to the customer's individual requirements. Various software applications and programing libraries are offered. Customizations and contract developments are possible.

Thermo Scientific

2 Radcliff Road
Tewksbury, MA 01876
www.thermoscientific.com/portableid

Booth #63

To accelerate materials science research and improve material verification, rely on Thermo Scientific™ Raman and IR instruments. The DXR™2xi Raman Imaging microscope provides highly usable, ultra-fast chemical imaging that speeds scientific investigations across a broad range of disciplines making it ideal for multi-user research facilities. Our portable optical analyzers are rugged, handheld spectrometers designed for rapid and precise chemical identification, authentication and screening directly at the point of need. The TruScan™ RM, based on Raman spectrometry, and the microPHAZIR™ RX, based on near-infrared spectrometry, enable companies to quickly identify materials from incoming receipt to final release.

Tornado Spectral Systems

555 Richmond Street West, Ste 402
Toronto, ON M5V 3B1 Canada
www.tornado-spectral.com

Booth #94

Think your chemical process is too complex, too fast, or too hazardous for Raman spectroscopy? The superior performance of Tornado's HyperFlux™ PRO Plus Raman spectroscopy system allows for more accurate chemical identification and quantitation even with challenging mixtures and low concentrations, faster measurements of dynamic reactions, and low laser power operation in

hazardous environments. HyperFlux PRO Plus uses a proprietary HTVS-enabled spectrometer to deliver better Raman sensitivity than ever before possible, making it an ideal solution for production line and laboratory settings. Combined with their small size and low cost, Tornado's non-destructive, real-time measurement solutions offer numerous benefits for established analytical practice and facilitate broader adoption of Raman methods for pharmaceutical, petrochemical, food, biotech, and other applications.

TSI Inc

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

Booth #83

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.

Wasatch Photonics

4020 Stirrup Creek Dr., Ste 115
Durham, NC 27703
www.wasatchphotonics.com

Booth #6

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.

Wiley

111 River Street
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WITec Instruments Corp.

130G Market Place Blvd
Knoxville, TN 37922
www.WITec-Instruments.com

Booth #32

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.

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 registration form for costs.

STEM WORKSHOP – INTRODUCTION TO ARDUINOS*

Celeste Morris, *Northern Kentucky University*

Sunday 9:00 am – 12:00 pm

*Attendee must bring laptop for workshop program to be uploaded

This hands-on workshop will be an opportunity for participants to learn about Arduinos and electronics for making basic scientific measurements. Arduinos, low-cost microcontrollers, are an ideal platform for creating simple and/or portable instruments for laboratory and education applications. We will explore electronic signals and use circuitry components, sensors, and arduino programs to create light, motion, and temperature sensors. More complex instrumentation for scientific applications such as an Arduino-powered UV/Vis spectrophotometer and a pH meter will be presented. No prior knowledge about circuitry, electronics, or computer coding is necessary, but participants are encouraged to bring a laptop and download arduino software compatible with their device from www.arduino.cc prior to the workshop. We encourage hobbyists, students, and educators to participate in this workshop for fun, to garner ideas for technology incorporation in teaching, and for cost-effective instrument development.

Note: Complimentary Arduino kits will be provided to the first 45 registrants (Sunday AM and Monday AM courses combined)

RAMAN SPECTROSCOPY AND IMAGING: APPLICATIONS OF "RAMAN CRYSTALLOGRAPHY" AND ANALYSIS OF 2D CRYSTALS

David Tuschel, *HORIBA Scientific*

Sunday 9:00 am – 12:00 pm

Title of the Class: Raman Spectroscopy and Imaging: Applications of "Raman Crystallography" and Analysis of 2D Crystals

Who should take this course?

In this course, you will learn the basics of applied Raman spectroscopy and imaging with a particular emphasis on 2D crystals such as few-layer transition metal dichalcogenides. In addition, students will be taught the application of group theory to crystalline materials and how to apply those symmetry rules to perform "Raman Crystallography". 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 and imaging at a practical level and cover those topics which will allow the student to apply the material learned in the laboratory, workplace and classroom. Students will learn about:

- Raman spectroscopy through the classical description
- Spatial resolution and confocality
- Raman imaging include 3D imaging
- Phonons and lattice vibrational modes
- Low-Energy phonon modes
- Chemical bond interactions and Raman band shape
- Group theory and spectral selection rules
- Crystal classes and Raman tensors
- Polarization-Orientation micro-Raman spectroscopy
- Application of "Raman crystallography"
- Raman spectroscopy and imaging of few-layer 2D crystals
- Raman sensitivity to number of crystal layers
- Course Outline
- Raman imaging
- Hyperspectral data and imaging rendering
- Spatial resolution
- Confocality
- 3D Raman imaging

- Raman Spectroscopy and Imaging of Low-Energy Phonons
- Phonons and lattice vibrational modes
- External and internal lattice vibrational modes
- Chemical bond interactions and Raman band shape
- Shear and layer breathing modes
- Application of "Raman Crystallography" With Group Theory
- Raman active normal vibrations
- Group theory and spectral selection rules
- Crystal classes and Raman tensors
- Raman polarization selection rules
- Polarization-Orientation Micro-Raman Spectroscopy
- Raman spectroscopy and Imaging of 2D Crystals
- Raman spectroscopy and imaging of few-layer 2D crystals
- Photoluminescence spectroscopy and imaging of few-layer 2D crystals
- Raman sensitivity to number of crystal layers
- Defects and crystal alignment
- Spectral quality and band shape
- Low-energy phonon modes

ITP WORKSHOP / MINI-COURSE: PRINCIPLES AND APPLICATIONS OF MODERN CE-MS

Govert Somsen, *VU University* and

Christian Klampfl, *Johannes Kepler University*

Sunday 9:30 am - 12:30 pm

Topics to be covered:

- Short basic introduction into capillary electrophoresis techniques
- Specifics in the coupling of capillary electrophoresis techniques with MS
- MS ion-source technology - impact on the choice of CE-MS parameters
- The co-axial sheath flow interface - the most widely used interface in CE-MS
- Choice of CE and MS parameters in CE-MS with the co-axial sheath flow interface
- Upsides and downsides of using sheath liquids
- Applications of CE-MS in other fields than bio-analysis
- Sheathless CE-MS interfacing - gaining sensitivity in CE-MS
- Other recently developed CE-MS interfaces
- Practical aspects of sheathless CE-MS
- Applications of CE-MS for biomolecular analysis
- CE-MS of pharmaceutical proteins

ITP WORKSHOP / MINI-COURSE: SEPARATION AND DETECTION ASPECTS OF MICROFLUIDIC DEVICES

Frantisek Foret, *Institute of Analytical Chemistry of the ASCR* and

Joerg Kutter, *University of Copenhagen*

Sunday 2:00 - 5:00 pm

The course starts of with a very brief introduction to the fundamentals of microfluidics and their immediate repercussions for applications in (analytical) chemistry. The remainder of the course then focuses on two main application areas within chemical analysis, where microfluidics as an enabling technology has been employed: separations and detection.

For the first part, emphasis will be on presenting rationales for performing chemical separations in a miniaturized formats, highlighting some attractive features and discussing still existing shortcomings.

WORKSHOPS

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In the second part, challenges and possibilities of “marrying” microfluidic approaches with state-of-the-art detectors (in particular, mass spectrometry) will be discussed, including a critical assessment on what fundamental limits apply.

Both parts will attempt to cover basic considerations, design aspects, but then also show a number of application examples, where microfluidic devices are used to attack problems in a variety of fields, such as analytical chemistry, biochemistry, pharmaceutical sciences, diagnostics and therapy, food safety and environmental protection.

STEM WORKSHOP – ADVANCED USES OF ARDUINOS*

Celeste Morris, *Northern Kentucky University*

Monday 9:00 am – 12:00 pm

*Attendee must bring laptop for workshop program to be uploaded

This hands-on workshop will be an opportunity for participants to learn about Arduinos and electronics for making basic scientific measurements. Arduinos, low-cost microcontrollers, are an ideal platform for creating simple and/or portable instruments for laboratory and education applications. We will explore electronic signals and use circuitry components, sensors, and arduino programs to create light, motion, and temperature sensors. More complex instrumentation for scientific applications such as an Arduino-powered UV/Vis spectrophotometer and a pH meter will be presented. No prior knowledge about circuitry, electronics, or computer coding is necessary, but participants are encouraged to bring a laptop and download arduino software compatible with their device from www.arduino.cc prior to the workshop. We encourage hobbyists, students, and educators to participate in this workshop for fun, to garner ideas for technology incorporation in teaching, and for cost-effective instrument development.

Note: Complimentary Arduino kits will be provided to the first 45 registrants (Sunday AM and Monday AM courses combined)

CLASSICAL LEAST SQUARES MODELS

Barry Wise, *Eigenvector*

Monday 9:00 am – 12:00 pm

Principal components analysis (PCA) and inverse least squares (ILS) methods such as partial least squares (PLS) are ubiquitous to chemometrics. However, classical least squares (CLS or forward least squares) techniques are seeing resurgence in popularity. Two major reasons are better interpretability and the ability to control aspects of the regression modeling. As with ILS, CLS methods can be used for exploratory analysis, detection, classification and quantification. This half-day course will start by covering CLS regression methods including classical, extended, weighted and generalized least squares. It will be shown how these methods can be used to account for interferents (i.e. analytes other than the one of interest) in spectroscopic systems. CLS also provides a natural framework for the development of popular de-cluttering methods such as External Parameter Orthogonalization (EPO) and Generalized Least Squares (GLS) weighting. The course includes hands-on computer time to work through example problems. It will also be shown how constraints can be easily employed with these methods to allow greater control over the modeling.

CALIBRATION MODEL MAINTENANCE

Barry Wise, *Eigenvector*

Monday 1:00 - 4:00 pm

Model maintenance can be defined as the on-going servicing of (primarily) multivariate calibration and fault detection models in order to preserve their predictive abilities. It is required because of changes to either the sample matrices or the instrument response. The goal of model maintenance is to sustain or improve models over time and changing conditions with the least amount of cost and effort. This course presents a roadmap for determining when model maintenance is required, the probable source of the response variations, and the appropriate approaches for achieving it. Hands-on exercises will be done using **MATLAB** and **PLS_Toolbox**.

3M FIELD TRIP

Monday 3:00 - 5:00 pm

The centerpiece of the 3M Innovation Center is the World of 3M Innovation. The World of 3M Innovation is comprised of interactive displays, films, presentations and stories. Join us on a tour of this fascinating local company. Shuttle bus will depart at 3:00 pm from the Hyatt Regency Hotel. Ticket required. Open to conference attendees and companions. *Shuttle bus will depart from the Hyatt Hotel promptly at 3:00 pm*

WORKSHOPS

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INTRODUCTION TO DOE AND CHEMOMETRICS

Heather Brooke, CAMO Software and Pat Whitcomb, Stat-Ease, Inc
Tuesday 9:00 am - 4:00 pm

Learn how design of experiments (DOE) and multivariate analysis (MVA) methods can be used together to optimize products and processes. First we will focus on using modern DOE tools, exploring relevant case studies to learn how to build designs and analyze your experimental data. Then we will discover how MVA methods can be used to gain a deeper understanding of your data and potentially replace time-consuming, difficult, or expensive “traditional” testing. We will wrap up the session by demonstrating how to build an optimal design from principal components and use the DOE results to find an optimal compound.

This will open new doors for researchers and data analysts with large or complex data sets. Scientists working in process analysis, chemometrics, spectroscopy, metabolomics or sensometrics, will gain valuable insights on how to enhance their work. Bring your laptops to get hands-on experience with Design-Expert® software from Stat-Ease and Unscrambler® software from Camo (time-limited copies will be provided).

STEM WORKSHOP: FLIPPING THE ANALYTICAL CHEMISTRY CLASSROOM

Christopher Harrison, San Diego State University

Tuesday 1:00 - 4:00 pm

Professor Christopher Harrison from San Diego State University has been using video demonstrations of laboratory techniques for over 8 years, and has been using a flipped classroom for his Analytical Chemistry course for the past three years with significant success. In this workshop professor Harrison will guide participants through best practices of developing and implementing recorded lecture materials, and considerations for how to make use of the classroom lecture time.

The workshop will provide participants with the opportunity to practice making their own recorded lectures, and peer evaluations of the final results. Participants are strongly encouraged to bring current classroom lecture materials with them to the workshop to develop these into flipped materials. Participants should also bring their own laptop, tablet and/or smartphone to the workshop.

HOW TO GET PUBLISHED

Louisa Strain, Naomi Blumson, SAGE Publishing and
Kristin MacDonald, Applied Spectroscopy

Tuesday 2:00 - 3:30 pm

This workshop will cover the fundamentals of preparing a manuscript for publication in an academic journal with direct reference to the Society of Applied Spectroscopy's own journal *Applied Spectroscopy*. The workshop will include an overview of the publishing landscape; how the publishing landscape is evolving; how to select a relevant publication; preparing your manuscript for submission to a journal; an overview of the peer review process; publication ethics and author rights and how to promote your article once published.

INTRO TO HPLC FOR NON-CHROMATOGRAPHERS

David Johnson, 3M and **Larry Felice**, Aspen Research Corp.

Wednesday 9:00 am - 4:00 pm

Designed for the novice chromatographer, this course will explore some of the fundamental concepts of HPLC. After establishing a foundation in basic chromatographic theory, concepts like manipulating resolution, understanding and minimizing band broadening, column selection (chemistry, format, and geometry) and detector selection will be investigated. At the end of our session we will attempt to synthesize these concepts by applying them to real method development scenarios. Topics will include an overview of basic chromatographic theory, exploring the parameters that impact resolution and their relative contributions, an overview of column chemistry fundamentals (silica types, bonding chemistry, endcapping), reverse phase solvents, reverse phase method development fundamentals, improving resolution in reverse phase systems, selectivity, pH affects, gradients, parameters that impact band broadening (both column and non-column contributions), and practical implications of the van Deemter equation. Time permitting; we will also explore advanced concepts in reverse phase chromatography (e.g. high vs. low pressure mixing, dwell volume, solvent purity, solvent viscosity, bonded phase stability). This session will also include a brief discussion about the strengths and limitations of the most commonly used LC detectors (UV-VIS, fluorescence, electro-chemical, conductivity, ELSD, and MS).

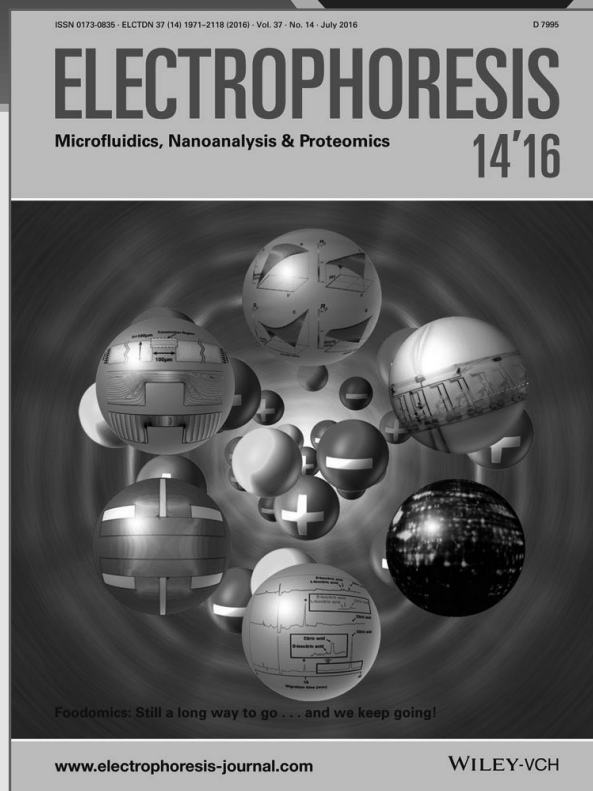
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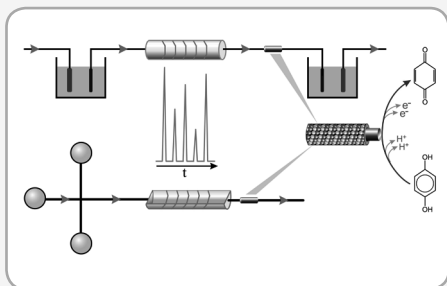
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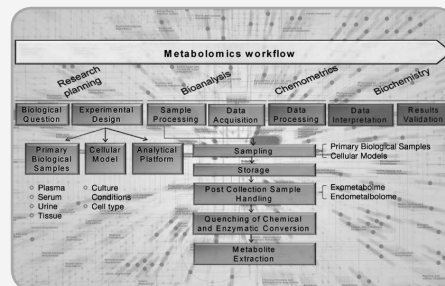
Electrochemistry

Submission deadline: November 15, 2016



Metabolomics

Submission deadline: January 15, 2017



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WILEY

PROGRAM OVERVIEW

SUNDAY	
4:20 – 6:00 pm	“What’s Hot” Vendor Presentations, <i>Nicollet B/C, page 52</i>
6:15 pm	KEYNOTE LECTURE. Democratization of Next-Generation Microscopy, Sensing and Diagnostics Tools through Computational Photonics; Aydogan Ozcan, <i>Nicollet B/C, page 52</i>
7:00 – 9:00 pm	Welcome Mixer, SAS Sponsored Student Poster Session, Coblenz Student Awards, FACSS Student and Tomas Hirschfeld Scholar Awards, <i>Nicollet A</i>

MONDAY MORNING	
7:50 am	Opening Address PLENARY LECTURES <i>Nicollet B/C, page 53</i>
8:00 am	Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award. Matthew Baker
8:30 am	ITP PLENARY LECTURE. Norman Dovichi
9:15 am	SYMPOSIA, page 53 Fundamentals and Novel Applications of Glow Discharge Spectroscopy, <i>Greenway A</i> Trace Detection in Forensics, <i>Lakeshore B</i> Molecular Spectroscopy - Selected Contributed Papers, <i>Greenway G</i> ITP - Dielectrophoresis I – Fundamentals, <i>Nicollet D2/D3</i> ITP - Electrophoresis - Instrumentation and Detection, <i>Nicollet B/C</i> LIBS Imaging, <i>Greenway J</i> Semiconducting Nanomaterials for Solar Energy Applications, <i>Greenway E</i> Raman and NIR Screening of Small Molecules and Biologics Based Counterfeits, <i>Greenway B/C</i> Emerging Raman I, <i>Nicollet D1</i> Raman Microscopy, <i>Lakeshore A</i> Topics in Microscopy, <i>Greenway H/I</i> Topics in Spectroscopy, <i>Greenway D</i> New Directions in Nanoplasmonics, <i>Lakeshore C</i>
11:00 am	POSTER SESSION AND BREAK, <i>Nicollet A,</i> page 56 Art & Archaeology Biomedical and Bioanalytical Sciences - Session I Forensics & Security Molecular/IR ITP - Electroreparation Methods Mass Spectrometry Raman SERS Deep and Far UV Spectroscopy XRay Fluorescence

MONDAY AFTERNOON	
1:20 pm	SYMPOSIA, page 60 Novel Applications of Laser Ablation - ICPMS and Related Techniques, <i>Greenway A</i> RSC Awards Symposium, <i>Greenway H/I</i> CLIRSPEC: Biological Fluids in Health and Disease, <i>Greenway G</i> New Frontiers in Chemometrics, <i>Greenway D</i> Nanoscale IR Spectroscopy, <i>Lakeshore B</i> ITP - Biomedical and Bioanalysis, <i>Nicollet D2/D3</i> ITP - Fundamentals of Electrophoresis, <i>Nicollet B/C</i> Nano-Facilitated Sensing, <i>Greenway E</i> Counterfeit Challenges in Biopharmaceuticals, <i>Greenway B/C</i> Bioanalytical SERS I, <i>Nicollet D1</i>

3:00 pm	Portable Raman, <i>Lakeshore A</i> New Directions in Plasmonic Applications and Instrumentation, <i>Lakeshore C</i> Topics in Mass Spectrometry, <i>Greenway J</i>
3:50 pm	POSTER VIEWING AND BREAK, <i>Nicollet A</i> SYMPOSIA, page 63 RSC-ACS Symposium - Solving Global Health Challenges: Elemental Techniques towards Characterization, Diagnostics, and Detection, <i>Greenway E</i> Innovations and Applications in X-Ray Fluorescence Spectrometry, <i>Greenway A</i> <i>Spectroscopy</i> Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Matthew Baker, <i>Greenway H/I</i> Vibrational Spectroscopy and Advanced Statistics for Medical Diagnostics, <i>Greenway G</i> Current Applications of Diffuse Reflectance Spectroscopy, <i>Lakeshore B</i> ITP - Microfluidics and Minaturization, <i>Nicollet D2/D3</i> ITP - Capillary Electrophoresis Applications, <i>Nicollet B/C</i> Integration of LIBS in the Analytical Laboratory, <i>Greenway J</i> Ion Mobility: Adding New Dimensions, <i>Greenway B/C</i> SAS PAT Technical Section: PAT in the Pharmaceutical Industries Session I, <i>Lakeshore C</i> Bioanalytical SERS II, <i>Nicollet D1</i> Industrial Raman, <i>Lakeshore A</i> Innovative Approaches to Teaching Analytical Chemistry, <i>Greenway D</i>

TUESDAY MORNING	
8:00 am	PLENARY LECTURES, <i>Nicollet B/C, page 66</i> Charles Mann Award for Raman Spectroscopy. Brian Marquardt
8:30 am	Coblenz Society Craver Award. Karen Faulds
9:15 am	SYMPOSIA, page 66 Atmospheric-pressure Plasmas as Tools for Atomic Analyses, Molecular Mass Spectrometry, and Chemical Synthesis, <i>Greenway A</i> Charles Mann Award Symposium Honoring Brian Marquardt, <i>Greenway H/I</i> Multimodal Imaging for Biomedical Diagnosis and Therapy Monitoring, <i>Greenway G</i> Nuclear Forensics, <i>Greenway D</i> Nano-IR/Nano-Raman - I, <i>Lakeshore B</i> ITP - Sample Preparation / Concentration, <i>Nicollet D2/D3</i> ITP - Proteomics /Glycoproteomics, <i>Nicollet B/C</i> Automated LIBS for Process Control, <i>Greenway J</i> Solving Industrial Problems with Vibrational Spectroscopy, <i>Greenway B/C</i> Emerging Raman II, <i>Nicollet D1</i> Bioanalytical SERS III, <i>Lakeshore A</i> Bottom-up Plasmonic Nanoparticles: Spectroscopic Applications, <i>Lakeshore C</i> IR, Raman and Nonlinear Spectroscopies of Surfaces & Boundaries, <i>Greenway E</i>

PROGRAM OVERVIEW

TUESDAY MORNING, continued			
11:00 am	POSTER SESSION AND BREAK , <i>Exhibit Hall</i> , page 68 ITP - Liquid Phase Separation Methods LIBS Raman	9:15 am	SYMPOSIA , page 78 Bioelectrokinetics: Biomolecules and Particles, <i>Greenway J</i> Glow Discharge Spectroscopy and Related Techniques, <i>Greenway A</i> ANACHEM Award Symposium Honoring Paul Cremer, <i>Greenway H/I</i> Chemometric Opportunities in Forensic Chemistry, <i>Greenway G</i> Quantum Cascade Lasers–II, <i>Lakeshore B</i> ITP - DNA Sequencing and Electrophoresis, <i>Nicollet B/C</i> ITP - Metabolomics, <i>Nicollet D2/D3</i> High-sensitivity Mass Spectrometry for Basic and Translational Research, <i>Greenway B/C</i> Biotemplate-Based Nanomaterials for Energy Applications, <i>Lakeshore A</i> Online Analysis of Industrial Processes and Reactions, <i>Greenway D</i> Standoff Raman Spectroscopy: Instrumentation and Applications, <i>Nicollet D1</i> The Power of Many: Supporting Diversity in Analytical Chemistry, <i>Greenway E</i> Surface Analysis of Biomaterials and Biological Materials, <i>Lakeshore C</i>
11:40 am	What's Hot Exhibitor Presentations, <i>Exhibit Hall</i> , page 71		
TUESDAY AFTERNOON			
Noon	Complimentary lunch in exhibit hall for all registered conferees		
1:20 pm	SYMPOSIA , page 71 Fundamentals and Applications of Laser Ablation, <i>Greenway A</i> Coblentz Craver Award Symposium Honoring Karen Faulds, <i>Greenway H/I</i> SERS and SESORS for Biomedical Applications, <i>Greenway G</i> Nano-IR / Nano Raman II, <i>Lakeshore B</i> ITP – HPLC and LC-MS, <i>Nicollet B/C</i> ITP – Delectrophoresis II – Applications and Methodologies, <i>Nicollet D2/D3</i> Fusion of LIBS with Other Techniques, <i>Greenway J</i> Ion Mobility: New Insights into Assembly, Interactions, and Structures, <i>Greenway B/C</i> Process Analytical Technology in the Biopharmaceutical Industries Session II, <i>Greenway D</i> Spatially Offset Raman Spectroscopy (SORS), <i>Nicollet D1</i> Raman SERS, <i>Lakeshore A</i> Bottom-up Plasmonic Nanoparticles: Synthetic Strategies, <i>Lakeshore C</i> Frontiers of Far-and Deep- Ultraviolet Spectroscopy I, <i>Greenway E</i>	11:00 am	POSTER SESSION AND BREAK , <i>Exhibit Hall</i> , page 80 Chemometrics Molecular Spectrometry - IR, Near IR, 2D Correlation, Imaging Mass Spectrometry Nanotechnology Raman - SERS/TERS Surface Plasmon Resonance and Surface Science
3:00 pm	POSTER VIEWING AND BREAK , <i>Exhibit Hall</i>	11:40 am	What's Hot Exhibitor Presentations, <i>Exhibit Hall</i> , page 83
3:50 pm	SYMPOSIA , page 74 Celebrating the Life and Legacy of Professor Joe Caruso, <i>Greenway A</i> Lipids and Lipodomics in Health and Disease, <i>Greenway G</i> Chemometrics in Chemical and Biological Imaging: From macro- to nano-, <i>Nicollet D2/D3</i> Quantum Cascade Lasers – I, <i>Lakeshore B</i> ITP - Youngs Scientists, <i>Nicollet B/C</i> Clinical and Forensic Applications of Ambient Ionization Mass Spectrometry, <i>Greenway J</i> Sustainable Nanotechnology, <i>Lakeshore C</i> Industrial Applications of Vibrational Spectroscopy, <i>Greenway D</i> Low Frequency Raman, a Pharmaceutical Approach, <i>Greenway B/C</i> Nano-IR/Nano-Raman- III, <i>Nicollet D1</i> Raman Spectroscopy for Security and Forensics Purposes, <i>Lakeshore A</i> Frontiers of Far-and Deep- Ultraviolet Spectroscopy II, <i>Greenway E</i>		
WEDNESDAY MORNING			
8:00 am	PLENARY LECTURES , <i>Nicollet B/C</i> , page 78 ANACHEM Award . Paul Cremer	Noon	Complimentary lunch in exhibit hall for all registered conferees
8:30 am	SAS's Applied Spectroscopy William F. Meggers Award . Mike George	1:20 pm	SYMPOSIA , page 83 RSC-ACS Symposium - Solving Global Health Challenges: Molecular Techniques towards Diagnostics and Detection, <i>Nicollet D2/D3</i> Micro- and Nanofluidics for Preparation, Separation and Detection of Biomolecules and Cells, <i>Greenway J</i> ICPMS: Fundamentals & Applications, <i>Greenway A</i> Meggers Award Symposium Honoring Mike George, <i>Greenway H/I</i> CLIRSPEC Biomedical Applications of Near-field Infrared Spectroscopy, <i>Greenway G</i> CLIRSPEC: Clinical Applications of IR Spectroscopy and Imaging, <i>Lakeshore B</i> ITP Closing Keynote Lectures I, <i>Nicollet B/C</i> ITP Closing Keynotes Lectures II, <i>Calhoun</i> Fundamentals of LIBS for Enhanced Analytical Performance, <i>Greenway B/C</i> Advances in On-line Process Analysis, <i>Greenway D</i> Novel Approaches to Biopharmaceutical Analysis, <i>Lakeshore C</i> Raman Spectroscopic Sensing, <i>Nicollet D1</i> Pharmaceutical Raman, <i>Lakeshore A</i> Making the Leap: Pathways from Graduate School to a Permanent Position, <i>Greenway E</i>

PROGRAM OVERVIEW

WEDNESDAY AFTERNOON, continued

- 3:00 pm **POSTER VIEWING AND BREAK**
Exhibit Hall
- 3:05 pm **ITP CLOSING PLENARY AND CLOSING REMARKS**, *Nicollet B/C*, page 85
- 3:50 pm **SYMPOSIA**, page 86
Nanoscopic Porous Sensors, *Greenway J*
Atomic Spectrometry with Glow Discharges at Atmospheric Pressure, *Greenway A*
Clinical Biomedical Imaging, *Greenway G*
Rethinking Calibration, *Nicollet D2/D3*
Forensic Analysis: From the Lab to the Crime Scene, *Greenway D*
Decoding Circulating Biomarkers with Spectroscopy: Next Generation Assays, *Lakeshore B*
Recent Advances in Spray Ionization Mass Spectrometry, *Greenway B/C*
Infrared and Raman Spectroscopy Group, *Nicollet D1*
Nano-Raman, *Lakeshore A*
Chemistry in Art and Archaeology, *Greenway H/I*
Recent Developments on Mass Cytometric Analysis, *Greenway E*
Bioanalytical Applications of Plasmonics, *Lakeshore C*

THURSDAY MORNING

- 8:00 am **PLENARY LECTURES**, *Nicollet B/C*, page 89
Lester W. Strock Award. Raymond Arvidson
- 8:30 am **AES Mid Career Award**. Amy Herr
- 9:15 am **SYMPOSIA**, page 89
Capillary Electrophoresis-Mass Spectrometry for Ultrasensitive Bioanalyses, *Greenway J*
Development and Applications of Atmospheric Pressure Glow Discharges, *Greenway A*
Lester Strock Award Symposium Honoring Raymond Arvidson, *Greenway H/I*
Novel Biomedical Technologies, *Greenway G*
Metabolite Pattern Recognition: The Key to Authentication, *Nicollet D2/D3*
Two-Dimensional Correlation Analysis – I, *Lakeshore B*
Mass Spectrometry-Based Metabolomics, *Greenway B/C*
Topics in Nanotechnology, *Lakeshore C*
PAT: Flow Chemistry and Continuous Manufacturing Monitoring, *Greenway E*
Chirality in Pharma, *Nicollet B/C*

Biomedical Raman Spectroscopy (CLIRSPEC), *Nicollet D1*

Bio Raman, *Lakeshore A*

Application of Photoelectron Spectroscopy Techniques to Analysis of Nanomaterials & Devices, *Greenway D*

- 11:00 am **POSTER SESSION**, *Nicollet A*, page 91
Electrokinetics-AES
Atomic Spectroscopy
Biomedical and Bioanalytical Sciences
Chromatography
Environmental and Oceanographic Sciences
LIBS
Microscopy and Materials Characterization
Process Analytical Technology
Pharmaceutical Analysis

THURSDAY AFTERNOON

- 1:20 pm **SYMPOSIA**, page 95
AES Mid-Career Award Symposium Honoring Amy Herr, *Greenway H/I*
Clinical Vibrational Spectroscopy, *Greenway G*
The Good, the Bad and the Ugly: Finding the Helpful Variables and Removing the Harmful Variables in Data, *Nicollet D2/D3*
CBRNE Detection, *Lakeshore C*
Two-Dimensional Correlation Analysis – II, *Lakeshore B*
LIBS for Forensic Analysis, *Greenway D*
Rapid Testing Using Field-Deployable Spectrometers, *Greenway J*
Pharmaceutical Applications of Transmission Raman Spectroscopy, *Nicollet D1*
Analytical Chemists Easing World Poverty, *Greenway E*
Handheld and Portable Spectroscopy Applications, *Lakeshore A*
Topics in Microfluidics, *Nicollet B/C*
Topics in Chromatography, *Greenway B/C*
Scanning Probe Methods for Surface Science Problems, *Greenway A*
- 3:00 PM **POSTER VIEWING AND BREAK**, *Nicollet A*
- 3:50 pm **PLENARY SESSION**, *Nicollet B/C*, page 97
FACSS Distinguished Service Award
FACSS Innovation Award Symposium

FRIDAY MORNING SPECIAL PLENARY SESSION

Lakeshore A, Page 98

- 8:00 am Announcement of Innovation Award Winners ,
- 8:15 am Science Beyond Borders
- 10:15 am SciX 2017 Preview



WEDNESDAY EVENING EVENT, 6:00 PM

AN ALL INCLUSIVE EVENT

Great Lakes Ballroom

The Great Outdoors Theme Party

Come experience the Great Outdoors of Minnesota at SciX 2016 in Minneapolis! Break out your favorite flannel shirt and be prepared for some outdoor fun at the Wednesday Evening Event. Think fishing, canoeing, hiking, and moose! The evening would not be complete without a DJ playing a wide variety of music and the opportunity to perform Karaoke. Enjoy an evening of food, beverage, and entertainment with your colleagues.

TECHNICAL PROGRAM OVERVIEW

ATOMIC SPECTROSCOPY

Monday (9:15 am session)

Fundamentals and Novel Applications of Glow Discharge Spectroscopy, *Greenway A*

Monday (1:20 pm session)

Novel Applications of Laser Ablation - ICPMS and Related Techniques, *Greenway A*

Monday (3:50 pm session)

Innovations and Applications in X-Ray Fluorescence Spectrometry, *Greenway A*

Tuesday (9:15 am session)

Atmospheric-pressure Plasmas as Tools for Atomic Analyses, Molecular Mass Spectrometry, and Chemical Synthesis, *Greenway A*

Tuesday (1:20 pm session)

Fundamentals and Applications of Laser Ablation, *Greenway A*

Tuesday (3:50 pm session)

Celebrating the Life and Legacy of Professor Joe Caruso, *Greenway A*

Wednesday (9:15 am session)

Glow Discharge Spectroscopy and Related Techniques, *Greenway A*

Wednesday (1:20 pm session)

ICPMS: Fundamentals and Applications, *Greenway A*

Wednesday (3:50 pm session)

Atomic Spectrometry with Glow Discharges at Atmospheric Pressure, *Greenway A*

Thursday (9:15 am session)

Development and Applications of Atmospheric Pressure Glow Discharges, *Greenway A*

AWARDS

Monday (1:20 pm session)

RSC Awards Symposium, *Greenway H/I*

Monday (3:50 pm session)

Spectroscopy Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Matthew Baker, *Greenway H/I*

Tuesday (9:15 am session)

Charles Mann Award Symposium Honoring Brian Marquart, *Greenway H/I*

Tuesday (1:20 pm session)

Coblentz Craver Award Symposium Honoring Karen Faulds, *Greenway H/I*

Wednesday (9:15 am session)

ANACHEM Award Symposium Honoring Paul Cremer, *Greenway H/I*

Wednesday (1:20 pm session)

Meggers Award Symposium Honoring Mike George, *Greenway H/I*

Thursday (9:15 am session)

Lester Strock Award Symposium Honoring Raymond Arvidson, *Greenway H/I*

Thursday (1:20 pm session)

AES Mid-Career Award Symposium Honoring Amy Herr, *Greenway H/I*

Thursday (3:50 pm session)

FACSS Innovation Award Symposium, *Nicollet B/C*

BIOLOGICAL/BIOMEDICAL

Monday (1:20 pm session)

CLIRSPEC: Biological Fluids in Health and Disease, *Greenway G*

Monday (3:50 pm session)

Vibrational Spectroscopy and Advanced Statistics for Medical Diagnostics, *Greenway G*

Tuesday (9:15 am session)

Multimodal Imaging for Biomedical Diagnosis and Therapy Monitoring, *Greenway G*

Tuesday (1:20 pm session)

SERS and SESORS for Biomedical Applications, *Greenway G*

Tuesday (3:50 pm session)

Lipids and Lipodomics in Health and Disease, *Greenway G*

Wednesday (1:20 pm session)

CLIRSPEC Biomedical Applications of Near-field Infrared Spectroscopy, *Greenway G*

Wednesday (3:50 pm session)

Clinical Biomedical Imaging, *Greenway G*

Thursday (9:15 am session)

Novel Biomedical Technologies, *Greenway G*

Thursday (1:20 pm session)

Clinical Vibrational Spectroscopy, *Greenway G*

CHEMOMETRICS

Monday (1:20 pm session)

New Frontiers in Chemometrics, *Greenway D*

Tuesday (3:50 pm session)

Chemometrics in Chemical and Biological Imaging: From macro- to nano-, *Nicollet D2/D3*

Wednesday (9:15 am session)

Chemometric Opportunities in Forensic Chemistry, *Greenway G*

Wednesday (3:50 pm session)

Rethinking Calibration, *Nicollet D2/D3*

Thursday (9:15 am session)

Metabolite Pattern Recognition: The Key to Authentication, *Nicollet D2/D3*

Thursday (1:20 pm session)

The Good, the Bad and the Ugly: Finding the Helpful Variables and Removing the Harmful Variables in Data, *Nicollet D2/D3*

ELECTRO- AND LIQUID PHASE-SEPARATION TECHNIQUES (ITP)

Monday (9:15 am session)

Dielectrophoresis I - Fundamentals, *Nicollet D2/D3*

Electrophoresis - Instrumentation and Detection, *Nicollet B/C*

Monday (1:20 pm session)

Biomedical and Bioanalysis, *Nicollet D2/D3*

Fundamentals of Electrophoresis, *Nicollet B/C*

Monday (3:50 pm session)

Microfluidics and Minaturization, *Nicollet D2/D3*

Capillary Electrophoresis Applications, *Nicollet B/C*

Tuesday (9:15 am session)

Sample Preparation / Concentration, *Nicollet D2/D3*

Proteomics / Glycoproteomics, *Nicollet B/C*

Tuesday (1:20 pm session)

Dielectrophoresis II - Applications and Methodologies, *Nicollet D2/D3*

HPLC and LC-MS, *Nicollet B/C*

Tuesday (3:50 pm session)

Youngs Scientists, *Nicollet B/C*

Wednesday (9:15 am session)

DNA Sequencing and Electrophoresis, *Nicollet B/C*

Metabolomics, *Nicollet D2/D3*

Wednesday (1:20 pm session)

ITP Closing Keynote Lectures I, *Nicollet B/C*

ITP Closing Keynote Lectures II, *Calhoun*

Wednesday (3:05 pm session)

ITP Closing Plenary and Closing Remarks, *Nicollet B/C*

TECHNICAL PROGRAM OVERVIEW

ELECTROPHORESIS AND MIROFLUIDICS

Wednesday (9:15 am session)

Bioelectrokinetics: Biomolecules and Particles, *Greenway J*

Wednesday (1:20 pm session)

Micro- and Nanofluidics for Preparation, Separation and Detection of Biomolecules and Cells, *Greenway J*

Wednesday (3:50 pm session)

Nanoscope Porous Sensors, *Greenway J*

Thursday (9:15 am)

Capillary Electrophoresis-Mass Spectrometry for Ultrasensitive Bioanalyses, *Greenway J*

FORENSICS AND SECURITY

Monday (9:15 am session)

Trace Detection in Forensics, *Lakeshore B*

Tuesday (9:15 am session)

Nuclear Forensics, *Greenway D*

Wednesday (3:50 pm session)

Forensic Analysis: From the Lab to the Crime Scene, *Greenway D*

Thursday (1:20 pm session)

CBRNE Detection, *Lakeshore C*

LASER INDUCED BREAKDOWN SPECTROSCOPY

Monday (9:15 am session)

LIBS Imaging, *Greenway J*

Monday (3:50 pm session)

Integration of LIBS in the Analytical Laboratory, *Greenway J*

Tuesday (9:15 am session)

Automated LIBS for Process Control, *Greenway J*

Tuesday (1:20 pm session)

Fusion of LIBS with Other Techniques, *Greenway J*

Wednesday (1:20 pm session)

Fundamentals of LIBS for Enhanced Analytical Performance, *Greenway B/C*

Thursday (1:20 pm session)

LIBS for Forensic Analysis, *Greenway D*

MASS SPECTROMETRY

Monday (1:20 pm session)

Topics in Mass Spectrometry, *Greenway J*

Monday (3:50 pm session)

Ion Mobility: Adding New Dimensions, *Greenway B/C*

Tuesday (1:20 pm session)

Ion Mobility: New Insights into Assembly, Interactions, and Structures, *Greenway B/C*

Tuesday (3:50 pm session)

Clinical and Forensic Applications of Ambient Ionization Mass Spectrometry, *Greenway J*

Wednesday (9:15 am session)

High-sensitivity Mass Spectrometry for Basic and Translational Research, *Greenway B/C*

Wednesday (3:50 pm session)

Recent Advances in Spray Ionization MS, *Greenway B/C*

Thursday (9:15 am session)

Mass Spectrometry-Based Metabolomics, *Greenway B/C*

MOLECULAR (IR AND NEAR IR)

Monday (9:15 am session)

Molecular Spectroscopy - Contributed Papers, *Greenway G*

Monday (1:20 pm session)

Nanoscale IR Spectroscopy, *Lakeshore B*

Monday (3:50 pm session)

Current Applications of Diffuse Reflectance Spectroscopy, *Lakeshore B*

Tuesday (9:15 am session)

Nano-IR/Nano-Raman - I, *Lakeshore B*

Tuesday (1:20 pm session)

Nano-IR/Nano-Raman - II, *Lakeshore B*

Tuesday (3:50 pm session)

Quantum Cascade Lasers - I, *Lakeshore B*

Wednesday (9:15 am session)

Quantum Cascade Lasers - II, *Lakeshore B*

Wednesday (1:20 pm session)

CLIRSPEC: Clinical Applications of IR Spectroscopy and Imaging, *Lakeshore B*

Wednesday (3:50 pm session)

Decoding Circulating Biomarkers with Spectroscopy: Next Generation Assays, *Lakeshore B*

Thursday (9:15 am session)

Two-Dimensional Correlation Analysis - I, *Lakeshore B*

Thursday (1:20 pm session)

Two-Dimensional Correlation Analysis - II, *Lakeshore B*

NANOTECHNOLOGY

Monday (9:15 am session)

Semiconducting Nanomaterials for Solar Energy Applications, *Greenway E*

Monday (1:20 pm session)

Nano-Facilitated Sensing, *Greenway E*

Tuesday (3:50 pm session)

Sustainable Nanotechnology, *Lakeshore C*

Wednesday (9:15 am session)

Bioteplate-Based Nanomaterials for Energy Applications, *Lakeshore A*

Thursday (9:15 am session)

Topics in Nanotechnology, *Lakeshore C*

PHARMACEUTICAL SPECTROSCOPY

Monday (9:15 am session)

Raman and NIR Screening of Small Molecules and Biologics Based Counterfeits, *Greenway B/C*

Monday (1:20 pm session)

Counterfeit Challenges in Biopharmaceuticals, *Greenway B/C*

Tuesday (9:15 am session)

Solving Industrial Problems with Vibrational Spectroscopy, *Greenway B/C*

Tuesday (3:50 pm session)

Low Frequency Raman, a Pharmaceutical Approach, *Greenway B/C*

Wednesday (1:20 pm session)

Novel Approaches to Biopharmaceutical Analysis, *Lakeshore C*

Thursday (9:15 am session)

A Chirality in Pharma, *Nicollet B/C*

PROCESS ANALYTICAL SPECTROSCOPY SURFACE SCIENCE

Monday (3:50 pm session)

SAS PAT Technical section: PAT in the Pharmaceutical Industries Session I, *Lakeshore C*

Tuesday (1:20 pm session)

Process Analytical Technology in the Biopharmaceutical Industries Session II, *Greenway D*

Tuesday (3:50 pm session)

Industrial Applications of Vibrational Spectroscopy, *Greenway D*

Wednesday (9:15 am session)

Online Analysis of Industrial Processes and Reactions, *Greenway D*

Wednesday (1:20 pm session)

Advances in On-line Process Analysis, *Greenway D*

Thursday (9:15 am session)

PAT: Flow Chemistry and Continuous Manufacturing Monitoring, *Greenway E*

Thursday (1:20 pm session)

Rapid Testing Using Field-Deployable Spectrometers, *Greenway J*

TECHNICAL PROGRAM OVERVIEW

RAMAN

Monday (9:15 am session)

Emerging Raman I, *Nicollet D1*
Raman Microscopy, *Lakeshore A*

Monday (1:20 pm session)

Bioanalytical SERS I, *Nicollet D1*
Portable Raman, *Lakeshore A*

Monday (3:50 pm session)

Bioanalytical SERS II, *Nicollet D1*
Industrial Raman, *Lakeshore A*

Tuesday (9:15 am session)

Emerging Raman II, *Nicollet D1*
Bioanalytical SERS III, *Lakeshore A*

Tuesday (1:20 pm session)

Spatially Offset Raman Spectroscopy (SORS), *Nicollet D1*
SERS, *Lakeshore A*

Tuesday (3:50 pm session)

Nano-IR/Nano-Raman- III, *Nicollet D1*
Raman Spectroscopy for Security and Forensics Purposes,
Lakeshore A

Wednesday (9:15 am session)

Standoff Raman Spectroscopy: Instrumentation and
Applications, *Nicollet D1*

Wednesday (1:20 pm session)

Raman Spectroscopic Sensing, *Nicollet D1*
Pharmaceutical Raman, *Lakeshore A*

Wednesday (3:50 pm session)

Infrared and Raman Spectroscopy Group, *Nicollet D1*
Nano-Raman, *Lakeshore A*

Thursday (9:15 am session)

Biomedical Raman Spectroscopy (CLIRSPEC), *Nicollet D1*
Bio Raman, *Lakeshore A*

Thursday (1:20 pm session)

Pharmaceutical Applications of Transmission Raman
Spectroscopy, *Nicollet D1*

SPECIAL TOPICS

Monday (9:15 am session)

Topics in Microscopy, *Greenway H/I*
Topics in Spectroscopy, *Greenway D*

Monday (3:50 pm session)

Innovative Approaches to Teaching Analytical Chemistry,
Greenway D

Wednesday (9:15 am session)

The Power of Many: Supporting Diversity in Analytical
Chemistry, *Greenway E*

Wednesday (1:20 pm session)

Making the Leap: Pathways from Graduate School to a
Permanent Position, *Greenway E*

Wednesday (3:50 pm session)

Chemistry in Art and Archaeology, *Greenway H/I*
Recent Developments on Mass Cytometric Analysis,
Greenway E

Thursday (1:20 pm session)

Analytical Chemists Easing World Poverty, *Greenway E*
Handheld and Portable Spectroscopy Applications, *Lakeshore A*
Topics in Microfluidics, *Nicollet B/C*
Topics in Chromatography, *Greenway B/C*

Friday (8:00 am session)

Science Beyond Borders, *Lakeshore A*

SURFACE PLASMON RESONANCE

Monday (9:15 am session)

New Directions in Nanoplasmonics, *Lakeshore C*

Monday (1:20 pm session)

New Directions in Plasmonic Applications and
Instrumentation, *Lakeshore C*

Tuesday (9:15 am session)

Bottom-up Plasmonic Nanoparticles: Spectroscopic
Applications, *Lakeshore C*

Tuesday (1:20 pm session)

Bottom-up Plasmonic Nanoparticles: Synthetic Strategies
Lakeshore C

Wednesday (3:50 pm session)

Bioanalytical Applications of Plasmonics, *Lakeshore C*

SURFACE SCIENCE

Wednesday (9:15 am session)

Surface Analysis of Biomaterials and Biological Materials,
Lakeshore C

Thursday (9:15 am session)

Application of Photoelectron Spectroscopy Techniques to
Analysis of Nanomaterials and Devices, *Greenway D*

Thursday (1:20 pm session)

Scanning Probe Methods for Surface Science Problems,
Greenway A

SCIX 2016 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 Coblenz 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
9:00 am – Noon SciX Bike Ride	<i>Nicollet Promenade</i> 7:30 am Wake Up Coffee	<i>Nicollet Promenade</i> 7:30 am Wake Up Coffee	<i>Nicollet Promenade</i> 7:30 am Wake Up Coffee	<i>Nicollet Promenade</i> 7:30 am Wake Up Coffee	<i>Lakeshore Prefunction</i> 7:30 am Wake Up Coffee and Muffins
9:00 am – 5:00 pm Workshops	<i>Nicollet B/C</i> 7:50 am Opening Remarks Alexandra Ros 8:00 am <i>Spectroscopy Magazine's</i> Emerging Leader in Molecular Spectroscopy Award Matthew Baker, <i>University of Strathclyde</i> 8:30 am ITP Plenary Lecture Norman Dovichi, <i>University of Notre Dame</i>	<i>Nicollet B/C</i> 8:00 am FACSS Charles Mann Award for Applied Raman Spectroscopy Brian Marquardt, <i>University of Washington</i> 8:30 am Coblentz Society Craver Award Karen Faulds, <i>University of Strathclyde</i>	<i>Nicollet B/C</i> 8:00 am ANACHEM Award Paul Cremer, <i>Pennsylvania State University</i> 8:30 am Applied Spectroscopy William F. Meggers Award Mike George, <i>Nottingham University</i>	<i>Nicollet B/C</i> 8:00 am Lester W. Strock Award Raymond Arvidson, <i>Washington University in Saint Louis</i> 8:30 am AES Mid Career Award Amy E. Herr, <i>UC Berkeley</i>	<i>Lakshore A</i> 8:00 – 10:30 am Announcement of Innovation Award Closing Session: Science Beyond Borders Preview of 2017 Conference
	9:00 – 4:30 pm Workshops	9:00 am – 4:00 pm Workshops	9:00 am – 4:30 pm Workshops		
		<i>Exhibit Hall</i> 10:00 am – 4:30 pm Exhibits Open	<i>Exhibit Hall</i> 10:00 am – 4:00 pm Exhibits Open		
	9:15 – 10:55 am Oral Symposia	9:15 – 10:55 am Oral Symposia	9:15 – 10:55 am Oral Symposia	9:15 – 10:55 am Oral Symposia	
	<i>Nicollet A</i> 11:00 – 12:00 pm Poster Session & Break	<i>Exhibit Hall</i> 11:00 – 12:00 pm Poster Session and Break	<i>Exhibit Hall</i> 11:00 – 12:00 pm Poster Session and Break	<i>Nicollet A</i> 11:00 – 12:00 pm Poster Session and Break	
		<i>Exhibit Hall</i> 11:40 am – 1:10 pm What's Hot Vendor Presentations	<i>Exhibit Hall</i> 11:40 am – 1:10 pm What's Hot Vendor Presentations		
	Noon Lunch on own	Noon Complimentary lunch in Exhibit Hall	Noon Complimentary lunch in Exhibit Hall	Noon Lunch on own	
	1:20 – 3:00 pm Oral Symposia	1:20 – 3:00 pm Oral Symposia	1:20 – 3:00 pm Oral Symposia	1:20 – 3:00 pm Oral Symposia	
	<i>Nicollet A</i> 3:00 – 3:50 Poster Viewing and Break	<i>Exhibit Hall</i> 3:00 – 3:50 Poster Viewing and Break	<i>Exhibit Hall</i> 3:00 – 3:50 Poster Viewing and Break	<i>Nicollet A</i> 3:00 – 3:50 Poster Viewing and Break	
<i>Nicollet B/C</i> 4:20 – 6:00 pm What's Hot Vendor Presentations	3:50 – 5:30 pm Oral Symposia	3:50 – 5:30 pm Oral Symposia	3:50 – 5:30 pm Oral Symposia	<i>Nicollet B/C</i> 3:50 – 5:30 pm Plenary Session FACSS DSA Awards Innovation Award Symposium	
<i>Nicollet B/C</i> 6:15 pm Keynote Lecture: Aydogan Ozcan <i>California NanoSystems Institute; UCLA</i>	<i>Exhibit Hall</i> 5:30 – 7:30 pm Exhibit Opening Reception	<i>Greenway H/I</i> 7:00 – 9:00 pm ITP Dinner Reception <i>Ticket Required</i>			
<i>Nicollet A</i> 7:15 – 9:15 pm Welcome Mixer and SAS Sponsored Student Poster Session Coblentz Student Awards FACSS Student and Tomas Hirschfeld Scholar Awards		<i>Great Lakes A</i> 6:00 pm Raman Reception, <i>Invitation Only</i> Sponsored by Kaiser Optical Systems, Inc.	<i>Great Lakes Ballroom</i> 6:00 pm Wednesday Evening All inclusive event		
		<i>Great Lakes B</i> 7:30 pm SAS Wine and Cheese Reception			

TECHNICAL PROGRAM

SUNDAY WORKSHOPS, see page 41 for a list

SUNDAY PROGRAM AND EVENTS

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

- 4:20 PM **Prism Analytical Technologies** "Introducing MAX™, a new GC-FTIR Gas Analyzer"
4:30 PM **Analytik Jena** "Sensitivity and Resolution - New Developments in Analytical Instruments"
4:40 PM **Keit Spectrometers** "Replacing off-line HPLC with Keit's in-line rugged FTIR: Case Studies from Bioprocess Industry"
4:50 PM **Hellma USA** "A New Raman Platform for Undergraduate Teaching and Research Laboratories"
5:00 PM **Bio-Rad, Informatics** "A Breakthrough Technology for IR & Raman Spectral Identification"
5:10 PM **MONTFORT Laser GmbH**
5:20 PM **Tornado Spectral Systems** "Taking Raman Spectroscopy by Storm"
5:30 PM **TSI Incorporated** "Solving Real-World Problems with TSI's ChemLogix Instruments"
5:40 PM **Bruker Corporation** "Advances in Raman Spectroscopy"
5:50 PM **Ibsen Photonics** "EAGLE Raman S, Cooler Than Ever"

6:15 **Keynote Lecture; Nicollet B/C**

(1) **Democratization of Next-Generation Microscopy, Sensing and Diagnostics Tools through Computational Photonics; Aydogan Ozcan**^{1,2}; ¹California NanoSystems Institute; ²University of California, Los Angeles

Dr. Ozcan is the Chancellor's Professor at UCLA and an HHMI Professor with the Howard Hughes Medical Institute, leading the Bio- and Nano-Photonics Laboratory at UCLA School of Engineering and is also the Associate Director of the California NanoSystems Institute (CNSI).



7:00 **Welcome Mixer**

SAS Sponsored Student Poster Session • Coblenz Student Awards • FACSS Student and Tomas Hirschfeld Scholar Awards – Nicollet A

TECHNICAL PROGRAM – MONDAY

Welcome – 7:50 am; Plenary Lectures – 8:00 am; *Nicollet B/C*

Presider: **Matthieu Baudelet**



8:00 am – Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award
(2) Serum Spectroscopic Diagnostics: The Future for Clinical Diagnostics?; Matthew Baker¹;
¹University of Strathclyde



8:30 am – ITP Plenary Lecture
(3) Capillary Electrophoresis for bottom-Up Proteomic Analysis of Complex Mixtures; Norman Dovichi¹, Liangliang Sun¹, Guijie Zhu¹; ¹University of Notre Dame

Orals 9:15 – 10:55 am

Monday Morning, *Greenway A* **FUNDAMENTALS AND NOVEL APPLICATIONS OF GLOW DISCHARGE SPECTROSCOPY**

Organizer: Jorge Pisonero; Presider: Matthieu Chausseau

- 9:15 (4) **Compressed Sensing Spectral Imaging Coupled to Glow Discharge Optical Emission Elemental Mapping;** Gerardo Gamez¹, John Usala¹, Adrian Maag², Thomas Nelis²; ¹Texas Tech University, Department of Chemistry and Biochemistry; ²Bern University of Applied Sciences, Institute of Applied Laser, Photonics and Surface Technologies
- 9:55 (5) **Pulsed Radiofrequency Glow Discharge Time-of-Flight Mass Spectrometry: A Versatile Analytical Technique for Fast Direct Solid and Gas Analysis;** Jorge Pisonero¹, Jonatan Fandiño¹, David Blanco², Alfredo Sanz-Medel³, Nerea Bordel³; ¹Department of Physics, University of Oviedo, c/ Calvo Sotelo s/n, Oviedo, Spain.; ²Department of Manufacturing Engineering, University of Oviedo, Campus of Gijón, Gijón, Spain.; ³Department of Analytical Chemistry, University of Oviedo, c/ Julian Clavería, Oviedo, Spain
- 10:15 (6) **The Realization of a New Solid-State Spectrometer for Glow Discharge Optical Emission;** Kim Marshall¹, Greg Schilling¹; ¹Leco Corporation
- 10:35 (7) **Use of Differential Interferometry for Direct Measurement of Depth with GD-OES, a Major Step for the Technique;** Matthieu Chausseau¹, Patrick Chapon¹, Sofia Gaiaschi¹, Simon Richard¹, Kayvon Savadkouei¹, Philippe Hunault¹; ¹HORIBA Scientific

Monday Morning, *Lakeshore B* **TRACE DETECTION IN FORENSICS**

Organizer and Presider: Edita Botonjic-Schic

- 9:15 (8) **Homemade Explosives Detection;** Hacene Boudries¹, Edita Botonjic-Schic¹, Vinh Lam¹; ¹Implant Sciences Corporation
- 9:55 (9) **The Use of FTIR for the Detection of Chemical Warfare Agents and Toxic Industrial Chemicals;** Larry McDermott, Mario Tongol¹, Norm Smith¹¹; ¹MKS Instruments
- 10:15 (10) **Solvent Effects in API Mass Spectrometry;** Jimmie Oxley¹; ¹University of Rhode Island
- 10:35 (11) **Commercial Rodenticide Repository and Attribution Signatures;** Evan Durnal¹, Krista Brady¹; ¹MRIGlobal

Monday Morning, *Greenway G* **MOLECULAR SPECTROSCOPY - SELECTED CONTRIBUTED PAPERS**

Organizer: Curtis Marcott; Presider: Anne Lemon

- 9:15 (12) **Re-invention of Rotational Spectroscopy - FT-MRR for Direct Composition Analysis of Complex Mixtures;** Brent J. Harris¹, Shelby S. Fields¹, Robin L. Pulliam¹, Justin L. Neill¹, Matthew T. Muckle¹, Linda H. Kidder¹; ¹BrightSpec

- 9:35 (13) **Microscopic Imaging of Structural Heterogeneity in Collagenous Tissue by Nonlinear Optical Stokes Ellipsometry;** Garth Simpson¹, Ximeng Y. Dow¹, Emma L. Kerian¹, Shane Z. Sullivan¹, James R. W. Ulcickas¹; ¹Purdue University
- 9:55 (14) **Photoacoustic FTIR Spectroscopy of Weathered Thermoplastics;** Michael Hall¹, Nancy Jestel¹, Pooja Bajaj¹, Eric Jiang²; ¹SABIC; ²Ddening LLC
- 10:15 (15) **A New Insight to Understand the Disease Pathology of Breast Cancer by Multimodal Spectroscopic Modalities;** Saroj Kumar¹, Xia Liu², Erik Goormaghtigh³, Fredrik Nikolajeff⁴; ¹Department of Engineering Science, Uppsala University, Uppsala, Sweden; ²Canadian Lightsource, Saskatoon, Canada; ³SFMB, Université Libre de Bruxelles, Belgium; ⁴Department of Engineering Science, Uppsala University, Uppsala, Sweden
- 10:35 (16) **Quantitative Analysis of Separated PAGE Proteins By Near Infrared Spectral Imaging;** Arash Hanifi¹, Nancy Pleshko¹; ¹Temple University

Monday Morning, *Nicollet B/C* **ITP - ELECTROPHORESIS - INSTRUMENTATION AND DETECTION**

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
 Presiders: Doo Soo Chung and Frantisek Foret

- 9:15 (17) **Searching for Signs of Life with Electrophoresis;** Peter Willis¹, Maria Mora¹, Jessica Creamer¹, Florian Kehl¹, Eric Tavares da Costa¹; ¹Caltech/JPL
- 9:55 (18) **Optical/Electrochemical Biosensing Using Micromotors as Novel Analytical Tools;** Beatriz Jurado-Sánchez¹, Alberto Escarpa¹; ¹University of Alcalá
- 10:15 (19) **Localized Surface Plasmon Resonance - A Novel Technique for Studying Interactions between Ionic Liquids and Lipid Vesicles;** Susanne Wiedmer¹, Joanna Witos¹, Suvi-Katriina Ruokonen¹; ¹Department of Chemistry, University of Helsinki, Finland
- 10:35 (20) **Simple and Low-Cost Point-of-Need Detection by AC Electrokinetics-Based Capacitive Biosensor;** Jayne Wu¹, Jiangang Chen¹, Shigetoshi Eda¹, Cheng Cheng¹, Rania Oueslati¹; ¹The University of Tennessee

Monday Morning, *Nicollet D2/D3* **ITP - DIELECTROPHORESIS I – FUNDAMENTALS**

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
 Presiders: Blanca Lapizco-Encinas and Nathan Swami

- 9:15 (21) **Engineering Nonlinear Electrokinetic Flows at Polarizable Interfaces;** Zachary Gagnon¹; ¹Johns Hopkins University
- 9:55 (22) **Dielectrophoresis: An Alternative to Chromatographic Techniques;** Sagnik Basuray¹; ¹New Jersey Institute of Technology
- 10:15 (23) **Enhancement of Dielectrophoresis Using Rough Electrodes;** Ali Beskok¹; ¹Southern Methodist University
- 10:35 (24) **Enabling Cell Co-culture and Cell Migration Studies in Microfluidic Systems;** Darwin R. Reyes¹; ¹National Institute of Standards and Technology

TECHNICAL PROGRAM – MONDAY

Orals 9:15 – 10:55 am

Monday Morning, Greenway J

LIBS IMAGING

Organizer and Presider: C. Derrick Quarles Jr

- 9:15 (25) **Laterally Resolved Analysis of Steels Using LIBS: Revealing the Distribution of Metallic and Non-Metallic Additions;** Maximilian Bonta¹, Raquel De Oro Calderon¹, Christian Gierl-Mayr¹, Herbert Danninger¹, Andreas Limbeck¹; ¹TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria
- 9:35 (26) **Laser Induced Breakdown SpeLaser Induced Breakdown Spectroscopy for High Resolution Mapping of Core Samples;** Francisco Lopez-Linares², C. Derrick Quarles Jr.¹, Toni Miao², Laura Poirier², Jhanis J. Gonzalez^{1,3}; ¹Applied Spectra, Inc.; ²Chevron Energy Technology Company, Richmond, CA; ³Lawrence Berkeley National Laboratory
- 9:55 (27) **Role of Interfacial Plasma Separation and Mixing Processes in Three-Dimensional Chemical Imaging with Femtosecond LIBS;** Vassilia Zorba¹, Ran Hai¹, Xianglei Mao¹, Richard Russo¹; ¹Lawrence Berkeley National Laboratory
- 10:15 (28) **The Tortuous Issues of Data Analysis in LIBS Imaging;** Vincent Motto-Ros¹, Florian Trichard¹, Jörg Hermann⁴, Bruno Bousquet², Frédéric Pélaschini³; ¹Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Villeurbanne, France; ²CELIA, UMR CNRS, Université Bordeaux, Talence Cedex, France; ³CRITT Matériaux Alsace, France; ⁴LP3, CNRS – Aix-Marseille Université, Marseille, France
- 10:35 (29) **Laser Induced Breakdown Spectroscopy of Simulated Used Nuclear Fuel;** Keri Campbell¹, Elizabeth Judge¹, James Barefield II¹, James Colgan¹, David Kilcrease¹; ¹Los Alamos National Laboratory

Monday Morning, Greenway E

SEMICONDUCTING NANOMATERIALS FOR SOLAR ENERGY APPLICATIONS

Organizer: Song Jin; Presider: Kyle Czech

- 9:15 (30) **Ultrafast Laser Spectroscopy of Two-Dimensional Materials and Their Heterostructures;** Hui Zhao¹, Yongsheng Wang², Dawei He²; ¹The University of Kansas; ²Beijing Jiaotong University, China
- 9:35 (31) **Spectroscopy of Quantum Dot Solar Energy Conversion Systems;** Matthew Beard¹, Daniel Kroupa¹, Yong Yan¹, Boris Chernomorkik¹, Jao van de Lagemaat¹, Jianbing Zhang¹, Ashley Marshall¹, Joseph Luther¹; ¹National Renewable Energy Laboratory
- 9:55 (32) **Electronic and Excitonic Properties of Monolayer Molybdenum Disulfide / Tungsten Disulfide Interfaces;** James Johns¹, Youngdong Yoo¹, Zachary Degregorio¹, Aaron Schulzetenberg¹; ¹University of Minnesota
- 10:15 (33) **Investigation of Transition Metal Dichalcogenide Exciton Dynamics Using State-Selective Multidimensional Spectroscopy;** Kyle Czech¹, Blaise Thompson¹, Song Jin¹, John Wright¹; ¹University of Wisconsin-Madison
- 10:35 (34) **Carrier Decay Process in Alloyed [HC(NH₂)₂][1-X][CH₃NH₃][XPbI₃ Nanostructures;** Jun Jun Dai¹; ¹University of Wisconsin-Madison

Monday Morning, Greenway B/C

RAMAN AND NIR SCREENING OF SMALL MOLECULES AND BIOLOGICS BASED COUNTERFEITS

Organizer and Presider: Anna Luczak

- 9:15 (35) **Raman Screening of Finished Medicines Using Surface Enhanced Raman Spectroscopy (SERS)-Based Approaches;** Latevi Lawson¹, Chelliah Navin¹, Jason Rodriguez¹; ¹FDA Division of Pharmaceutical Analysis
- 9:35 (36) **Past, Present and Future Analytical Techniques to Screen Counterfeit Drugs;** Ravi Kalyanaraman¹; ¹Bristol-Myers Squibb
- 9:55 (37) **Optimizing Detection of Milk Protein Adulterants Utilizing a Custom SERS Substrate;** Milo Overbay¹, Anita Rogacs¹, Viktor Shkolnikov¹, Michael Delos-Reyes¹; ¹HP Inc
- 10:15 (38) **Fluorescence Suppressed Time Resolved Raman Spectroscopy of Adulterated Herbal Products;** Clare Strachan^{1,3}, Sara Miller^{1,2}, Friederike Foltmann^{2,3}, Keith Gordon², Mari Tenhunen⁴; ¹Division of Pharmaceutical Chemistry and Technology, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland; ²Department of Chemistry, University of Otago, Dunedin, New Zealand; ³School of Pharmacy, University of Otago, Dunedin, New Zealand; ⁴TimeGate Instruments, Oulu, Finland
- 10:35 (39) **An Application of Rapid Detection Technologies in a National Regulatory Laboratory Setting: Differentiating Imported and Domestic Drug Products of Oxcarbazepine Using Handheld Raman, Near Infrared, and Portable FTIR Analyzers;** Bei Ma¹, Lingbo Wang²; ¹The U.S. Pharmacopeial Convention (USP); ²China Shanghai Institute for Food and Drug Control

Monday Morning, Nicollet D1

EMERGING RAMAN I

Organizers and Presiders: Ian Lewis, Duncan Graham and Pavel Matousek

- 9:15 (40) **A Multifocal Approach for Parallel Hyperspectral Detection in Confocal Raman Microscopy;** James Chan¹, Maria Navas-Moreno¹, Lingbo Kong¹; ¹University of California, Davis
- 9:35 (41) **Coherent Raman Imaging of Pheomelanin;** Conor Evans¹, Tracy Wang¹, Sam Osseiran¹, Vivien Ingrass¹, Alexander Nichols¹, Elizabeth Roider¹, Joachim Prussner¹, Hensin Tsao¹, David Fisher¹, Conor Evans¹; ¹Massachusetts General Hospital
- 9:55 (42) **Extreme Red-Shifted SERS;** Duncan Graham¹, Hayleigh Kearns¹, Matthew Bedics², Neil Shand³, Michael Detty², Karen Faulds¹; ¹University of Strathclyde; ²University at Buffalo; ³Dstl
- 10:15 (43) **SLIPSERS: When a Pitcher Plant meets with SERS;** Tak-Sing Wong¹, Shikuan Yang¹, Xianming Dai¹, Birgitt Boschitsch Stogin¹; ¹The Pennsylvania State University
- 10:35 (44) **Standoff Spatial Heterodyne Raman Spectrometer for Mineralogical Analysis;** Miles Egan¹, Stanley Angel², Shiv Sharma¹; ¹Hawaii Institute of Geophysics & Planetology, University of Hawaii at Manoa, Honolulu, HI; ²Department of Chemistry and Biochemistry, The University of South Carolina, Columbia, SC

TECHNICAL PROGRAM – MONDAY

Orals 9:15 – 10:55 am

Monday Morning, Lakeshore A

RAMAN MICROSCOPY

Organizer and Presider: Katsumasa Fujita

- 9:15 (45) **Live Cell Imaging of Nanoparticle Trafficking: A surface-Enhanced Raman Scattering Perspective;** Maria Navas-Moreno¹, Majid Mehrpouyen², Tatyana Chernenko², Demet Candas⁴, Jian Jian Li³, James W. Chan^{1,4}; ¹Center for Biophotonics, University of California, Davis, Sacramento, CA; ²BD Biosciences, San Jose, CA; ³Department of Radiation Oncology, University of California, Davis, Sacramento, CA; ⁴Department of Pathology and Laboratory Medicine, University of California, Davis, Sacramento, CA
- 9:35 (46) **Hyperspectral Raman microscopy Enables Robust and Flexible Molecular Sensing and Imaging on Nanoporous Gold Nanoparticles;** Wei-Chuan Shih¹; ¹University of Houston
- 9:55 (47) **High-Speed Multicolor Chemical Imaging with Stimulated Raman Scattering;** Yasuyuki Ozeki¹; ¹University of Tokyo
- 10:15 (48) **Surface-Enhanced Hyper-Raman Scattering from Optically Trapped Silver Nanoparticles on Yeast;** Yasutaka Kitahama¹, Hiroaki Hayashi¹, Tamitake Itoh², Yukihiro Ozaki¹; ¹Kwansei Gakuin University; ²AIST
- 10:35 (49) **3D Raman Imaging of Transparent and Opaque Samples – Applications in Pharmaceuticals ;** Wei Liu², Andrea Richter¹, Thomas Dieing¹, Joachim Koenen¹, Ute Schmidt¹; ¹WITec GmbH; ²WITec Instruments

Monday Morning, Greenway H/I

TOPICS IN MICROSCOPY

Organizer: Alexandr Ros; Presider: Garth Simpson

- 9:15 (50) **Nanoparticle Diffusion on Sub-Micrometer Oil Droplet-Water Interface Studied with Three Dimensional Single Particle Tracking;** Gufeng Wang¹, Yaning Zhong¹; ¹North Carolina State University
- 9:35 (51) **Scanning Angle Raman Spectroscopy Measurements of Thin Polymer Film Thickness, Domain Size and Index of Refraction;** Emily A Smith^{1,2}, Jonathan Bobbitt^{1,2}, Deyny Mendivelso^{1,2}; ¹Ames Laboratory; ²Iowa State University
- 9:55 (52) **In situ Raman Mapping of Materials under Mechanical Loading: Spatial Variation of Strain Evolution and Phase Transformation;** Chris Michaels¹, Yvonne Gerbig², Robert Cook¹; ¹Material Measurement Laboratory, NIST; ²School of Engineering and Applied Science, The George Washington University
- 10:15 (53) **Quantitative Analysis of Powdered Solids by Second Harmonic Generation Microscopy;** Azhad Chowdhury¹, Shijie Zhang¹, Garth Simpson¹; ¹Purdue University
- 10:35 (54) **Probing the Morphology, Nanomechanics and Tribology of Biomedical Gels with AFM;** Greg Haugstad¹, Joram Slager², Maggie Zeng³, Alon McCormick¹, Bob Tranquillo¹, Anne Ellis¹; ¹University of Minnesota; ²Surmodics, Inc.; ³Boston Scientific, Inc.

Monday Morning, Greenway D

TOPICS IN SPECTROSCOPY

Organizer: Alexandr Ros; Presider: Xiaohong Bi

- 9:15 (55) **A Search for the (most) Perfect Speciation Method of Arsenic in Rice;** Patrick Gray¹; ¹US Food and Drug Administration Center for Food Safety and Applied Nutrition
- 9:35 (56) **Computational Modeling of GC-VUV Spectra;** Jeremy Reyes¹, Bill Winniford¹, Eldad Hecceg², Kefu Sun², Anna Sandlin¹, James Griffith², Chris Siegler², Phillip Walsh³, Dale Harrison³; ¹Core R&D Analytical Sciences, The Dow Chemical Company, Freeport, TX; ²Analytical Technology Center, The Dow Chemical Company, Freeport, TX; ³VUV Analytics, Inc., Austin, TX
- 9:55 (57) **Tunable Laser Absorption Spectroscopy in Femtosecond Laser Ablation;** Mark Phillips¹, Jeremy Yeak², Sivanandan Harilal¹; ¹Pacific Northwest National Laboratory; ²Physics, Materials, and Advanced Mathematics Research
- 10:15 (58) **Spatial Characterizations of Aluminum Laser-Induced Plasma;** David Surnick¹, Christian Parigger¹; ¹University of Tennessee Space Institute
- 10:35 (59) **Sensitivity of in vivo Raman Measurements to Physiological Variability;** Xiaohong Bi¹, Andrew W. Dupont¹, Shashideep Singhal¹, Larry D. Scott¹, Sushovan Guha¹, Mamoun Younes¹, Yuanqing Ye², Hao Ding¹; ¹The University of Texas Health Science Center at Houston; ²The University of Texas M.D. Anderson Cancer Center

Monday Morning, Lakeshore C

NEW DIRECTIONS IN NANOPLASMONICS

Organizer and Presider: Jean-Francois Masson

- 9:15 (60) **Plasmon-in-a-Box;** Prashant Jain¹; ¹University of Illinois at Urbana-Champaign
- 9:35 (61) **Monitoring Plasmon Resonance Shifts upon Plasmon Excitation with Ultrafast Surface-Enhanced Raman Spectroscopy;** Emily Keller¹, Renee Frontiera¹; ¹University of Minnesota
- 9:55 (62) **Active Control of Near-Field Distribution in Plasmonic Nanorods;** Emilie Ringe¹, Sadeh Yazdi¹, Josee R. Daniel², Nicolas Large³, George C. Schatz³, Denis Boudreau²; ¹Department of Materials Science & Nano Engineering, Rice University; ²The Center for Optics, Photonics and Lasers (COPL), Department of Physics, Laval University; ³Department of Chemistry, Northwestern University
- 10:15 (63) **Detecting Nanoscale Structural Changes with Plasmonics: From Self-Assembled Plasmon Rulers to Tunable Circular Dichroism;** Vivian Ferry¹; ¹University of Minnesota - Twin Cities
- 10:35 (64) **Molecular Structure and Solvent Factors Influencing SERS on Planar Gold Substrates;** Ashish Tripathi¹, Erik D. Emmons¹, Jason A. Guicheteau¹, Augustus W. Fountain III¹, Steven D. Christesen¹; ¹US Army ECBC

TECHNICAL PROGRAM – MONDAY

Posters 11:00 am – 12:00 pm, *Nicollet A*

All Monday posters should be put up between 9:00 – 10:00 am and removed by 4:30 pm

Art and Archaeology Posters

Poster Board #1

(65) **Handheld X-ray Fluorescence Spectrometry for Characterization of Archaeological Materials from an Etruscan/Roman Archaeological Site near Orvieto, Italy;** Kaliopi Konomi¹, Mary Kate Donais¹, David George¹; ¹Saint Anselm College

Poster Board #2

(66) **Microchemical and Microstructural Investigation of Islamic Green and Manganese Glazed Pottery from Mertola (Portugal): Preliminary Results;** Jose Mirao¹, Massimo Beltrame^{1,2}, Susana Gómez Martínez³, Antonio Candeias¹; ¹HERCULES Laboratory, Universidade of Évora, Portugal; ²UNESCO Chair in Intangible Heritage and Traditional Know-How: Linking Heritage, Universidade of Évora, Portugal; ³Campo Arqueológico de Mértola, Mértola, Portugal

Poster Board #3

(67) **HERCULES Laboratory: An Portuguese Analytical Facility Fully Committed to the Material Study of Cultural Heritage;** Jose Mirao^{1,3}, Antonio Candeias^{1,2}, Cristina Dias^{1,3}, Ana Teresa Caldeira^{1,2}; ¹Hercules Laboratory, Universidade of Évora, Portugal; ²Chemistry Department, Sciences and Technology School, Portugal; ³Geosciences Department, Sciences and Technology School, Portugal

Poster Board #4

(68) **Sepsis: Serum Spectroscopic Sensing;** Matthew Baker¹, Lila Lovergne^{1,2}, Ganesh Sockalingum², Valerie Untereiner^{2,3}, Roman Lukaszewski⁴; ¹WESTChem, Department of Pure and Applied Chemistry, University of Strathclyde; ²Université de Reims Champagne-Ardenne, CNRS UMR 7369-MEDyC, Equipe MéDIAN-Biophotonique et Technologies pour la Santé; ³Plateforme en Imagerie Cellulaire et Tissulaire, Université de Reims Champagne-Ardenne, Reims Cedex, France; ⁴Chemical Biological Radiological Division, Dstl Porton Down, Salisbury Wiltshire, UK

Biomedical and Bioanalytical Sciences

Poster Board #5

(69) **Tunable Luminescent Carbon Nanospheres with Well-Defined Nanoscale Chemistry for Synchronized Imaging and Therapy;** Prabuddha Mukherjee¹, Santosh Misra¹, William Wilson¹, John Scott¹, Dipanjan Pan¹, Rohit Bhargava¹; ¹University of Illinois

Poster Board #6

(70) **Synergy of Cold Atmospheric Plasma and Electroporation for Treatment of Cancer Cells;** Arianna Avellan^{1,2}, Rohil Jain³, Prasoon Diwakar¹, Cagri Savran^{3,4}, Ahmed Hassanein¹; ¹Center for Materials Under eXtreme Environment, School of Nuclear Engineering Purdue University, West Lafayette, IN; ²Department of Materials Science and Engineering, University of Maryland, College Park, MD; ³Department of Mechanical Engineering, Purdue University, West Lafayette, IN; ⁴Birck Nanotechnology Center, Purdue University, West Lafayette, IN

Poster Board #7

(71) **Early Prediction of Renal Graft Outcomes by Interrogation of Fibrotic Regions;** Vishal Varma^{1,3}, Andre Kajdacsy-Balla¹, Sanjeev Akkina², Suman Setty¹, Michael Walsh^{1,3}; ¹University of Illinois at Chicago, Department of Pathology; ²Loyola University Chicago

Health Sciences Division; ³University of Illinois at Chicago, Department of BioEngineering

Poster Board #8

(72) **Kidney Stone Analysis Utilizing Fourier Transform Infrared Spectroscopy;** Olivia Maleki¹; ¹Mayo Clinic

Poster Board #9

(73) **Comparison of Multivariate Analysis Techniques for Investigating Paraffin-Embedded Cancer Tissue Section Using Raman Imaging System;** Phiranuphon Meksiarun¹, Ishigaki Mika¹, Verena A.C. Huck-Pezzei², Christian W. Huck², Hidetoshi Sato¹, Yukihiro Ozaki¹; ¹Kwansei Gakuin University, Sanda, Hyogo, Japan; ²Universität Innsbruck, Institut für Analytische Chemie und Radiochemie, Innsbruck, Austria

Forensic and Security Posters

Poster Board #10

(74) **Sublimation Dynamics of Explosives Particles under Various Environmental Conditions;** Michael Papantonakis¹, Robert Furstenberg¹, Viet Nguyen¹, Thomas Fischer², Christopher Kendziora¹, Andrew McGill¹; ¹U.S. Naval Research Laboratory; ²Federal Office of Bundeswehr Equipment, IT and In-Service Support

Poster Board #11

(75) **Mechanistic Studies of Particle Depositions in a Fingerprint;** Michael Papantonakis¹, Viet Nguyen¹, Robert Furstenberg¹, Thomas Fischer², Lily Zehfus³, Christine Mahoney⁴, Andrew McGill¹; ¹U.S. Naval Research Laboratory; ²Federal Office of Bundeswehr Equipment, IT and In-Service Support; ³Northland College; ⁴Nova Research

Poster Board #12

(76) **DHS Chemical Forensics Program – REACTS;** Evan Durnal¹, Krista Brady¹, Keith Broekhuizen¹, Peter Deardorff¹; ¹MRIGlobal

Poster Board #13

(77) **Identification of Individual Red Blood Cells by Raman Microspectroscopy for Forensic Purposes;** Claire Muro¹, Igor Lednev¹; ¹Chemistry Department, University at Albany

Poster Board #14

(78) **Use of FIB/SEM for Spatially Resolved Mass Spectrometry Measurements;** Dallas Reilly¹, Edgar Buck¹; ¹Pacific Northwest National Laboratory

Poster Board #15

(79) **Identification of Pen Inks Using Grating-Based Spectral Imaging Microscopy and Electrospray Ionization Mass Spectrometry;** Emily Horton¹, Michael R. Webb¹; ¹University of North Carolina at Wilmington

Poster Board #16

(80) **DART-MS Imaging of Adulterated Bread to Suggest Route of Contamination;** Travis Falconer¹; ¹U.S. Food and Drug Administration, Forensic Chemistry Center

Poster Board #17

(81) **Detection of Explosives from Surface Swabs Using Thermal Desorption DART-MS and Reverse Library Search;** Frederick Li¹, Joseph Tice¹, Steve Shrader², Paul Liang¹, Brian Musselman¹; ¹IonSense, Inc.; ²Shrader Software Solutions

TECHNICAL PROGRAM – MONDAY

Posters 11:00 am – 12:00 pm

Poster Board #18

(82) Analysis of IED Wires by Isotope Ratio Mass Spectrometry; Jane Vezina¹, Douglas Beussman¹; ¹St. Olaf College

Poster Board #19

(83) Isotope Ratio Mass Spectrometry Analysis of Natural and Synthetic Fibers and Effects of Chemical and Environmental Factors for Forensic Applications; Hannah Brown¹, Dat Le¹, Douglas Beussman¹; ¹St. Olaf College

Molecular/IR Posters

Poster Board #20

(84) Conformational Stability and Enthalpy Difference of Some Silane and Cyclopentane Compounds; Dattatray Sawant¹; ¹University of Missouri - Kansas City

Poster Board #21

(85) Infrared Analysis of Oil in Water: Traditional Liquid Cells versus Uniquely Designed More User Friendly DialPath Transmission Cells; Dipak Mainali¹, Frank Higgins¹; ¹Agilent Technologies

Poster Board #22

(86) High Resolution, High Sensitivity FT-IR for Industrial Analysis of Gas Phase Samples; Steve Lowry¹, Jay Roberts¹, Frank Wasacz¹, Karmel Walker¹; ¹Thermo Fisher Scientific

Poster Board #23

(87) The Potential of FTIR Spectroscopy and Computational Analysis in Characterizing the Mechanism of Action of Blue-Light against Methicillin-resistant *Staphylococcus aureus*; Ebrahim Aboualizadeh¹, Violet Bumah¹, Daniela Masson-Meyers¹, Janis Eells¹, Chukuka Enwemeka², Carol Hirschmugl¹; ¹University of Wisconsin-Milwaukee; ²San Diego State University

Poster Board #24

(88) Accurate Diagnosis of Thyroid Carcinoma Subtypes: Addressing Tissue Heterogeneity in Infrared Spectroscopic Imaging; David Martinez Marin¹, Hari Sreedhar¹, Vishal Varma¹, Catarina Eloy², Manuel Sobrinho-Simões², André Kajdacsy-Ballaa¹, Michael Walsh¹; ¹University of Illinois at Chicago Department of Pathology; ²Instituto de Patologia e Imunologia Molecular da Universidade do Porto

Poster Board #25

(89) Study on the Molecular Interaction of Hydration Water with the Sulfonic Acid Group Involved in Nafion; Takafumi Shimoaka¹, Chihiro Wakai¹, Takeshi Hasegawa¹; ¹Institute for Chemical Research, Kyoto University

Poster Board #26

(90) Strategy for Creating 3-aminopropyltriethoxysilane-derived Microarrays on Porous Silicon; Sidney Coombs¹, Frank Bright¹; ¹University at Buffalo

Poster Board #27

(91) Digital Confocal FTIR Microscopy; Alex Schofield¹, Carol Hirschmugl¹; ¹University of Wisconsin-Milwaukee

Poster Board #28

(92) Investigating the Heavy Atom Effect in Triphenyl Metal Hydrides via IR pump-probe and 2D-IR Spectroscopies; Cynthia Pyles¹, Courtney Olson¹, Ivan Spector¹, Aaron Massari¹; ¹Department of Chemistry, University of Minnesota Twin Cities

Poster Board #29

(93) Mid-IR spectral Histopathology: Classification of Biomedical Images with Spectral Markers Selected by GA-FDA; Rupali Mankar¹, Vishal Varma², Michael Walsh³, Carlos Bueso-Ramos⁴, David Mayerich¹; ¹Department of Electrical and Computer Engineering at the University of Houston; ²Department of Bioengineering at the University of Illinois at Chicago; ³Department of Pathology at the University of Illinois at Chicago; ⁴Division of Pathology/Lab Medicine, University of Texas MD Anderson Cancer Center, Houston, TX

ITP-Electro separation Methods Posters

Poster Board #30

(94) Direct Analysis of Ionogenic Substances in Thermoreversible Gel Samples by Capillary Isotachopheresis; Róbert Bodor¹, Marián Koval², Marián Masár¹; ¹Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovak Republic.; ²Villa Labeco spol. s r. o., Spišská Nová Ves, Slovak Republic

Poster Board #31

(95) Measuring Extracellular Amino Acid Dynamics From 3T3-L1 Adipocytes Using Online Microdialysis-Capillary Electrophoresis; Rachel Harstad¹, Michael Bowser¹; ¹University of Minnesota, Twin Cities

Poster Board #32

(96) Capillary Electrophoresis Coupled with Micro Free Flow Electrophoresis for High Speed Comprehensive Two Dimensional Analysis of Peptides; Alexander Johnson¹, Michael Bowser¹; ¹University of Minnesota

Poster Board #33

(97) Electroextraction Coupled On-Line to Capillary Electrophoresis – Mass Spectrometry: An Innovative Tool for Metabolomic Profiling of Biomass-Limited Samples; Amar Oedit¹, Thomas Hankemeier¹, Peter Lindenburg¹; ¹Leiden University, Leiden Academic Centre for Drug Research, Division of Analytical BioSciences

Poster Board #34

(98) Mechanism of Sequence-Based Separation of Single-Stranded DNA in Capillary Zone Electrophoresis; Jia Zhao¹, Steven Cramer¹, Linda McGown¹; ¹Rensselaer Polytechnic Institute

Poster Board #35

(99) Increasing the Separation Capability of Insulator-based Dielectrophoresis; Claire Crowther¹, Mark Hayes¹; ¹Arizona State University

Poster Board #36

(100) Dielectrophoretic Differentiation and Separation Based on Antibiotic Resistance; Shannon Huey Hilton¹, Mark A. Hayes¹; ¹Arizona State University

Poster Board #37

(101) Design of Experiments for Amino Acid Extraction from *Nicotiana Tabacum* and Their Subsequent Determination by Capillary Zone Electrophoresis; Ondřej Hodek¹, Tomáš Křížek¹; ¹Charles University in Prague, Faculty of Science, Department of Analytical Chemistry

TECHNICAL PROGRAM – MONDAY

Posters 11:00 am – 12:00 pm

Poster Board #38

(102) **An Influence of Various Operational Conditions on Offgel Isoelectric Focusing;** Magda Ördögová¹;

¹Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, Prague 2, Czech Republic

Poster Board #39

(103) **Glycoform Analysis of Alpha1-acid Glycoprotein by Capillary Electrophoresis with Electroosmotic Flow Absent Field Enhanced Sample Injection;** Chenhua Zhang¹, Cong Bi¹, William Clarke², David Hage¹;

¹University of Nebraska-Lincoln; ²Johns Hopkins School of Medicine

Poster Board #40

(104) **Interactions of Helquats with Chiral Acidic Aromatic Analytes Studied by Partial-Filling Affinity Capillary Electrophoresis;** Vaclav Kasicka¹, Martin Ruzicka^{1,2}, Dusan Koval¹, Jan Vavra¹, Paul Reyes-Gutierrez¹, Filip Teply¹;

¹The Czech Academy of Sciences, Institute of Organic Chemistry and Biochemistry, Prague 6, Czech Republic; ²Charles University in Prague, Faculty of Science, Prague 2, Czech Republic

Poster Board #41

(105) **Development of Capillary Separation System for Complex Characterization of Glycomic Samples;** Jana Vanova¹, Petr Cesla¹, Vaclav Simanek¹, Jana Krenkova², Jan Fischer¹;

¹Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic; ²Institute of Analytical Chemistry of the CAS, Brno, Czech Republic

Poster Board #42

(106) **Solving Complex-Forming Equilibria in Capillary Electromigration Theory;** Michal Malý¹, Magda Ördögová¹, Pavel Dubský¹;

¹Charles University in Prague, Department of Physical and Macromolecular Chemistry

Poster Board #43

(107) **Particle-Particle Interactions in Insulator Based Dielectrophoresis;** Mario Saucedo-Espinosa¹, Blanca Lapizco-Encinas¹;

¹Rochester Institute of Technology

Poster Board #44

(108) **Capillary Electrophoretic Determination of Ceftazidime in Human Blood and Microdialysates from Diabetic Foot after Acetonitrile-Based Sample Stacking;** Petr Tuma¹, Martin Jacek¹, Vladimira Fejfarova², Jan Polak¹;

¹Charles University in Prague, Third Faculty of Medicine; ²Institute for Clinical and Experimental Medicine, Czech Republic

Poster Board #45

(109) **Headspace In-Tube Microextraction Coupled with Micellar Electrokinetic Chromatography of Neutral Aromatic Compounds;** Yoon Jeong Choi¹, Sung Min Cho¹, Bum Su Park², Woo Sung Jung², Sang Won Lee², Yunhwan Jung²;

¹Seoul National University; ²Seoul Science High School

Poster Board #46

(110) **Assessment of Complex Biological Samples with Insulator-Based Dielectrophoresis;** Maria F. Romero-Creel¹, Alexandra LaLonde¹, Blanca H. Lapizco-Encinas¹;

¹Rochester Institute of Technology

Poster Board #47

(111) **Joule Heating Effects in Dielectrophoretic Devices of Optimized Posts Geometry;** Laura M. Arciniegas¹, Victor H. Pérez-González², Roberto C. Gallo-Villanueva², Blanca H. Lapizco-Encinas¹;

¹Microscale Bioseparations Laboratory, Rochester Institute of Technology; ²Sensors and Devices, Instituto Tecnológico y de Estudios Superiores de Monterrey

Poster Board #48

(112) **A Novel Image Analysis Based Capillary Electrophoresis Detection System;** Andras Guttman^{1,3},

Marton Szigeti^{1,3}, Mate Szarka^{1,2}, ¹Horvath Csaba Memorial Institute of Bioanalytical Research, University of Debrecen, Hungary; ²Vitrolink Ilc, Debrecen; ³MTA-PE Translational Glycomics Research Group, MUKKI, University of Pannonia, Veszprem, Hungary

Mass Spectrometry Posters

Poster Board #49

(113) **Simulation of a Helium DC Glow Discharge Used as an Ambient Desorption/Ionization Source for Mass Spectrometry;** Wade C Ellis¹, Ross L Spencer¹, Paul B Farnsworth¹;

¹Brigham Young University

Poster Board #50

(114) **Modeling Gas-Skimmer Cone Interactions in the ICP-MS Using DSMC;** Ross Spencer¹, Michael Carlson¹;

¹Brigham Young University

Poster Board #51

(115) **Stability and Precision of a Liquid Sampling - Atmospheric Pressure Glow Discharge Ion Source Interfaced with a Orbitrap Mass Analyzer;** Edward Hoegg^{1,2}, Garret Hart², George Hager², David Koppenaal², Kenneth Marcus¹;

¹Clemson University; ²Pacific Northwest National Lab

Poster Board #52

(116) **Determination of SeMet by HPLC- MP-AES with Post-Column Hydride Generation.;** Eunice Yañez Barrientos¹, Kazimierz Wrobel¹, Alma Rosa Corrales Escobosa¹, Francisco Acevedo Aguilar¹, Katarzyna Wrobel¹;

¹University of Guanajuato

Poster Board #53

(117) **HPLC-qTOF Analysis for Screening and Quantification of Drugs of Abuse Using Diagnostic Ions for Analytes and Internal Standards;** McCauley Reardon¹, Aditya Kulkarni¹, Matt Willetts¹, Howard Taylor², Shannon Johnson², Stephanie Whitson²;

¹Bruker Corporation; ²Addiction Labs of America

Poster Board #54

(118) **Correcting Saturation in Mass Spectrometry Data Using Principal Components Analysis;** Stephanie DeJong¹, James Hochrein¹, Lance Miller¹, Mark Van Benthem¹;

¹Sandia National Laboratories

Poster Board #55

(119) **Investigating the Potential of Transition Metal Cations to Probe the Gas Phase Structures of Isomeric Carbohydrates;** Yuting Huang¹, Lauren M. Petros¹, Katherine N. Schumacher¹, Eric D. Dodds¹;

¹Department of Chemistry, University of Nebraska - Lincoln

Poster Board #56

(120) **Spectral Comparison of Dielectric Barrier Discharge Ionization Sources;** Daniel F. Thurston¹, David Klute², Joachim Franzke², Paul B. Farnsworth¹;

¹Brigham Young University; ²ISAS—Leibniz Institut für analytische Wissenschaften

TECHNICAL PROGRAM – MONDAY

Posters 11:00 am – 12:00 pm

Poster Board #57

(121) **Improved Instrument Robustness via a Hot Source Induced Desolvation (HSID) Interface for Tandem Mass Spectrometry Instrumentation;** Frank Kero¹; ¹PerkinElmer

Poster Board #58

(122) **Desorption/Ionization System for Skin-Surface Compounds Mapping Using Low Power Laser and Non-Thermal Plasma;** Mari Aida¹, Yuya Yamashita¹, Ken Kakegawa¹, Hidekazu Miyahara¹, Akitoshi Okino¹¹; ¹FIRST, Tokyo Institute of Technology

Poster Board #59

(123) **MWCNT Functionalized APCI Corona Pin for PAH Sampling;** Keaton Nahan¹, Vesselin Shanov³, Anne Vonderheide^{2,3}; ¹University of Cincinnati, McMicken College of Arts and Sciences, Department of Chemistry, Metallomics Center of the Americas; ²University of Cincinnati, McMicken College of Arts and Sciences, Department of Chemistry; ³University of Cincinnati, College of Engineering and Applied Sciences

Raman-SERS Posters

Poster Board #60

(124) **Diverse SERS Substrates Nanofabricated On-Demand by Electroless Plating;** Jason Dwyer¹; ¹University of Rhode Island

Poster Board #61

(125) **A Stable, Disposable, Homogeneous Nanostructured Substrate for Surface Enhanced Raman Spectroscopy (SERS) Detection of Various Analyte Molecules;** Honey Madupalli¹, Mary Tecklenburg¹; ¹Central Michigan University

Poster Board #62

(126) **Long Term Stability of Gold and Silver Nanoparticle Activity in Polymer Films for SERS Applications;** Mary Tecklenburg¹, Honey Madupalli², Md. Shah Alam²; ¹Chemistry and Biochemistry, Central Michigan University; ²Science of Advanced Materials, Central Michigan University

Poster Board #63

(127) **Quantitative Online Sheath-Flow Surface Enhanced Raman Spectroscopy Detection for Liquid Chromatography;** Anh Nguyen¹, Zachary D. Schultz¹; ¹University of Notre Dame, Notre Dame, IN

Poster Board #64

(128) **Exploring the Effect of Intermolecular H-bond and the Application in Enantioselective Discrimination by SERS;** Bing Zhao¹, Yue Wang^{1,2}, Yukihiro Ozaki²; ¹State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, P. R. China; ²Department of Chemistry, School of Science and Technology, Kwansei Gakuin University, Sanda, Hyogo, Japan

Poster Board #65

(129) **Application of the Superhydrophobic Biomimetic Chip in SERS Analysis;** Qian Cong¹, Zhi Yu^{1,2}, Young Mee Jung²; ¹Key Laboratory for Bionic Engineering of Ministry of Education, Jilin University, Changchun, China.; ²Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chunchon, Korea

Poster Board #66

(130) **Label-Free Protein Detection on Silver Nanodomes Using Surface-enhanced Raman Scattering;** Aysun Korkmaz¹, Handan Yuksek², Ramazan Solmaz^{2,3},

Adile Gürkan¹, Mehmet Kahraman¹; ¹Gaziantep University; ²Bingöl University

Poster Board #67

(131) **Multiplex DNA Analysis Using Surface-Enhanced Raman Scattering;** Tugce Yigit¹, Ebru Akdogan¹, Isik Didem Karagoz¹, Mehmet Kahraman¹; ¹Gaziantep University

Poster Board #68

(132) **Detection of Bacteria Using SERS-Based Immunoassay;** Gamze Yaman¹, Okkes Celik¹, Nese Erdogan¹, Ibrahim Halil Kilic¹, Dilek Buyukbesel¹, Mehmet Kahraman¹; ¹Gaziantep University

Poster Board #69

(133) **Enhancing Raman Signaling under High Pressure;** Abdullah Al Balushi¹, Kirsten Gracie², Duncan Graham², Alexander Mullen¹, Iain Oswald¹; ¹University of Strathclyde, Strathclyde Institute of Pharmacy & Biomedical Sciences; ²University of Strathclyde, Department of Pure and Applied Chemistry

Poster Board #70

(134) **Reproducibility and Stability of SERS Signal of Analytes on a PEI Polymer Matrix Embedded with Gold Nanoparticles;** Md Shah Alam, Mary M. J. Tecklenburg¹; ¹Central Michigan University; ²Central Michigan University

Poster Board #71

(135) **Filter Based Surface-Enhanced Raman Scattering (SERS) Substrates for Aqueous Environmental Analyte Detection;** Kyle Bantz¹, Garrett Briggs¹, Michael Parsons¹; ¹Virginia Military Institute

Poster Board #72

(136) **3-Dimensional SERS Imaging Using Highly Symmetric Silver Microparticles with Nanopores as a Substrate;** Sanpon Vantasin¹, Wei Ji¹, Yoshito Tanaka¹, Yasutaka Kitahama¹, Kanet Wongravee², Harnchana Gatemala², Sanong Ekgasit², Yukihiro Ozaki²; ¹School of Science and Technology, Kwansei Gakuin University; ²Department of Chemistry, Faculty of Science, Chulalongkorn University

Poster Board #73

(137) **A Gold Nanohole Array Based Biosensor for Mercury Detection in Human Saliva;** Peng Zheng¹, Nianqiang Wu¹; ¹West Virginia University

Deep and Far UV Spectroscopy Posters

Poster Board #74

(138) **First Electronic Transition of Interfacial Water Adsorbed on Alumina Surface Studied by Far-Ultraviolet Spectroscopy;** Takeyoshi Goto¹, Yukihiro Ozaki¹; ¹Kwansei Gakuin University

Poster Board #75

(139) **Cation Size Effects on A←X transition of Proton-Water Cluster: Electronic Delocalization of Hydrated Proton in Liquid Water;** Takeyoshi Goto¹, Krzysztof Bec¹, Yukihiro Ozaki¹; ¹Kwansei Gakuin University

Poster Board #76

(140) **Electronic States of Composite Polymer Electrolyte Composed of PEG and Lithium-salts;** Nami Ueno¹, Tomonari Wakabayashi¹, Yusuke Morisawa¹; ¹Graduate School of Science and Engineering Research, Kindai University

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

Poster Board #77

(141) **The Electronic States of Composite Polymer Electrolytes Composed of Poly(ethylene glycol) and Lithium salt;** Nami Ueno¹, Tomonari Wakabayashi¹, Yusuke Morisawa¹; ¹Graduate School of Science and Engineering Research of Kindai University

X-Ray and Fluorescence Posters

Poster Board #78

(142) **Use of Synchrotron X-Ray Fluorescence Microprobe to the Study of Inks and Their Separation Using Paper Chromatography;** Dale L Perry¹, Tom J Wilkinson¹, Albert C Thompson¹; ¹Lawrence Berkeley National Laboratory, University of California

Poster Board #79

(143) **X-ray Based Analytical Methods and the Color of Marbles and Limestones Used in Architecture;** Jose Mirao^{1,3}, Luis Dias¹, Pedro Barrulas¹, Luis Lopes^{2,3}, Patricia Moita^{1,3}, Ana Teresa Caldeira^{1,4}, Antonio Candeias^{1,4}; ¹Hercules Laboratory, Universidade of Évora, Portugal; ²Institute of Earth Sciences, Universidade of Évora, Portugal; ³Geosciences Department, Sciences and Technology School, Universidade of Évora, Portugal; ⁴Chemistry Department, Sciences and Technology School, Universidade of Évora, Portugal

Monday Afternoon, Greenway A
NOVEL APPLICATIONS OF LASER ABLATION - ICPMS AND RELATED TECHNIQUES

Organizer and Presider: Jorge Pisonero

- 1:20 (144) **Detection of Engineered Nanoparticles in Water, Soil and Sediments: From Bulk Analysis to Single Particle ICP-TOF-MS;** Frank von der Kammer¹, Antonia Praetorius¹, Andreas Gondikas¹, Jana Navratilova¹, Olga Borovinskaya², Alexander Gundlach-Graham³, Detlev Gunther³, Thilo Hofmann¹; ¹University of Vienna - Department of Environmental Geosciences; ²TOFWERK; ³ETH Zurich
- 1:40 (145) **Novel "Filter Pellet" Sample Preparation Strategy for Analysis of Filter-Bound Sediment Samples by Laser Ablation ICP-MS- application to Sediment Fingerprinting;** Ruthmara Corzo¹, Sarah Jantzi¹, Christopher Dutton², Amartya Saha³, Jose Almirall¹; ¹Department of Chemistry and Biochemistry and International Forensic Research Institute, Florida International University, Miami, FL; ²Department of Ecology and Evolutionary Biology, Yale University, New Haven, CT; ³Global Water for Sustainability Program (GLOWS), Florida International University, Miami, FL
- 2:00 (146) **Bioimaging of Metals and Biomolecules in Breast Tissues by LA-MS;** Raquel Gonzalez de Vega¹, Maria Luisa Fernández Sánchez¹, Jorge Pisonero², Noemí Eiró³, Francisco J. Vizoso³, Uwe Karst⁴, Alfredo Sanz-Medel¹; ¹Department of Physical and Analytical Chemistry, Faculty of Chemistry, University of Oviedo, Spain; ²Department of Physics, University of Oviedo, Spain; ³Research Unit, Hospital de Jove Foundation, Gijón, Spain; ⁴Institute of Inorganic and Analytical Chemistry, University of Münster, Germany
- 2:20 (147) **Climate Variability in the Northwest Iberian Peninsula during the Last Millennium Based on LA-ICP-MS Analysis of Speleothems Records;** Miguel Iglesias¹, Jorge Pisonero¹, Wolfgang Muller³, Hai Cheng², R. Lawrence Edwards², Heather Stoll¹; ¹University of Oviedo, Geology Department, Oviedo, Spain; ²University of Minnesota, Department of Earth Sciences, Minneapolis,

MN; ³Royal Holloway University of London, Department of Earth Sciences, Egham, UK.; ⁴Xian Jiaotong University, Institute of Global Environmental Change, Xian, China.

- 2:40 (148) **Bio-imaging by LA-ICP-MS: Quantification and Uncertainty Estimation;** David Douglas¹, Jennifer O'Reilly¹, Heidi Goenaga-Infante¹; ¹Science and Innovation, LGC, Queens Road, Teddington, Middlesex, UK

Monday Afternoon, Greenway H/I

RSC AWARDS SYMPOSIUM

Organizer and Presider: Philippa Hughes

- 1:20 (149) **Quantification of the Composition, Volatility, and Sources of Particulate Matter by Field-Deployable Mass Spectrometry: Implications for Air Quality and Health;** Patrick Hayes¹; ¹Université de Montréal
- 1:40 (150) **Single Particle Mass Spectrometric Studies of Carbonaceous Aerosol;** Jonathan Abbott¹; ¹University of Toronto
- 2:00 (151) **Life, Death and SERS;** Colin Campbell¹, Lauren Jamieson¹, Victoria Camus¹, Hannah Johnston¹, William Nailon², Duncan McLaren², David Harrison³; ¹University of Edinburgh; ²NHS Lothian; ³St Andrews University
- 2:20 (152) **Biosensing Using SERS;** Karen Faulds¹; ¹University of Strathclyde
- 2:40 (153) **Yet another SERS Talk!;** Duncan Graham¹; ¹University of Strathclyde

Monday Afternoon, Greenway G

CLIRSPEC: BIOLOGICAL FLUIDS IN HEALTH AND DISEASE

Organizer and Presider: Matthew Baker

- 1:20 (154) **Towards Non-invasive Spectroscopy of Red Blood Cells Stored in Transfusion Bags;** Michael Blades¹, Kevin Buckley², Robin F.B. Turner³, H.G. Schulze³, Deborah Chen⁴, Dana Devine⁴; ¹Department of Chemistry, The University of British Columbia, Vancouver, BC, Canada; ²National University of Ireland, Galway, Gaillimh, Co. Galway, Ireland; ³Michael Smith Laboratories, The University of British Columbia, Vancouver, BC, Canada; ⁴Department of Pathology and Laboratory Medicine, The University of British Columbia, Vancouver, BC, Canada and Centre for Blood Research, The University of British Columbia, Vancouver, BC, Canada
- 1:40 (155) **Lipids or Basic Calcium Phosphates: A Novel Family of Synovial Fluid Crystals Identified by Raman Spectroscopy;** Ozan Akkus¹, Bolan Li¹, Nora Singer²; ¹Case Western Reserve University; ²MetroHealth Medical Center
- 2:00 (156) **Development and Analysis of Liquid, Liquid Serum Biopsies;** Katie Spalding¹, Ruth Board², Benjamin Bird³, Caryn Hughes¹, Matthew James Baker¹; ¹WestCHEM, Department of Pure and Applied Chemistry, Technology and Innovation Centre, University of Strathclyde, Glasgow, UK; ²Rosemere Cancer Centre, Lancashire Teaching Hospitals NHS Trust, Royal Preston Hospital, Preston, UK; ³Daylight Solutions, San Diego, CA
- 2:20 (157) **SERS-based in vitro Assays for the Sensitive Detection of Cardiovascular Disease Biomarkers in Clinical Samples;** Lee Barrett¹, Naveed Sattar², Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde; ²University of Glasgow
- 2:40 (158) **Quantitative Raman Spectroscopy for Protein Therapeutics;** William Herrington¹, Gajendra Singh¹, Di Wu², Paul Barone¹, William Hancock², Rajeev Ram¹; ¹MIT; ²Northeastern University

TECHNICAL PROGRAM – MONDAY

Orals 1:20 – 3:00 pm

Monday Afternoon, Greenway D NEW FRONTIERS IN CHEMOMETRICS

Organizer and Presider: Peter Harrington

- 1:20 (159) **Data Preprocessing- The Main Bottleneck in Data Analysis**; Beata Walczak¹; ¹University of Silesia
- 1:40 (160) **Single Bacteria Identification by Raman Spectroscopy and Topological Data Analysis**; Ludovic Duponchel¹; ¹Lille University
- 2:00 (161) **ILS to CLS: Synergistic Regression Modeling for Improved Control and Interpretability**; Neal Gallagher¹; ¹Eigenvector Research, Inc.
- 2:20 (162) **Whole Spectrum Unmixing for Raman and FTIR Applications**; CJ Carey¹, M. Darby Dyar²; ¹University of Massachusetts - Amherst; ²Mount Holyoke College
- 2:40 (163) **Parameter-Free Support Vector Machines for Calibration with Hybrid Penalty Function**; Peter Harrington¹; ¹Ohio University

Monday Afternoon, Lakeshore B NANOSCALE IR SPECTROSCOPY

Organizer and Presider: Curtis Marcott

- 1:20 (164) **Applications of Nanoscale Chemical Imaging to Polymeric Systems**; Mark Rickard¹, Gregory Meyers¹, Carl Reinhardt¹, Jamie Stanley¹; ¹The Dow Chemical Company
- 1:40 (165) **Nanoscale Characterization of Engineered Thermoplastic Materials by Atomic Force Microscopy – Infrared Spectroscopy (AFM-IR) in Combination with Traditional Microscopy and Spectroscopy Methods**; Anne Lemon¹, Liang Gong², Lanti Yang¹, Pooja Bajaj¹, John Rabolt², Bruce Chase²; ¹SABIC; ²University of Delaware
- 2:00 (166) **AFM-IR Studies of Collagen Microstructure and Chemical Composition for Estrogen Depleted and Drug Treated Cortical Bone and Lumbar Vertebrae**; Mark Banaszak Holl¹, Meagan Cauble¹, Matthew Muckley¹, Taeyong Ahn¹, Sriram Vaidyanathan¹, Rachel Merzel¹, Jeffrey Fessler¹, Bradford Orr¹, Le Duong²; ¹University of Michigan; ²Merck Research Laboratories
- 2:20 (167) **AFM-IR of a Nanostructured Bioadhesive Produced by Acorn Barnacles**; Daniel Barlow¹, Kenan Fears¹, Christopher So¹, Jenifer Scancelli¹, Kedar Manandhar¹, Boris Feygelson¹, Beatriz Orihuela², Daniel Rittschof², Kathryn Wahl¹; ¹US Naval Research Laboratory; ²Duke University Marine Lab
- 2:40 (168) **Nanoscale Investigation of Nanoscale Structure Transitions in Silk Proteins Using Near-Field Optics**; Shaoqing Zhang¹, Woonsoo Lee¹; ¹University of Texas at Austin

Monday Afternoon, Nicollet B/C ITP - FUNDAMENTALS OF ELECTROPHORESIS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Neil Cornelius Ivory and Dutta Prashanta

- 1:20 (169) **Capillary Electrophoresis and Density Functional Theory Employed for Characterization of Biopeptide Complexes with Ammonium and Alkali Metal Ions**; Vaclav Kasicka¹, Sachinkumar Pangavhane¹, Stanislav Boehm², Emanuel Maklik³, Paolo Ruzza⁴; ¹The Czech Academy of Sciences, Institute of Organic Chemistry and Biochemistry, Prague 6, Czech Republic; ²University of Chemistry and Technology, Prague 6, Czech Republic; ³Czech University of Life Sciences, Faculty of Environmental Sciences, Prague 6, Czech Republic; ⁴Institute of Biomolecular Chemistry of CNR, Padua Unit, Padua, Italy

- 1:40 (170) **The Relationship between Electrophoretic Mobility and Polyion Charge**; Nancy Stellwagen¹; ¹University of Iowa
- 2:00 (171) **The Dynamics of Comigration: An Insight into a Cluster of Two Semi-Separated Peaks**; Pavel Dubský¹, Martin Dvořák¹; ¹Charles University in Prague, Faculty of Science, Praha 2
- 2:20 (172) **Exploring the Promise of Microgradient Electrophoretic Separations**; Mark Hayes¹, Fanyi Zhu¹, Michael Keebaugh¹; ¹Arizona State University
- 2:40 (173) **Size and Charge Characterization of Nanomolecular Entities by Taylor Dispersion Analysis and Capillary Electrophoresis**; Hervé Cottet¹, Joseph Chamieh¹, Laurent Leclercq¹, Michel Martin³, Luca Cipelletti²; ²IBMM, University of Montpellier, France; ²L2C, University of Montpellier, France; ³PMMH, ESPCI, Paris, France

Monday Afternoon, Nicollet D2/D3 ITP - BIOMEDICAL AND BIOANALYSIS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Yehia Mechref and Michael Bowser

- 1:20 (174) **Study on the Protein-Protein Interaction in Single Living Cells by Microfluidic Chip with Single Molecule Fluorescence Correlation Spectroscopy**; Jicun Ren¹, Chaoping Dong¹; ¹Shanghai Jiaotong University, Shanghai
- 1:40 (175) **Quantitative Method Development for the Simultaneous Determination of Tocopherols and Tocotrienols in Human Adipose Tissue and Serum**; Danuta Siluk¹, Ewa Bartosińska¹, Magdalena Buszewska-Forajta¹, Wiktoria Struck-Lewicka¹, Julia Jacyna¹, Agnieszka Borsuk¹, Paweł Wiczling¹, Roman Kaliszan¹; ¹Medical University of Gdańsk
- 2:00 (176) **Insights into Protein Tyrosine Nitration in Brain Cancers**; Xianquan Zhan¹; ¹Xiangya Hospital, Central South University
- 2:20 (177) **Electrophysiological Rhythms in Blood**; Fatima Labeed¹, Erin Henslee¹, Malcolm von Schantz¹, Rita Jabr¹, Akhilesh Reddy², John O'Neill³, Daan Van Der Veen¹, Rula Abdallat⁴; ¹University of Surrey; ²University of Cambridge; ³Medical Research Council-Laboratory for Molecular Biology (MRC-LMB); ⁴Hashemite University, Jordan
- 2:40 (178) **Low-copy Number Biomolecular Analysis with Dielectrophoretic Enrichment /Trapping via Molecular Dam and Plasmonic Electrode Nanogaps**; Chia-Fu Chou¹; ¹Academia Sinica

Monday Afternoon, Greenway J TOPICS IN MASS SPECTROMETRY

Organizer: Alexandra Ros; Presider: John Olesik

- 1:20 (179) **Tuning Soft Ionization Strength for Organic Mass Spectrometry**; Alexander Schütz¹, Sebastian Brandt¹, Felix David Klute¹, Joachim Franzke¹; ¹Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V.
- 1:40 (180) **3D Printing: Intermediate Fast Prototyping and Enlarging Possibilities for Analytical ScienceS**; Sebastian Brandt¹, Alexander Schütz¹, Felix David Klute¹, Joachim Franzke¹; ¹Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.
- 2:00 (181) **High-Resolution Atmospheric Pressure Drift Tube Ion Mobility Spectrometry Coupled with Ultra-Accurate Mass Orbitrap Mass Spectrometry**; Stephen Zambrzycki¹, Anyin Li¹, Joel Keelor¹, Brian Clowers², Facundo Fernandez¹; ¹Georgia Institute of Technology; ²Washington State University

TECHNICAL PROGRAM – MONDAY

Orals 1:20 – 3:00 pm

- 2:20 (182) **A Novel Gas Chromatography Mass Spectrometry Approach for the Determination of Inorganic Anions;** Enea Pagliano¹, Beatrice Campanella^{2,3}, Massimo Onor², Emilia Bramanti², Alessandro D², Zoltan Mester¹; ¹National Research Council of Canada; ²Consiglio Nazionale delle Ricerche
- 2:40 (183) **Single Particle Inductively Coupled Plasma Mass Spectrometry for Nanoparticle Characterization: Calibration Techniques and Fundamental Processes that Generate Signals from Solutions vs. Nanoparticles;** John Olesik¹, Austin Wilson¹; ¹The Ohio State University

Monday Afternoon, Greenway E NANO-FACILITATED SENSING

Organizer and Presider: David E. Thompson

- 1:20 (184) **Changing Plasmonic Nanoparticle Shape and Resonance Frequency via Mechanical Deformation;** Jeffrey Anker¹; ¹Clemson University
- 1:40 (185) **Single Nanoparticle Plasmonic Spectroscopy for Single-Molecule Sensing and Super-resolution Imaging of Single Live Cells;** X. Nancy Xu¹, Pavan K. Cherukuri¹, Kerry J. Lee¹, Tao Huang¹, Feng Ding¹; ¹Old Dominion University
- 2:00 (186) **Ultrasensitive Detection with SEHRS: From Single Molecules to NIR Imaging;** Jon Camden¹; ¹University of Notre Dame
- 2:20 (187) **Plasmon-Driven Photocatalytic Molecular Transformations: A Plasmon-Enhanced Spectroscopic Study;** Hui Wang¹; ¹University of South Carolina
- 2:40 (188) **Wetting Effects on Surface Enhanced Signals from Gold Coated Nanopillar Substrates;** David E. Thompson¹, Manpinder Kaur¹, Alam Nure Md.¹, Alyssa Noonan¹, Xinmei Dong¹; ¹Sam Houston State University

Monday Afternoon, Greenway B/C COUNTERFEIT CHALLENGES IN BIOPHARMACEUTICALS

Organizer and Presider: Sulaf Assi

- 1:20 (189) **Pharmaceutical Evaluation of Atorvastatin Calcium Tablets Available on the Internet;** Toshiro Fukami¹, Motoki Inoue¹, Hiroshi Hisada¹, Tatsuo Koide²; ¹Meiji Pharmaceutical University; ²National Institute of Health Sciences
- 1:40 (190) **Combating counterfeit Medicines: The Use of NMR and MS Techniques;** Ian Jones¹; ¹AstraZeneca
- 2:00 (191) **Assessment of the Effectiveness of the CD3+ Tool to Detect Counterfeit and Substandard Anti-Malarials;** Mustapha Hajjou¹; ¹United States Pharmacopeial Convention; Promoting the Quality of Medicines Program
- 2:20 (192) **Complementarity of PDA and MS Detection for Chromatographic Fingerprinting of Genuine and Counterfeit Viagra®;** Deborah Custers^{1,2}, Barbara Krakowska³, Patricia Courselle¹, Michal Daszykowski³, Sandra Apers², Eric Deconinck¹; ¹Section Medicinal Products, Scientific Institute of Public Health (WIV-ISP), Brussels, Belgium; ²Research group NatuRA (Natural products and Food - Research and Analysis), Department of Pharmaceutical Sciences, University of Antwerp, Wilrijk, Belgium; ³Institute of Chemistry, University of Silesia, Katowice, Poland
- 2:40 (193) **MHRA Sampling Programme and Choice of Target Products;** Stephen Young¹; ¹Medicines and Healthcare Products Regulatory Agency

Monday Afternoon, Nicollet D1

BIOANALYTICAL SERS I

Organizers and Presiders: Roy Goodacre and Duncan Graham

- 1:20 (194) **Development of Aluminum Substrates for UV Surface-Enhanced Resonance Raman Spectroscopy;** Bhavya Sharma¹; ¹University of Tennessee
- 1:40 (195) **Optimisation of Surface Enhanced Raman Scattering and Isotopic Labelling for Unambiguous Bacterial Identification;** Howbeer Muhamadali¹, Abdu Subaihi¹, Yun Xu¹, David Ellis¹, Royston Goodacre¹; ¹The University of Manchester
- 2:00 (196) **Rapid Detection and Identification of Bacterial Meningitis Pathogens in ex vivo Clinical Samples by SERS Method and Principal Component Analysis;** Agnieszka Kamińska¹; ¹Institute of Physical Chemistry Polish Academy of Sciences
- 2:20 (197) **Single-Bacteria Analysis by Surface Enhanced Raman Spectroscopy SERS;** Christoph Haisch¹, Haibo Zhou³, Nicoleta Mircescu², Natalie Ivleva¹, Reinhard Niessner¹, Andreas Wieser⁴; ¹Technical University Munich, Germany; ²National Institute of R&D of Isotopic and Molecular Technology, Romania; ³Jinan University, P.R. China; ⁴Max von Pettenkofer-Institute for Hygiene and Clinical Microbiology, Ludwig Maximilians-University, Germany
- 2:40 (198) **Improved lateral flow SERS Immunoassay Performance Using a New Approach to Antibody Conjugation of Gold Nanoparticles;** Pietro Gancitano¹, Stephen Carmichael², Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde; ²BBI Solution Ltd

Monday Afternoon, Lakeshore A

PORTABLE RAMAN

Organizer and Presider: Neil Shand

- 1:20 (199) **Portable Raman: Then, Now, and Beyond;** Keith Carron¹; ¹Metrohm Raman
- 1:40 (200) **Applications of Portable and Handheld Raman Systems to Military Detection Scenarios;** Jason Guicheteau¹, Steven Christesen¹, Ashish Tripathi¹, Erik Emmons¹, Phillip Wilcox¹, Augustus W. Fountain III¹; ¹USA RDECOM Edgewood Chemical Biological Center
- 2:00 (201) **Implementation of a Cell Phone Camera as a Detector for a Miniature Spatial Heterodyne Raman Spectrometer;** Patrick D. Barnett¹, S. Michael Angel¹; ¹University of South Carolina
- 2:20 (202) **Complex Mixture Analysis Using Hand-Held Raman Chemical Detectors and Novel Spectral Deconvolution Algorithms;** Rhea Clewes¹, Mehrdad Yaghoob², Di Wu², Mike Davies²; ¹Dstl, UK; ²School of Engineering, University of Edinburgh, UK
- 2:40 (203) **Time-gated Raman Spectroscopy Using SPAD Matrix Detectors: Towards Hand-Held Scale;** Lauri Kurki¹, Jouni Takalo¹, Mari Tenhunen¹, Jussi Tenhunen²; ¹TimeGate Instruments Oy; ²VTT Technical Research Centre of Finland

Monday Afternoon, Lakeshore C

NEW DIRECTIONS IN PLASMONIC APPLICATIONS AND INSTRUMENTATION

Organizer and Presider: Jean-Francois Masson

- 1:20 (204) **Applications of SERS pH Nanoprobes Produced by Co-Solvent Controlled AuNP Aggregation;** Peter Vikesland^{1,2}, Haoran Wei^{1,2}, Marjorie Willner^{1,2}, Linsey Marr^{1,2}; ¹Department of Civil and Environmental Engineering, Virginia Tech; ²Institute for Critical Technology and Applied Science, Virginia Tech

Future SciX Meeting: October 8 – 13, 2017, Reno, Nevada

TECHNICAL PROGRAM – MONDAY

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

- 1:40 (205) **Single Nanoparticle SPR Imaging Microscopy of Bioaffinity, Uptake and Surface Enzymatic Reactions;** Adam Maley¹, Robert M. Corn¹; ¹University of California-Irvine
- 2:00 (206) **Cell imaging with Metal Clad Waveguide (MCWG) Microscopy;** Paul G. Charette¹, Thomas Söllradl¹, Frédéric A. Banville¹, Ulrike Fröhlich¹, Vincent Chabot¹, Pierre-Jean Zermatten¹, Michael T. Canva¹, Michel Grandbois¹; ¹Université de Sherbrooke
- 2:20 (207) **Characterization and Applications of Nanoporous Gold Nanoparticles in the Near-Infrared;** Wei-Chuan Shih¹; ¹University of Houston
- 2:40 (208) **Insight into Plasmon-driven Photochemistry via Surface-enhanced Raman Spectroscopy;** James Brooks¹, Renee Frontiera¹; ¹University of Minnesota
- 3:00 **Poster Viewing and Coffee Break, Nicollet A**

Monday Afternoon, Greenway E

RSC-ACS SYMPOSIUM - SOLVING GLOBAL HEALTH CHALLENGES: ELEMENTAL TECHNIQUES TOWARDS CHARACTERIZATION, DIAGNOSTICS, AND DETECTION

Organizers: Philippa Hughes and Douglas Duckworth;
 President: Douglas Duckworth

- 3:50 (209) **Arsenic-related Health Challenges: Making Students Aware and Getting Them Involved;** Julian Tyson¹, Ray Kronquist²; ¹University of Massachusetts; ²Chemists without Borders
- 4:10 (210) **Lab on Paper for Quantification of Analytes at PPM and PPB Levels;** Marya Lieberman¹, Nicholas Myers¹; ¹University of Notre Dame
- 4:30 (211) **Electrochemically Modulated Separation for Iodine and Cesium for Detection and Diagnosis;** Sandra Pratt¹, Douglas Duckworth¹, Shane Peper¹, Kate Magee³, Katy Fordyce², Janet Cloutier¹; ¹Pacific Northwest National Laboratory; ²Bioanalytical Systems, Inc; ³W&M Environmental Group
- 4:50 (212) **Imaging iron: The Key to Understanding Aging and Neurodegeneration?;** Dominic Hare^{1,2}, Philip Doble¹; ¹University of Technology Sydney; ²The Florey Institute of Neuroscience and Mental Health
- 5:10 (213) **Elemental Speciation of Environmental and Biological Materials Using Ultra-High Resolution Mass Spectrometry;** David Koppelaar¹, Walker Larry¹, Tfaily Malak¹, Jared Shaw¹, Nancy Hess¹, Pasa-Tolic Lilijana¹; ¹EMSL, Pacific Northwest National Laboratory

Monday Afternoon, Greenway A

INNOVATIONS AND APPLICATIONS IN X-RAY FLUORESCENCE SPECTROMETRY

Organizer and President: Christine Vanhoof

- 3:50 (214) **Micro-XRF and XRF Microanalysis Trade-Offs between Large Facility (Synchrotron) and Laboratory Approaches;** Ursula Fittschen¹; ¹Washington State University
- 4:30 (215) **Total Element Determination and Speciation of Arsenic in Airborne Particulate Matter by Combining ED/WDXRF, HPLC-ICP-MS and XANES Analyses;** Christine Vanhoof¹, Kristof Tirez¹, Jan Peters¹, Patrick Berghmans¹, Elke Adriaenssens², Edward Roekens², Florian Meirer³, Christina Strel⁴; ¹Flemish Institute for Technological Research (VITO); ²Flemish Environment Agency, Department Air, Communication and Environment, Section Air; ³Utrecht University, Inorganic Chemistry and Catalysis; ⁴Vienna University of Technology, Atominstitut

- 4:50 (216) **On the Use of X-Ray Fluorescence in Cultural Heritage Studies: A Portuguese Testimony;** Jose Mirao¹, Antonio Candeias¹; ¹Hercules Laboratory - University of Evora, Portugal
- 5:10 (217) **Geographical Profiling of Sand Using Micro-XRF and Trace Element Analysis;** Sergey Mamedov¹; ¹Horiba Scientific

Monday Afternoon, Greenway H/I

SPECTROSCOPY EMERGING LEADER IN MOLECULAR SPECTROSCOPY AWARD SYMPOSIUM HONORING MATTHEW BAKER

Organizers: Laura Bush and Matthew Baker;
 President: Matthew Baker

- 3:50 (218) **Discrete Frequency Vibrational Spectroscopic Imaging: Development and Prospects;** Rohit Bhargava¹; ¹University of Illinois at Urbana-Champaign
- 4:10 (219) **Recent Applications of ATR-FTIR Spectroscopic Imaging;** Sergei Kazarian¹, Andrew Ewing¹; ¹Imperial College London
- 4:30 (220) **SESORS for Subsurface Tissue Monitoring;** Nick Stone¹, Ben Gardner¹, Pavel Matousek²; ¹University of Exeter; ²STFC Rutherford Appleton Laboratory
- 4:50 (221) **Clinical Applications for Far-Field and Near-Field FTIR Imaging;** Kathleen Gough¹; ¹University of Manitoba
- 5:10 (222) **Take My Breath Away: Non-Invasive Breathomics for Bacterial Detection;** Roy Goodacre¹; ¹University of Manchester, UK

Monday Afternoon, Greenway G

VIBRATIONAL SPECTROSCOPY AND ADVANCED STATISTICS FOR MEDICAL DIAGNOSTICS

Organizer and President: Igor Lednev

- 3:50 (223) **Label-free Diagnostics by FTIR Spectroscopy;** Klaus Gerwert¹; ¹Ruhr-University Bochum
- 4:10 (224) **A Novel Raman Spectroscopic Method for Early Diagnosis of Osteoarthritis;** Mustafa Unal¹, Ozan Akkus¹; ¹Case Western Reserve University
- 4:30 (225) **Optimization of the Analysis Routines for Raman Spectra;** Thomas Bocklitz^{1,2}, Shuxia Guo^{1,2}, Oleg Ryabchykov^{1,2}, Ralf Heinke^{1,2}, Thomas Doerfer^{1,2}, Stephan Stoeckel^{1,2}, Jürgen Popp^{1,2}; ¹Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Jena, Germany; ²Leibniz Institute of Photonic Technology, Jena, Germany
- 4:50 (226) **Raman Microscopy of Bladder Cancer Cells Expressing Green Fluorescent Protein;** Gurjit S. Mandair¹, Amy Han², Evan T. Keller², Michael D. Morris³; ¹Department of Biologic and Materials Sciences, School of Dentistry, University of Michigan, Ann Arbor, MI; ²NCRC Building 20, University of Michigan, Ann Arbor, Michigan; ³Department of Chemistry, University of Michigan, Ann Arbor, MI
- 5:10 (227) **DDR2 Detection Leading to Cancer Diagnostics;** Alexandre Girard¹, Corinna Wetherill¹, Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde

Monday Afternoon, Lakeshore B

CURRENT APPLICATIONS OF DIFFUSE REFLECTANCE SPECTROSCOPY

Organizer and President: Benoit Inge

- 3:50 (228) **The Interfacing of Diffuse Reflectance Probes to Monitor and Control Continuous Solid Dose Manufacturing;** Ke Hong¹, Angela Liu¹, Stephen Hammond¹; ¹Pfizer Inc
- 4:10 (229) **Penalty Based Methods for Calibration Maintenance;** John Kalivas¹; ¹Idaho State University

TECHNICAL PROGRAM – MONDAY

Orals 3:50 – 5:30 pm

- 4:30 (230) **Infrared Reflectance Spectroscopy for Detection and Classification of Mineral Components**; Neal Gallagher¹, Toya Beiswenger², James Szecsody², Timothy Johnson²; ¹Eigenvector Research, Inc.; ²Pacific Northwest National Laboratory
- 4:50 (231) **Chemometrics for NIR in the Real World: What We've Learned over 20 Years**; Wendy Flory¹, Mary Beth Seasholtz¹; ¹The Dow Chemical Company
- 5:10 (232) **Near Infrared Spectroscopic Remote Sensing of Pulses from Extrasolar Planets**; Robert Lodder¹, Anne Brooks¹; ¹University of Kentucky

Monday Afternoon, Nicollet B/C

ITP - CAPILLARY ELECTROPHORESIS APPLICATIONS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Bezhan Chankvetadze and Christian Kalmpfl

- 3:50 (233) **Sequence-Dependent Electrophoretic Migration of DNA at High Salt Concentration in CZE**; Linda McGown¹, Jia Zhao¹, Steven Cramer¹; ¹Rensselaer Polytechnic Institute
- 4:10 (234) **Recent Development in Complex Glycan Analysis by CE-MS**; David Chen¹; ¹University of British Columbia
- 4:30 (235) **Tetrabutylammonium, a DNA Denaturant**; Earle Stellwagen¹, Nancy Stellwagen¹; ¹University of Iowa
- 4:50 (236) **Multiple Modes Application of Capillary Electrophoresis in Aptamers Selection**; Qu Feng¹; ¹Beijing Institute of Technology
- 5:10 (237) **Characterization of Novel Chiral Helical Molecules by Capillary Electrophoresis**; Dusan Koval¹, Harish Talele¹, Lukas Severa¹, Jan Vavra¹, Paul E. Reyes-Gutierrez¹, Filip Tepy¹, Vaclav Kasicka¹; ¹Institute of Organic Chemistry & Biochemistry, Czech Academy of Sciences

Monday Afternoon, Nicollet D2/D3

ITP - MICROFLUIDICS AND MINATURIZATION

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Rafael Davalos and Rodrigo Martinez-Duarte

- 3:50 (238) **Thiolene-based Microfluidic Devices for Applications in Drug Metabolism Studies**; Jörg Kutter¹, Cornelia Zapp², Unai Ortiz de Orruno Cuesta³, Josiane Lafleur¹; ¹University of Copenhagen; ²University of Heidelberg; ³Universitat Autònoma de Barcelona
- 4:10 (239) **Coupling Frequency-Selective Dielectrophoretic Biomarker Enrichment within Physiological Media to Electrochemical Detection**; Nathan Swami¹, Ali Rohani¹, Walter Varhue¹, Kuo-Tang Liao², Chia-Fu Chou²; ¹University of Virginia, Charlottesville, VA; ²Institute of Physics, Academia Sinica, Taiwan
- 4:30 (240) **Assembled Microfluidic Platforms and Moonshine**; Carlos Garcia¹, Mauro S. Ferreira Santos², Eric da Costa¹, Ivano Gutiz²; ¹Clemson University; ²University of Sao Paulo
- 4:50 (241) **Nanogels: New Materials to Program, Erase, and Redesign Liquid Phase Separations**; Lisa Holland¹, Srikanth Gattu¹, Cassandra Carihfield¹, Brandon Durney¹, Grace Weisenmiller¹; ¹West Virginia University Chemistry
- 5:10 (242) **Bioanalytical Applications of Microchip Electrophoresis with Coupled Channels**; Marián Masár¹, Peter Troška¹, Marina Rudašová¹, Jasna Hradski¹, Róbert Bodor¹; ¹Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Slovakia

Monday Afternoon, Greenway J

INTEGRATION OF LIBS IN THE ANALYTICAL LABORATORY

Organizer: Vincent Motto-Ros; Presider: Matthieu Baudelet

- 3:50 (243) **Towards the Integration of LIBS in the CRITT Matériaux Alsace Analytical Laboratory**; Frederic Pelascini¹, Vincent Motto-Ros²; ¹CRITT Matériaux Alsace, 67305 Schiltigheim, France; ²Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, 69622 Villeurbanne, France
- 4:10 (244) **The Critical Aspects of Data Analysis for Quantification in LIBS**; B. Bousquet¹, L. Bassel¹, D. Syvilay², E. Negre³, F. Trichard⁴, F. Pelascini³, J. El Haddad⁵, A. Harhira⁵, S. Moncayo⁶, J. Picard⁷, D. Devisme⁸, V. Motto-Ros⁴; ¹CELIA, UMR CNRS 5107, Université de Bordeaux, 351 Cours de la Libération, France; ²LRMH Laboratory, CNRS USR3224 CRC-LRMH, Champs-sur-Marne, France; ³CRITT Matériaux Alsace, France; ⁴Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, France; ⁵National Research Council Canada, Energy, Mining and Environment Portfolio, Boucherville (QC), Canada; ⁶Department of Analytical Chemistry, Faculty of Chemical Sciences, Complutense University, Madrid, Spain; ⁷CEA, DSM, IRAMIS, NIMBE-UMR 3685, LEDNA, France; ⁸NASA PostDoc Program ORAU-USRA, Marshall Space Flight Center, Huntsville, AL
- 4:30 (245) **Laser Induced Breakdown Spectroscopy, an Example of Its use as a Complete Analytical Solution**; Jhanis Gonzalez^{1,2}, Robb Hunt², Charles Sisson², Alexandre Bolshakov², C. Derrick Quarles², Chunyi Liu², Jong Yoo², Richard E. Russo^{1,2}; ¹L. Berkeley National Lab; ²Applied Spectra, Inc
- 4:50 (246) **LIBS for Monitoring the Fabrication of Optical Ceramics**; Mauro Martinez¹, Matthieu Baudelet^{1,3}, Romain Gaume³, Sudeep Jung Pandey⁴, Jan Hostasa², Laura Esposito²; ¹National Center of Forensic Science/Chemistry Department, University of Central Florida; ²CNR ISTE National Research Council, Institute of Science and Technology for Ceramics; ³CREOL-The College of Optics and Photonics, University of Central Florida; ⁴Physics Department, University of Central Florida
- 5:10 (247) **Certified Analyses with Calibration-Free Laser-Induced Breakdown Spectroscopy: A Dream?**; Jörg Hermann^{1,2}; ¹Aix-Marseille University; ²Centre National de la Recherche Scientifique

Monday Afternoon, Greenway B/C

ION MOBILITY: ADDING NEW DIMENSIONS

Organizer and Presider: Brian Clowers

- 3:50 (248) **Recent Developments in Structures for Lossless Ion Manipulations (SLIM) for Enhanced Ion Mobility Separation**; Yehia Ibrahim¹, Liulin Deng¹, Ahmed Hamid¹, Sandilya Garimella¹, Ian Webb¹, Xueyun Zheng¹, Erin Baker¹, Spencer Prost¹, Randolph Norheim¹, Richard Smith¹; ¹Pacific Northwest National Laboratory
- 4:10 (249) **Gas-Phase Adsorption to Improve Ion Mobility-Mass Spectrometry Orthogonality: Linking Observed Mobility Shifts to Collision Cross Section and Binding Models**; Chris Hogan¹, Vivek Rawat¹, Carlos Larriba-Andaluz³, Derek Oberreit³, Hui Ouyang¹, Jikku Thomas¹; ¹University of Minnesota; ²Kanomax-FMT; ³Indiana University-Purdue University Indianapolis

TECHNICAL PROGRAM – MONDAY

Orals 3:50 – 5:30 pm

- 4:30 (250) **Ion Modification - A New Technology to Enhance the Selectivity of TOF-IMS Detectors**; Jonathan Atkinson¹, Alastair Clark¹, Bruce Grant¹, Steve Taylor¹; ¹Smiths Detection - Watford Ltd
- 4:50 (251) **Drift Gas Modifiers to Elucidate Chemical Class**; Brian Clowers¹, Pearl Kwantwi-Barima¹, Kelsey Morrison¹, Zhihao Yu¹; ¹Washington State University
- 5:10 (252) **Recent Advancement in FAIMS and Future Direction**; Satendra Prasad¹, Mike Belford¹, Jean-Jacques Duniach¹; ¹Thermo Fisher Scientific

Monday Afternoon, Lakeshore C PROCESS ANALYTICAL TECHNOLOGY IN THE PHARMACEUTICAL INDUSTRIES SESSION I

Organizers: Brandye Smith-Goettler and Saly Romero-Torres;
President: Saly Romero-Torres

- 3:50 (253) **Residence Time Distribution Analysis for a Hot Melt Granulation Process Using Positron Emission Particle Tracking and NIR Spectroscopic Probes**; Patrick Wray¹, John Jones¹, Martin Vernon¹, Gary McGeorge¹; ¹Bristol Myers Squibb
- 4:10 (254) **Applications of PAT-based Feedback Control Approaches Pharmaceutical Crystallization Development**; Zoltan Nagy¹; ¹Purdue University
- 4:30 (255) **Process Development and Design Space Definition of a Pharmaceutical Intermediate Azeotropic Drying System via *in situ* FT-IR & Raman Spectroscopies and FBRM**; Zachary Dance¹, Morgan Crawford¹, Aaron Moment¹, Busolo Wabuyele¹; ¹Merck & Co., Inc.
- 4:50 (256) **Combining Fluid Bed Process Data with Spectral Data to Improve Model Prediction of Product Performance**; Stephen W. Hoag¹, Ahmed Ibrahim¹; ¹University of Maryland, Baltimore
- 5:10 (257) **Managing Uncertainty in Design Space**; Mark Anderson¹, Patrick Whitcomb¹; ¹Stat-Ease, Inc.

Monday Afternoon, Nicollet D1 BIOANALYTICAL SERS II

Organizers and Presiders: Roy Goodacre and Duncan Graham

- 3:50 (258) **Targeted Molecular Detection in Human Biofluids**; Zachary Schultz¹; ¹University of Notre Dame
- 4:10 (259) ***In situ* Redox Assessments Using SERS**; Colin Campbell¹, Victoria Camus¹, Kate Fisher¹, Lauren Jamieson¹, Bill Nailon², Duncan McLaren²; ¹University of Edinburgh, School of Chemistry; ²NHS Lothian, Edinburgh Cancer Centre
- 4:30 (260) **SERS-based Lateral Flow Assay for the Rapid and Sensitive Detection of Specific Biomarkers**; Jaebum Choo¹; ¹Hanyang University

- 4:50 (261) **Challenges in Applying SERS to Quantitative Bioanalytical Measurements**; Marc Porter¹, Alexis Crawford¹, Aleksander Skuratovsky¹, Colin Young¹; ¹University of Utah
- 5:10 (262) **Highly Controlled Assembly of Molecules for Optimisation of SERS Detection Methods**; Stacey Laing¹, Karen Faulds¹; ¹University of Strathclyde

Monday Afternoon, Lakeshore A INDUSTRIAL RAMAN

Organizer and Presider: Karen Esmonde-White

- 3:50 (263) **Some Insights into Principal Component Analysis of Industrial Raman Spectra**; Douglas Elmore¹; ¹3M
- 4:10 (264) **Raman Spectroscopy Study of Frying Oil Quality**; Jinping Dong¹; ¹Cargill
- 4:30 (265) **Flying with Molecular Spectroscopy Instruments**; Xiaoyun Chen¹; ¹The Dow Chemical Company
- 4:50 (266) **Basic Aspects of Experimental Design in Raman Microscopy**; Alexander Rzhetskii¹; ¹Thermo Fisher Scientific
- 5:10 (267) **Enhanced Gas Phase Raman Scattering Using Substrate-Integrated Hollow Waveguides (iHWG) Coupled to Optical Fiber Probes**; J. Chance Carter¹, S. Michael Angel², Boris Mizaikoff³, William E. Hunt¹, Anastacia M. Manuel¹, Josh Huntington²; ¹Lawrence Livermore National Laboratory; ²University of South Carolina; ³Ulm University

Monday Afternoon, Greenway D INNOVATIVE APPROACHES TO TEACHING ANALYTICAL CHEMISTRY

Organizers: Mary Kate Donais, Alexandra Ros, Celeste Morris, Christopher Harrison; President: Celeste Morris

- 3:50 (268) **An Active Learning and Reduced Seat Time Approach to General Chemistry**; Michelle Driessen¹; ¹University of Minnesota
- 4:10 (269) **The Evolving Use of Electronic Tools in Undergraduate Analytical Teaching and Research**; Dwight Stoll¹; ¹Gustavus Adolphus College
- 4:30 (270) **Teaching Chemical Instrumentation Through Team-Based Research Projects**; Deanna O'Donnell¹; ¹Hamline University
- 4:50 (271) **In-Class Measurements of Academic Progress and Class Morale**; Allen R. White¹; ¹Rose-Holman Institute of Technology
- 5:10 (272) **Creating a Course Redesign Strategy: Examining an Instrumental Analysis Laboratory Course**; Anna Donnell¹; ¹University of Cincinnati, Center for the Enhancement of Teaching & Learning

TECHNICAL PROGRAM - TUESDAY

Plenary Lectures – *Nicollet B/C*

President: **Matthieu Baudelet**



8:00 am – FACSS Charles Mann Award for Applied Raman Spectroscopy
(273) **Process Raman: Reproducibility Drove Capability;** Brian Marquardt^{1,2}; ¹MarqMetrix Inc.; ²University of Washington, APL



8:30 am – Coblenz Society Craver Award
(274) **Multiplexed and Quantitative Bioanalysis Using Surface Enhanced Raman Spectroscopy (SERS);** Karen Faulds¹; ¹University of Strathclyde

Orals 9:15 – 10:55 am

Tuesday Morning, *Greenway A* ATMOSPHERIC-PRESSURE PLASMAS AS TOOLS FOR ATOMIC ANALYSES, MOLECULAR MASS SPECTROMETRY, AND CHEMICAL SYNTHESIS

Organizer and President: Jacob Shelley

- 9:15 (275) **Alternative Ionization Chemistries with Mixed-Gas Flowing Atmospheric-Pressure Afterglow (FAPA) Ambient Desorption/Ionization (ADI) Source;** Sunil Badal¹, Shawn Michalak², Yi You¹, Jacob Shelley¹; ¹Department of Chemistry and Biochemistry, Kent State University, Kent, OH; ²Stark State College, North Canton, OH
- 9:35 (276) **Atmospheric-pressure Plasmas as Electrochemical Electrodes for Nanomaterial Synthesis;** R. Mohan Sankaran¹; ¹Case Western Reserve University
- 9:55 (277) **Understanding and Advancing Solution-Cathode Glow Discharge - Optical Emission Spectrometry;** Michael Webb¹, Denise Moon¹, Wade Maresh¹, Christian Decker¹; ¹University of North Carolina Wilmington
- 10:15 (278) **Atmospheric-Pressure Ionization and Tunable Fragmentation of Peptides by Solution-Cathode Glow Discharge;** Andrew Schwartz¹, Jacob Shelley², Kelsey Williams², Courtney Walton², Gary Hieftje¹; ¹Indiana University; ²Kent State University
- 10:35 (279) **Negative Ion Chemistry in the FAPA-APGD Source;** Jaime Orejas¹, Jorge Pisonero², Nerea Bordel², Alfredo Sanz-Medel², Steven J. Ray¹; ¹University at Buffalo; ²University of Oviedo

Tuesday Morning, *Greenway H/I* CHARLES MANN AWARD SYMPOSIUM HONORING BRIAN MARQUART

Organizer and President: Brian Marquardt

- 9:15 (280) **UV Raman Spectroscopy Using A Spatial Heterodyne Raman Spectrometer: Planetary Exploration and On-line Applications;** S. Michael Angel¹, Nirmal Lamsal¹, K. Alicia Strange¹, Patrick Barnett¹; ¹University of South Carolina
- 9:35 (281) **Quantitative Characterization of Heterogeneous Processes by Raman Spectroscopy;** Sergey Mozharov¹, Brian Marquardt¹; ¹University of Washington
- 9:55 (282) **Raman Spectroscopy - No Longer the Technique of Last Resort in PAC/PAT;** Ian R. Lewis¹, David J. Strachan¹, Maryann Cuellar¹, Sean Gilliam¹, Karen Esmonde-White¹, Carsten Uerpmann², Herve Lucas², Alex Pitters², Bruno Lenain²; ¹Kaiser Optical Systems, Ann Arbor, MI; ²Kaiser Optical Systems, SARL, Ecully, France
- 10:15 (283) **Simultaneous Measurements of the Physical and Chemical Properties of Proteins by the Combination of Raman Spectroscopy and Dynamic Light Scattering;** E. Neil Lewis¹, John F. Carpenter², Matthew Brown³; ¹Mettler-Toledo; ²University of Colorado; ³Malvern Instruments, Ltd.
- 10:35 (284) **Transforming Raman Spectroscopy from Academic Theory to a Workhorse Tool for Industry;** Andrew Whitley¹; ¹HORIBA

Tuesday Morning, *Greenway G* MULTIMODAL IMAGING FOR BIOMEDICAL DIAGNOSIS AND THERAPY MONITORING

Organizer and President: Juergen Popp

- 9:15 (285) **A Fiber-Delivered Optoacoustic Guide for Precise Breast-Conserving Surgery;** Ji-Xin Cheng¹; ¹Purdue University
- 9:55 (286) **Fluorescence Lifetime-Based Augmented Reality Multimodal Imaging: Applications for Intraoperative Delineation of Surgical Margins and Biopsy Guidance;** Laura Marcu¹; ¹University of California Davis
- 9:55 (287) **Multimodal Morpho-Functional Optical Diagnosis of tissue Tumor;** Francesco Pavone¹; ¹LENS
- 10:15 (288) **Non-linear Multimodal Imaging a Possible Solution towards Intraoperative Diagnosis;** Michael Schmitt¹, Sandro Heuke², Fisseha Bekele Legesse^{1,2}, Tobias Meyer², Olga Chernavskaia², Thomas Bocklitz^{1,2}, Juergen Popp^{1,2}; ¹Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Jena, Germany; ²Leibniz-Institute of Photonic Technology Jena (IPHT), Jena, Germany
- 10:35 (289) **Differentiating Responses of Lung Cancer Cell Lines to Doxorubicin Exposure: *in vitro* Raman Micro Spectroscopy, Oxidative Stress and bcl-2 Protein Expression;** Zeineb Farhane¹, Franck Bonnier², Marcus Alexander Maher¹, Jane Bryant¹, Alan Casey¹, Hugh James Byrne¹; ¹DIT-FOCAS Research Institute; ²Université François-Rabelais de Tours, Faculty of Pharmacy

Tuesday Morning, *Greenway D* NUCLEAR FORENSICS

Organizer and President: Andrew Duffin

- 9:15 (290) **Monitoring Chromometer Fractionation in Actinide Metals;** Dallas Reilly¹, Jordan Corbey¹, Matthew Athon¹, Jon Schwantes¹, Kellen Springer¹; ¹Pacific Northwest National Laboratory
- 9:35 (291) **Spectroscopic Characterization of Uranyl-Nitric Acid Extraction by Tributylphosphate in Hydrocarbon Solvent;** Gregory Klunder¹, Paul Spackman¹, Patrick Grant¹; ¹Lawrence Livermore National Laboratory
- 9:55 (292) **Elemental Analysis of Impurity Content in Glasses by Extreme Ultraviolet Mass Spectrometry;** Carmen Menoni¹, Tyler Green¹, Ilya Kuznetsov¹, Weilun Chao³, Jorge Rocca¹, Andrew Duffin²; ¹Colorado State University; ²Pacific Northwest National Laboratory; ³Center for X-Ray Optics, Lawrence Berkeley Laboratory
- 10:15 (293) **Rapid Debris Analysis via Femtosecond Laser Ablation Sampling;** Jesse Ward¹, Andrew Duffin¹, Gregory Eiden¹; ¹Pacific Northwest National Laboratory
- 10:35 (294) **Applications of Absorption Spectroscopy and Chemometrics for Plutonium Monitoring in Nuclear Materials Processing Facilities;** Robert Lascola¹, Patrick O'Rourke¹, Edward Kyser¹, Michael Phillips¹; ¹Savannah River National Laboratory

TECHNICAL PROGRAM – TUESDAY

Orals 9:15 – 10:55 am

Tuesday Morning, Lakeshore B

NANO-IR/NANO-RAMAN - I

Organizers: Curtis Marcott and Andrew Whitley;

Presider: Curtis Marcott

- 9:15 (295) **The Imaging Advantage in Molecular Spectroscopy**; John Reffner¹; ¹John Jay College, CUNY
- 9:35 (296) **Raman Microscopy – from the Diffraction Limitations of Optics to NanoSpectroscopy**; Fran Adar¹, Maruda Shanmugasundaram¹; ¹HORIBA Scientific
- 9:55 (297) **Improved Sensitivity of Non-Resonantly Excited PTIR Probes Enables Monolayer Detection from the Visible through Mid-IR**; Andrea Centrone¹, Jungseok Chae^{1,2}, SangMin An^{1,2}, Yohan Yoon^{1,2}, Vladimir Aksyuk¹; ¹National Institute of Standards and Technology; ²University of Maryland
- 10:15 (298) **Tip-Enhanced Photo-Thermal Expansion with TERS**; Raul D. Rodriguez¹, Teresa Madeira¹, Harsha Shah¹, Eugene Bortchagovsky¹, Zoheb Khan¹, Dietrich R.T. Zahn¹; ¹Technische Universität Chemnitz
- 10:35 (299) **Studies of Polymer Ultrathin Films, Nanofibers and Single Crystals by AFM-IR and Selected Area Electron Diffraction**; John Rabolt¹; ¹University of Delaware

Tuesday Morning, Nicollet B/C

ITP - PROTEOMICS / GLYCOPROTEOMICS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;

Presiders: Rawi Ramutar and Coral Barbas

- 9:15 (300) **The Roles of Glycan and Glycopeptide Isomers in the Development and Progression of Diseases**; Yehia Mechref¹, Rui Zhu¹, Shiyue Zhou¹, Yifan Huang¹; ¹Texas Tech University
- 9:55 (301) **Deciphering the Proteome of Lymphoblastoid Cells from Nasu-Hakola Patients through a Complementary 2-DE and LC-MS Approach.**; Paolo Iadarola¹, Roberta Salvini², Anna Maria Agresta³, Antonella De Palma³, Pier Luigi Mauri³, Simona Viglio², Laura Fossati⁴, Anna Bardoni²; ¹Department of Biology and Biotechnology, Biochemistry Unit, University of Pavia, Italy.; ²Department of Molecular Medicine, University of Pavia, Italy.; ³Institute for Biochemical Technologies, Proteomics and Metabolomics Unit, National Research Council, Segrate (Milano), Italy.; ⁴Department of Brain and Behavioral Sciences, University of Pavia, Pavia, Italy
- 10:15 (302) **Nano-LC-Orbitrap MS/MS-Based Quantitative Proteomics and Transcriptomics for Uncovering the Mechanisms of Action of Rosemary Bioactives in Colon Cancer: A New Foodomics Approach**; Alberto Valdés¹, Virginia Garcia-Cañas¹, Konstantin Artemenko², Jonas Bergquist², Alejandro Cifuentes¹; ¹Laboratory of Foodomics, Institute of Food Science Research (CIAL, CSIC), Madrid, Spain; ²Analytical Chemistry, Department of Chemistry-BMC, Uppsala University, Uppsala, Sweden
- 10:35 (303) **New Enrichment and Separation Methods for Phosphoproteomics Analysis**; Mingliang Ye¹, Hanfa Zou¹; ¹Dalian Institute of Chemical Physics, CAS

Tuesday Morning, Nicollet D2/D3

ITP - SAMPLE PREPARATION / CONCENTRATION

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;

Presiders: Marja-Liisa Riekkola and Michal Markuszewski

- 9:15 (304) **Liquid Phase Microextraction Techniques for Capillary Electrophoresis/Mass Spectrometry**; Doo Soo Chung¹, Joon Yub Kwon¹, Hye Ryoo Lee¹, Jihye Kim²;

¹Seoul National University; ²Korea Atomic Energy Research Institute

- 9:55 (305) **Extraction, Concentration and Separation of dsDNAs Using an Open Capillary without an Applied Electric Field**; Cornelius Ivory¹, Jeffrey Burke², Sarah Friedrich³, Tza-Huei Wang³, Kelvin Liu²; ¹Washington State University; ²Circulomics, Inc.; ³Johns Hopkins University
- 10:15 (306) **Micro-electromembrane Extraction across Multiple Organic and Aqueous Phases. A New Tool for Selective Pretreatment of Biological Fluids**; Pavel Kubán¹, Petr Boček¹, Knut Fredrik Seip², Astrid Gjelstad², Stig Pedersen-Bjergaard²; ¹Institute of Analytical Chemistry of CAS, Brno, Czech Republic; ²School of Pharmacy, University of Oslo, Blindern, Oslo, Norway
- 10:35 (307) **Challenges Encountered Using CE-LEDIF/ High Throughput DNA Sequencing for Aptamer Selection.**; Francois Couderc¹, Audrey Ric^{1,2}, Vincent Ecochard², Audrey Boutonnet³, Frederic Giot³, Varravaddheay Ong-Meang¹; ¹Université de Toulouse, Paul Sabatier, IMRCP; ²Université de Toulouse, Paul Sabatier, IPBS; ³Picometrics

Tuesday Morning, Greenway J

AUTOMATED LIBS FOR PROCESS CONTROL

Organizer and Presider: Francois Doucet

- 9:15 (308) **Automated LIBS for Process Control**; Reinhard Noll¹, C. Fricke-Begemann¹, S. Connemann¹, C. Meinhardt², V. Sturm¹; ¹Fraunhofer Institute for Laser Technology; ²RWTH Aachen University
- 9:55 (309) **Automated Process Analysis – LIBS takes root**; Tino Seger¹, Dominik Schiller¹, Christoph Scholz¹; ¹LTB Lasertechnik Berlin GmbH
- 10:15 (310) **Cereal Analysis with Laser Induced Breakdown Spectroscopy**; Gonca Bilge¹, Banu Sezer¹, Ismail Hakkı Boyacı¹, Kemal Efe Eseller², Halil Berberoglu³, Hamit Koksel¹; ¹Department of Food Engineering, Hacettepe University; ²Department of Electrical and Electronics Engineering, Atilim University; ³Department of Physics, Gazi University
- 10:35 (311) **High Throughput Online LIBS Monitoring**; Francois Doucet¹, Lutfu Ozcan¹; ¹ELEMISSION Inc.

Tuesday Morning, Greenway B/C

Solving Industrial Problems with Vibrational Spectroscopy

Organizers and Presiders: Patrick Wray and John Bobiak

- 9:15 (312) **Solving Problems in Tablet Dissolution Using FTIR Spectroscopic Imaging**; Sergei Kazarian¹, Andrew Ewing¹; ¹Imperial College London
- 9:35 (313) **The Influence of Intermolecular Forces on Amorphous Stability Probed by Terahertz and Low-Frequency Raman Spectroscopy**; Michael Ruggiero¹, J. Axel Zeitler¹; ¹University of Cambridge
- 9:55 (314) **Studying The Effect of Humidity on Nifedipine/PVP Solid Dispersion stability Using FT-IR Spectroscopy**; Abdulrahman Aloumi¹, Ka Lung Andrew Chan¹; ¹King
- 10:15 (315) **Rapid Discrimination of Polymorphic Crystal Forms by Nonlinear Optical Stokes Ellipsometric Microscopy**; Garth Simpson¹, Paul D. Schmitt¹, Emma L. Kerian¹, Ximeng Y. Dow¹; ¹Purdue University

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

- 10:35 (316) **A Systematic Evaluation of Spectroscopic Process Analytical Technologies to Inform Implementation into a Continuous Process**; David Myers¹, Lukas Barnes¹, Bryan Castle¹, Tony Cooper¹, Jimmy Engle¹, Aaron Garrett¹, Evan Hetrick¹, Michael Miller¹, Zhenqi Shi¹, Robert Glenn Rupard¹; ¹Eli Lilly and Company

Tuesday Morning, Nicollet D1
EMERGING RAMAN II
 Organizers and Presiders: Ian Lewis, Duncan Graham and Pavel Matousek

- 9:15 (317) **Raman Microscopy Beyond the Resolution Limit**; Katsumasa Fujita¹; ¹Osaka University
- 9:35 (318) **Seeing Things in a New Light: Brillouin/Raman Microscope for Physico-Chemical Microscopic Analysis**; Vladislav Yakovlev¹; ¹Texas A&M University
- 9:55 (319) **Raman Signal Enhancement via Quantum Coherence**; Dmitri Voronine³, Marlan Scully^{1,2,3}; ¹Baylor University; ²Princeton University; ³Texas A&M University
- 10:15 (320) **Low Content and Multiple Analyte Quantification in the Solid-State by Raman Spectroscopy: An Alternative to HPLC?**; Alan Ryder¹, Boyan Li¹, Amandine Calvet¹, Yannick Casamayou-Boucau¹, Cheryl Morris¹; ¹Nanoscale Biophotonics Lab., School of Chemistry, National University of Ireland Galway.
- 10:35 (321) **Anti-reflection coating for boosting tip-enhanced Raman spectroscopy performance**; Evgeniya Sheremet¹, Raul D. Rodriguez¹, Ashutosh Mukherjee¹, Michael Hietschold¹, Dietrich R.T. Zahn¹; ¹Technische Universität Chemnitz

Tuesday Morning, Lakeshore A
BIOANALYTICAL SERS III
 Organizers and Presiders: Roy Goodacre and Duncan Graham

- 9:15 (322) **Development and Deployment of Robust SERS for Multiplexed Microbial Quantification**; Karen Faulds¹, Kirsten Gracie¹, Duncan Graham¹, Samuel Mabbott¹, Hayleigh Kearns¹, Roy Goodacre²; ¹University of Strathclyde; ²University of Manchester
- 9:35 (323) **SERS as a Novel Approach for Ultra-Sensitive Magnetic Immunoassays**; Jianlin Yao¹; ¹Soochow University
- 9:55 (324) **Electrochemical Surface-Enhanced Raman Spectroscopy (EC-SERS) – A Tool for Exploring Protein-Biomembrane Interactions at the Molecular Level**; Christa Brosseau¹, Reem Karaballi¹, Soraya Merchant¹, Sasha Power¹; ¹Saint Mary
- 10:15 (325) **SERS for the Detection of Low Molecular Weight Biothiols in Umbilical Cord Whole Blood**; Bernhard Lendl¹, Julia Kuligowski¹, Marwa R. El-Zahry¹, Ángel Sánchez-Illana², Guillermo Quintás³, Máximo Vento²; ¹Technische Universität Wien, Austria; ²Neonatal Research Unit, Health Research Institute Hospital La Fe, Valencia,

- Spain; ³Safety & Sustainability, Leitat Technological Center, Valencia, Spain
- 10:35 (326) **Surface Enhanced Raman Spectroscopy-based Nanosensors for *in vivo* in situ Oxidation-Reduction-Potential Sensing in Lung Injury**; Samuel Stanfield¹, Sarah McAughtrie¹, Mark Bradley¹, Colin Campbell¹; ¹University of Edinburgh

Tuesday Morning, Lakeshore C
BOTTOM-UP PLASMONIC NANOPARTICLES: SPECTROSCOPIC APPLICATIONS
 Organizers: Jennifer Shumaker-Parry and Amanda Haes; Presider: Jennifer Shumaker-Parry

- 9:15 (327) **Controlling the Plasmon Excitation of Triangular Gold Nanoprisms Enables Detection of Yoctomole microRNAs**; Rajesh Sardar¹, Thakshila Liyanage¹; ¹IUPUI
- 9:35 (328) **Colloidal Lithography On Flexible Plastic Substrates**; Laura Sagie¹, Jie He¹, Sarah Unser¹; ¹University of Cincinnati
- 9:55 (329) **How to Make Surface Chemistry on Gold Nanostars Promote Reproducible Small Molecule Detection**; Amanda Haes¹, Wenjing Xi¹; ¹University of Iowa
- 10:15 (330) **Plasmonic Molecules for Probing Conductivity with Light**; Bjoern Reinhard¹; ¹Boston University
- 10:35 (331) **Flexible SERS Substrates for the Detection of Small Molecules**; Li-Lin Tay¹, John Hulse¹, Jeff Fraser¹, Sarah Milliken¹, Shawn Poirier¹; ¹National Research Council Canada

Tuesday Morning, Greenway E
IR, RAMAN AND NONLINEAR SPECTROSCOPIES OF SURFACES AND BOUNDARIES
 Organizers and Presiders: Takeshi Hasegawa and Masanari Okuno

- 9:15 (332) **IR pMAIRS: A Cutting-Edge Tool to Reveal the Molecular Orientation in an Ultrathin Film**; Takeshi Hasegawa¹; ¹ICR, Kyoto University
- 9:35 (333) **Molecular Orientation and Conformation of Fluorinated Polymers at Interface Studied by Vibrational Sum Frequency Generation Spectroscopy**; Masanari Okuno¹, Taka-aki Ishibashi¹; ¹University of Tsukuba
- 9:55 (334) **Molecular Structures of Peptides and Proteins at Interfaces Studied by Linear and Nonlinear Vibrational Spectroscopic Techniques**; Zhan Chen¹; ¹University of Michigan
- 10:15 (335) **Infrared Spectroscopy as a Tool for Studying Interstellar Dust Chemistry**; Tetsuya Hama¹, Akira Kouchi¹, Naoki Watanabe¹; ¹Institute of Low Temperature Science, Hokkaido Univ.
- 10:35 (336) **Total Internal Reflection (TIR) Raman Spectroscopy**; Colin Bain¹; ¹Durham University

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

All Tuesday posters should be put up between 9:00 – 10:00 am and removed by 4:30 pm

ITP – Liquid Phase Separation Methods Posters

Poster Board #1

- (337) **HPLC Analysis of Fluorescently Labelled Fatty Acids in Food Samples Using an Organic Monolithic Column and a Butyl Silica Column**; Murthy Jonnada¹, Ziad El Rassi¹, Guadalupe Davila El Rassi²; ¹Department of Chemistry, Oklahoma State University; ²Robert M. Kerr

Food & Agricultural Products Center, Oklahoma State University

Poster Board #2

- (338) **How to Select Relevant Variables in Non-Targeted Metabolomics Data? Different Statistical Approaches**; Renata Bujak¹, Emilia Daghir - Wojtkowiak¹, Roman Kaliszan¹, Michał Jan Markuszewski¹; ¹Department

TECHNICAL PROGRAM – TUESDAY

Posters 11:00 am – 12:00 pm

of Biopharmaceutics and Pharmacodynamics, Medical University of Gdańsk

Poster Board #3

(339) **Stratified Polar Silica Bonded Stationary Phases for HILIC and Affinity Chromatography at Reduced Nonspecific Interactions;** Renuka Rathnasekara¹, Ziad El Rassi¹; ¹Oklahoma State University

Poster Board #4

(340) **Designing Highly-Sensitive Electrical Impedance Based Microfluidic Flow Sensors;** Pengfei Niu¹, Brian J. Nablo¹, Darwin R. Reyes¹; ¹BioMEMS and Microsystem Metrology, Nanoscale Metrology Group, Engineering Physics Division, Physical Measurement Laboratory, National Institute of Standards and Technology, Gaithersburg, MD

Poster Board #5

(341) **Simultaneous Determination of Human Biogenic Amines and Their Metabolites with the use of Hydrophilic Interaction Chromatography Preceded by Microextraction as the Preconcentration Tool;** Tomasz Bączek¹, Lucyna Konieczna¹, Anna Roszkowska¹; ¹Medical University of Gdansk

Poster Board #6

(342) **Tunable Short-Pass filter for Recovering Long DNA Using an Entropic Trap;** Pranav Agrawal¹, Kevin D. Dorfman¹; ¹University of Minnesota

Poster Board #7

(343) **Non-targeted High Resolution Tandem Mass Spectrometry (HR-MS/MS) Screening and Mutagenicity Evaluation of Photo-Degradation Products of Tartrazine (E102) in a Commercial Soft Drink;** Karthik Yamjala¹, Meyyanathan Subramania Nainar¹; ¹JSS College of Pharmacy, Udhagamandalam

Poster Board #8

(344) **The Effect of pH on the Partitioning of Polychlorinated Biphenyls (PCBs) between Sediment Grain Sizes and Water;** Gbadebo Adeyinka¹, Brenda Moodley¹; ¹University of KwaZulu-Natal

Poster Board #9

(345) **Monolithic Stationary Phases with Incorporated Nanoparticles as Chromatographic Separation Media for High Performance Liquid Chromatography and Capillary Electrochromatography;** Nisansala Ganewatta¹, Ziad El Rassi¹; ¹Oklahoma State University

Poster Board #10

(346) **Comparison of Liposome- and Octanol-water Distribution Constants of Antioxidants;** Susanne Wiedmer¹, Jana Vanova², Petr Cesla²; ¹Department of Chemistry, University of Helsinki, Finland; ²Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Pardubice, Czech Republic

Poster Board #11

(347) **Distribution Constants of Local Anesthetics between Aqueous and Liposome Phases;** Susanne Wiedmer¹, Suvi-Katriina Ruokonen¹, Filip Dusa¹, Paula Holma¹, Alexandra Robciuc², Antti Rantamäki¹, Juha Holopainen²; ¹Department of Chemistry - University of Helsinki, University of Helsinki, Finland; ²Department of Ophthalmology - University of Helsinki and Helsinki University Hospital, Helsinki, Finland

Poster Board #12

(348) **Prediction of Gradient Retention Data of Oligomeric Series in HILIC;** Nikola Vankova¹, Petr Cesla¹; ¹University of Pardubice, Faculty of Chemical

Technology, Department of Analytical Chemistry, Pardubice, Czech Republic, CZ

Poster Board #13

(349) **Development and Validation of HPLC-MS/MS Method for the Simultaneous Determination of Seventeen Metabolites in Human Urine;** Michał Jan Markuszewski¹, Arlette Yumba Mpanga¹, Danuta Siluk¹, Julia Jacyna¹, Oliwia Szerkus¹, Renata Bujak¹, Marcin Markuszewski², Marcin Matuszewski², Roman Kaliszan¹; ¹Department of Biopharmaceutics and Pharmacodynamics, Medical University of Gdańsk, Gdańsk, Poland; ²Department of Urology, Medical University of Gdańsk, Gdańsk, Poland

Poster Board #14

(350) **A New Approach to Investigate Microfluidic Substrates: Examination of Air Plasma Treated PDMS Samples by Inverse Gas Chromatography;** András Guttman^{1,2}, Gábor Járvas^{1,2}, Márton Szigeti^{1,2}, László Hajba², András Dallos³, Brigitta Mészáros¹; ¹Horváth Csaba Memorial Institute of Bioanalytical Research, University of Debrecen, Debrecen, Hungary; ²MTA-PE Translational Glycomics Research Group, MUKKI, University of Pannonia, Veszprem, Hungary; ³Department of Physical Chemistry, University of Pannonia, Veszprem, Hungary

Poster Board #15

(351) **μLAS, a Disruptive Technology for Size Analysis of DNA with Unrivalled Sensitivity : Application for Circulating Cell Free DNA Analysis;** Audrey Boutonnet¹, Comtet Louis Andriamanampisoa¹, Aurélien Bancaud², Jacques Favre¹, Frédéric Ginot¹, Arnaud Morin¹, Vincent Picot¹, Laure Saia¹; ¹Picometrics Technologies; ²LAAS-CNRS

Poster Board #16

(352) **Development of a scanning Microfluidic Chromatography System for Binding Assays with Near Infrared Fluorescence Detection;** Elliott Rodriguez¹, John Vargas¹, Benjamin Hage¹, Michael Stoller¹, Stephen Morrin¹, David Hage¹; ¹University of Nebraska-Lincoln

Poster Board #17

(353) **¹H-NMR Spectroscopy to Analyze the Metabolome of Exhaled Breath Condensate from alpha1-antitrypsin Deficient (AATD) Patients and Healthy Controls ;** Marco Fumagalli¹, Jan Stolk², Carlotta Ciarra³, Rita Bussei³, Valeria Mazzoni³, Simona Viglio⁴, Paolo Iadarola¹, Cristina Airolti³; ¹Department of Biology and Biotechnologies, Biochemistry Unit, University of Pavia, Italy; ²Department of Pulmonology, Leiden University Medical Center, Leiden, the Netherlands; ³Department of Biotechnology and Biosciences, University of Milano-Bicocca, Italy; ⁴Department of Molecular Medicine, University of Pavia, Italy

Poster Board #18

(354) **Development of a NMR-Based Approach to Evaluate the Metabolome of BALf for Biomarker Identification of Bronchiolitis Obliterans Syndrome (BOS);** Cristina Airolti¹, Carlotta Ciarra¹, Marco Fumagalli², Sara Magni³, Simona Viglio⁴, Davide Piloni³, Annamaria Bardoni⁴, Maddalena Cagnone⁴, Federica Meloni³, Paolo Iadarola²; ¹Department of Biotechnology and Biosciences, University of Milano-Bicocca, Milano, Italy; ²Department of Biology and Biotechnologies, University of Pavia, Italy; ³Cardiothoracic and Vascular Department, Pneumology Unit, IRCCS

TECHNICAL PROGRAM – TUESDAY

Posters 11:00 am – 12:00 pm

Policlinico San Matteo Foundation, Pavia, Italy;
⁴Department of Molecular Medicine, University of Pavia,
 Italy

Poster Board #19

(355) **Optimization of On-Column Entrapment Containing Human Serum Albumin for the Study of drug-Protein Binding by High Performance Affinity Chromatography;** Shiden Azaria¹, John Vargas¹, David Hage¹; ¹University of Nebraska- Lincoln

Poster Board #20

(356) **Analysis of Drug Binding with Soluble Proteins by Using Ultrafast Affinity Extraction and Alpha1-Acid glycoprotein Microcolumns;** Sandya Rani Beeram¹, Xiwei Zheng¹, David Hage¹; ¹University of Nebraska

Poster Board #21

(357) **LC-MS, CE-MS and GC-MS Urine Metabolic Fingerprinting in Renal Cell Carcinoma;** Michał J. Markuszewski¹, Marta Kordalewska¹, Renata Bujak¹, Joanna Godziń², Arlette Yumba Mpanga¹, Ángeles López Gonzálves², Marcin Markuszewski³, Marcin Matuszewski³, Roman Kaliszan¹, Coral Barbas²; ¹Department of Biopharmaceutics and Pharmacodynamics, Medical University of Gdansk, Gdansk, Poland; ²CEMBIO, Centre for Metabolomics and Bioanalysis, San Pablo CEU University, Madrid, Spain; ³Department of Urology, Medical University of Gdansk, Gdansk, Poland

Poster Board #22

(358) **Affinity Purification of Monoclonal Antibody Using a lab-On-A-Chip Device;** Mehnaz Mursalat¹, Mengxin He¹, Natalija Tasovac¹, Sagnik Basuray¹; ¹New Jersey Institute of Technology

LIBS Posters

Poster Board #23

(359) **Radial Distribution of Electron Density and Temperature in Laser-Induced Plasma;** Ghaneshwar Gautam¹, Christian Parigger¹; ¹University of Tennessee Space Institute

Poster Board #24

(360) **In-situ Measurements of Calcium Carbonate Dissolution under Rising pCO₂ Using Underwater Laser Induced Breakdown Spectroscopy;** Jinesh Jain¹, Christian Goueguel¹, Dustin McIntyre¹, Cantwell Carson, Harry Edenborn¹; ¹National Energy Technology Laboratory

Poster Board #25

(361) **In-situ Applications of Field-Portable Handheld LIBS Analyzers with Expanded Spectral Range;** Brendan Connors¹, David Day¹, Morgan Jennings¹; ¹SciAps, Inc.

Poster Board #26

(362) **Laser Induced Fluorescence for Arsenic Detection in Laser Induced Plasmas;** Jonathan Merten¹, Christopher Jones¹; ¹Arkansas State University

Poster Board #27

(363) **Substrate-Enhanced LIBS for Analyzing Liquid Samples;** Qun Li¹, Sean Wang¹; ¹B&W TEK

Poster Board #28

(364) **Laser-Induced Breakdown Spectroscopy for Elemental Characterization of Calcitic Alterations on Cave Walls;** Bruno Bousquet¹, Lena Bassel², Vincent Motto-Ros³, Florian Trichard³, Frederic Pelascini⁴, Faten Ammari², Remy Chapoulie², Catherine Ferrier¹, Delphine Lacanette¹; ¹University of Bordeaux; ²University Bordeaux Montaigne; ³University of Lyon; ⁴CRIT Matériaux Alsace

Poster Board #29

(365) **Multi-block Analysis Coupled to Laser-Induced Breakdown Spectroscopy for Elemental Characterization of Geological Materials from Caves;** Bruno Bousquet¹, Faten Ammari², Lena Bassel², Catherine Ferrier¹, Delphine Lacanette¹, Remy Chapoulie²; ¹University of Bordeaux; ²University Bordeaux Montaigne

Poster Board #30

(366) **Investigating Analyte Transport in Solution-Cathode Glow Discharge Using Wavelength-Resolved Imaging;** Denise Moon¹, Michael R. Webb¹; ¹University of North Carolina Wilmington

Poster Board #31

(367) **A Depth Profiling Method for Measuring Helium Retention in Tungsten Using Laser Based Characterization Techniques;** Guinevere Shaw¹; ¹University of Tennessee; ²Oak Ridge National Laboratory

Poster Board #32

(368) **Facilitating Diatomic Metal Oxide Formation in Femtosecond-Laser-Induced Plasmas;** Yonghoon Lee^{1,2}, Xianglei Mao¹, George C.-Y. Chan¹, Jhanis J. Gonzalez¹, Richard E. Russo¹, Vassilia Zorba¹; ¹Lawrence Berkeley National Laboratory, Berkeley CA; ²Department of Chemistry, Mokpo National University, Republic of Korea

Poster Board #33

(369) **Accurate Analysis of Sulfur in Edible Salts by Using Laser-Ablation Sampling;** Yonghoon Lee^{1,2}, Jose Chirinos³, Jhanis Gonzalez^{1,4}, Dayana Oropeza¹, Vassilia Zorba¹, Xianglei Mao¹, Jonghyun Yoo⁴, Richard E. Russo¹; ¹Lawrence Berkeley National Laboratory, Berkeley CA; ²Department of Chemistry, Mokpo National University, Republic of Korea; ³Escuela de Química, Facultad de Ciencias, Universidad Central de Venezuela 1041a, Venezuela; ⁴Applied Spectra, Inc., Fremont, CA

Raman Posters

Poster Board #34

(370) **Probing the Mechanism of Charge Transfer in Organic Crystals Using Femtosecond Stimulated Raman Spectroscopy;** Alyssa Cassabum¹, Renee Frontiera¹; ¹University of Minnesota

Poster Board #35

(371) **Elucidating Molecular Structure in New Zealand Native Chiton and Feathers Using Raman Spectroscopy and Density Functional Theory;** Keith Gordon¹; ¹University of Otago

Poster Board #36

(372) **Human and Animal Blood Differentiation Using Raman Spectroscopy and Chemometrics;** Kyle C. Doty¹, Gregory McLaughlin¹, Igor K. Lednev¹; ¹University at Albany, SUNY

Poster Board #37

(373) **Vibrational Assignments and Conformer Stability Determination of Cyclobutylchlorosilane by Variable Temperature Raman Spectra in Krypton Solution;** Reid Brenner¹, Bhushan Deodhar¹, Dattatray Sawant¹, Gamil Guirgis², Yannick Geboes³, Wouter Herrebout³, James Durig¹; ¹University of Missouri-Kansas City; ²College of Charleston; ³Universitair Centrum Antwerpen

Poster Board #38

(374) **Innovative Applications of Raman Microscopy;** Sergey Shilov¹, Peng Wang¹, Juergen Sawatzki², Thomas Tague¹; ¹Bruker Optics, Inc.; ²Bruker Optik GmbH

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 #39

(375) **Microcavity Raman Sensing: Improved System Stability for Quantitative Analysis;** Adam J. Hopkins¹, Benjamin Petrak², Andreas Muller²; ¹Alakai Defense Systems; ²University of South Florida

Poster Board #40

(376) **Study the Interaction between Monoclonal Antibody (mAb) Pharmaceuticals and SDS by Using Deep-UV Resonance Raman (DUVRR) Spectroscopy with Two-Dimensional (2D) Correlation Analysis;** Chen Qiu¹, Sergey Arzhantsev¹, John Kauffman¹; ¹Division of Pharmaceutical Analysis, Center for Drug Evaluation and Research, US Food and Drug Administration

Poster Board #41

(377) **Advanced Chemical Imaging of Hair Fiber: the Combination of Confocal Raman Microscopy and Band Target Entropy Minimization;** Shuying Cheng¹, Liangfeng Guo¹, Nuan Qin Ong¹, Marc Garland¹; ¹Institute of Chemical and Engineering Sciences

Poster Board #42

(378) **Temperature- and Ultraviolet Irradiation - Induced Structural Changes of polylactide and Poly(L-lactide)/Poly(D-lactide) Stereocomplex Studied by Raman and Terahertz Spectroscopies;** Moe Nakamura¹, Harumi Sato², Hiromichi Hoshina³, Yukihiro OZAKI¹; ¹Grad. Sch. of Sci. and Tech., Kwansei Gakuin Univ.; ²Grad. Sch. of Human Develop., Kobe Univ.; ³RIKEN, Sendai

Poster Board #43

(379) **Piezoresistance Strain Sensing in Single Carbon Fibers Epoxy Composites Using Raman Spectroscopy;** Nataliya Kalashnyk¹, Eric Faulques², Jan Schjødt-Thomsen, Lars R Jensen³, Jens Chr M Rauhe³, Ryszard Pyrz³, Dale L Perry⁴; ¹Institut Jean Lamour, UMR 7198 CNRS - Université de Lorraine, Nancy, France; ²Institut des Matériaux Jean Rouxel, UMR 6502 CNRS - Université de Nantes, Nantes, France; ³Department of Mechanical and Manufacturing Engineering, Aalborg University, Aalborg East, Denmark; ⁴Lawrence Berkeley National Laboratory, University of California, Berkeley, CA

Poster Board #44

(380) **Probing the Mechanism of Photoinduced Electron Transfer in Betaine-30 in Solution and Solid Phases;** Ruchira Silva¹, Alyssa Cassabaum¹, Renee Frontiera¹¹; ¹Department of Chemistry, University of Minnesota

Poster Board #45

(381) **Investigation of β -carotene and Lycopene Aggregation Structure in Tomato Using UV-VIS and Raman Spectroscopy;** Phiranuphon Meksiarun¹, Ishigaki Mika¹, Hideki Hashimoto¹, Toshihiko Kakitsubo², Takuma Genkawa³, Yukihiro Ozaki¹¹; ¹Kwansei Gakuin University, Sanda, Hyogo, Japan; ²Takii & Co., Ltd., Shimogyo-ku, Kyoto city, Kyoto, Japan; ³Tsukuba University, Tsukuba, Ibaraki, Japan

Poster Board #46

(382) **Raman Spectroscopic Screening Methods for Lung Cancer Detection;** Jeongho Kim¹, Wansun Kim Kim¹, Seungho Lee¹, Yongjin An An¹, Eunjung Kim¹, Hyung Woo Choi¹, Jae Hyung Kim¹, Boksoon Chang¹, Samjin Choi¹, Hun-Kuk Park¹; ¹Kyung Hee University

Poster Board #47

(383) **Development of an Efficient Robust Calibration Model of Spectroscopic Systems by Incorporating Variations of Pure Components: A Pharmaceutical Tablet Assay Example;** Md Nayeem Hossain¹, Carl Anderson¹, James Drennen¹; ¹Graduate School of Pharmaceutical Sciences, Duquesne University

Poster Board #48

(384) **Gated Raman to Support Mining Operations;** Paul Bartholomew^{1,3}, Jouni Takalo², Mari Tenhunen²; ¹University of New Haven; ²Timegate Instruments; ³Superb LLC

Poster Board #49

(385) **Representative Sampling in Solids and Turbid Media for Process Raman Measurements during Continuous or Batch Manufacturing Operations;** Karen Esmonde-White^{1,2}, Carsten Uerpman³, Sean Gilliam¹, Lisa Ganster¹, Ian Lewis¹; ¹Kaiser Optical Systems Inc.; ²University of Michigan Medical School; ³Kaiser Optical Systems SARL

Poster Board #50

(386) **Raman Spectroscopy in Polymer Processing Applications;** Lisa Ganster¹, Karen Esmonde-White^{1,2}, Ian Lewis¹; ¹Kaiser Optical Systems, Inc.; ²University of Michigan Medical School

11:40AM – 1:10 PM

WHAT'S HOT VENDOR PRESENTATIONS, Exhibit Hall

Presider: Brian Dable, *Arete Associates*

Free lunch available in exhibit hall for all conferees, ticket required

- | | |
|-------|--|
| 11:40 | Wasatch Photonics "Advantage of High Throughput Spectrometers" |
| 11:50 | B&W Tek "Handheld LIBS for the Pharmaceutical Industry" |
| 12:00 | Renishaw "Raman Imaging of Samples with Complex surface Topographies Using Renishaw's inVia Qontor" |
| 12:10 | HORIBA "NanoRaman/TERS Solutions - Beyond Ready...PROVEN!" |
| 12:20 | Ocean Optics "Soaked in SERS: New Gold/Silver Nanosponges Enhance Sensitivity" |
| 12:30 | Innovative Photonic Solutions "Advances in Laser Technology for Raman Spectroscopy" |
| 12:40 | Kaiser Optical Systems "Let Your Production Flow-Raman Spectroscopy for Continuous Manufacturing" |
| 12:50 | BioTools "The Power of 532 nm Excitation for Handheld Raman: From Explosives to Counterfeit Biologics" |
| 1:00 | Thermo Fisher Scientific "Accelerate Research and Improve Material Verification with Thermo Scientific Raman Instruments" |

Tuesday Afternoon, Greenway A

FUNDAMENTALS AND APPLICATIONS OF LASER ABLATION

Organizer and Presider: Jorge Pisonero

- | | |
|------|---|
| 1:20 | (387) Femtosecond Laser Ablation-ICPMS: Beam Homogenization and Delivery by Two-Stage Fourier Optical Processing; <u>Joachim Koch</u> ¹ , Debora Käser ¹ , Detlef Günther ¹ ; ¹ ETH Zurich, Laboratory of Inorganic Chemistry, Switzerland |
| 1:40 | (388) Laser Ionization Mass Spectrometry is Not the Poor Man; <u>Jose Vadillo</u> ¹ , Samara Medina ¹ , J. Javier Laserna ¹ ; ¹ University of Málaga |
| 2:00 | (389) Solid Sample Analysis by a Tandem LIBS and LA-ICP-MS System: Use of Chemometrics Tools for Data Reduction and Interpretation; <u>Jhanis Gonzalez</u> ^{1,2} ; ¹ L. Berkeley National Lab; ² Applied Spectra, Inc. |

TECHNICAL PROGRAM – TUESDAY

Orals 1:20 – 3:00 pm

- 2:20 (390) **Mapping the Elemental Distribution in Different Types of Rice Grains Using laser Ablation ICP-MS;** Todor Todorov¹, Patrick Gray¹; ¹Food and Drug Administration
- 2:40 (391) **Matrix-Free Ambient Pressure UV-LAESI Mass Spectrometry for Plant Metabolite Imaging;** Patrick McVey^{1,2}, Katherine-Jo Galayda^{1,2}, Liza Alexander^{1,2}, Basil Nikolau^{1,2}, R.S. Houk^{1,2}; ¹Iowa State University; ²Ames Laboratory US DOE

Tuesday Afternoon, Greenway H/I COBLENTZ CRAVER AWARD SYMPOSIUM HONORING KAREN FAULDS

Organizer: Karen Faulds; President: Duncan Graham

- 1:20 (392) **Detection of Drugs and Drug Metabolites Using SERS;** Roy Goodacre¹, Abdu Subaihi¹, Omar Alharbi¹, Yun Xu¹; ¹University of Manchester, UK
- 1:40 (393) **Detection of Mycoplasma with SERS. Progress Towards Clinical Applications.;** Richard Dluhy¹; ¹University of Alabama at Birmingham
- 2:00 (394) **Development of Micro-Scale Spatially Offset Raman Spectroscopy (Micro-SORS) for Analysis of Thin Turbid Layers;** Pavel Matousek¹, Claudia Conti², Chiara Colombo², Marco Realini²; ¹Rutherford Appleton Laboratory, Oxford, UK; ²ICVBC-CNR, Milan, Italy
- 2:20 (395) **What Factors Really Matter in Quantitative SERS?;** Steven Bell¹; ¹Queen
- 2:40 (396) **SHE – SERS, Hats and Enzymes;** Duncan Graham¹, Karen Faulds¹, Ewen Smith¹; ¹University of Strathclyde

Tuesday Afternoon, Greenway G SERS AND SESORS FOR BIOMEDICAL APPLICATIONS

Organizer and President: Bhavya Sharma

- 1:20 (397) **SERS as Powerful Tool in Food and Drug Monitoring;** Dana Cialla-May^{1,2,3}, Karina Weber^{1,2,3}, Juergen Popp^{1,2,3}; ¹Leibniz Institute of Photonic Technology (IPHT), Jena, Germany; ²Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics, Jena, Germany; ³InfectoGnostics Research Campus Jena, Centre for Applied Research, Jena, Germany
- 1:40 (398) **Surface-enhanced Spatially-offset Raman Spectroscopy (SESORS) in Tissues;** Steven Asiala¹, Jonathan Noonan², Gianluca Grassia², Neil MacRitchie², Neil Shand³, Pasquale Maffia², Paul Garside², Iain McInnes², Karen Faulds¹, Duncan Graham²; ¹University of Strathclyde; ²University of Glasgow; ³Defence Science and Technology Laboratory
- 2:00 (399) **SESORS for Neuroscience;** Amber Moody¹, Bhavya Sharma¹; ¹University of Tennessee
- 2:20 (400) **Dynamic SERS Optophysiology: Plasmonic Nanosensing for Monitoring Cell Secretion Events;** Jean-Francois Masson¹, Felix Lussier¹, Thibault Brule¹; ¹Universite de Montreal
- 2:40 (401) **Development of Nanosensors for the Detection of Cardiovascular Disease Biomarkers Using SERS;** Kirsten Gracie¹, Steven Asiala¹, Jonathan Noonan², Neil MacRitchie², Gianluca Grassia², Pasquale Maffia², Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde; ²University of Glasgow

Tuesday Afternoon, Lakeshore B NANO-IR/NANO-RAMAN - II

Organizers: Curtis Marcott and Andrew Whitley;
President: Curtis Marcott

- 1:20 (402) **Etalon Tip-Enhanced Raman Spectroscopy;** Evgeniya Sheremet¹, Raul D. Rodriguez¹, Ashutosh Mukherjee¹, Michael Hietschold¹, Dietrich R.T. Zahn¹; ¹Technische Universität Chemnitz
- 1:40 (403) **How to Investigate Parchment Alteration by AFM-IR;** Ariane Deniset-Besseau¹, Alexandre Dazzi¹, Laurianne Robinet², Gael Latour³, Marie-Claire Schanne-Klein⁴; ¹Laboratoire de Chimie Physique, Université Paris-Sud; ²Centre de recherche sur la conservation, Sorbonne Universités, Muséum National; ³Laboratoire Imagerie et Modélisation en Neurobiologie et Cancérologie, Université Paris-Sud; ⁴Laboratoire d'Optique et Biosciences, Ecole Polytechnique
- 2:00 (404) **TERS: Per aspera ad astra;** Andrey Kravayev¹; ¹AIST-NT Inc
- 2:20 (405) **Nanoscale Chemical Imaging by Photo-induced Force Microscopy;** Ryan Murdick¹, Will Morrison¹, Katie Park¹, Derek Nowak¹, Tom Albrecht¹, Sung Park¹; ¹Molecular Vista
- 2:40 (406) **Tip Enhanced Raman Spectroscopy Imaging of Opaque Samples in Organic Liquid;** Emmanuel Maisonhaute¹, Thomas Touzaline¹, Alice Dauphin¹, Suzanne Joiret¹, Ivan Lucas¹; ¹Université Pierre et Marie Curie

Tuesday Afternoon, Nicollet B/C

ITP - HPLC AND LC-MS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Govert Somsen and David Chen

- 1:20 (407) **Microscale Specific Separations Using Fullerenes;** Koji Otsuka¹, Madoka Tsuzuki¹, Eisuke Kanao¹, Toyohiro Naito¹, Takuya Kubo¹; ¹Graduate School of Engineering, Kyoto University
- 1:40 (408) **Uptake and Metabolization of Pharmaceuticals in Plants;** Christian Klampfl¹, Lisa Emhofer¹, Markus Himmelsbach¹; ¹Johannes Kepler University Linz, Institute of Analytical Chemistry, Austria
- 2:00 (409) **Deep Proteomic Profiling of Limited Samples Using Ultra-Low Flow Liquid Phase Separation Techniques Coupled To Advanced Mass Spectrometry;** Alexander Ivanov¹; ¹Northeastern University, Barnett Institute
- 2:20 (410) **Hybrid Technology for CE-MS Interfacing;** Frantisek Foret¹, Jana Krenkova¹, Karel Kleparnik¹, Anna Tycova¹; ¹Institute of Analytical Chemistry CAS, v.v.i.
- 2:40 (411) **Two-Dimensional Liquid Phase Separations Coupled with Mass Spectrometry;** Petr Cesla¹, Nikola Vankova¹, Jana Vanova¹, Zuzana Novakova¹; ¹University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry

Tuesday Afternoon, Nicollet D2/D3 ITP - DIELECTROPHORESIS II - APPLICATIONS AND METHODOLOGIES

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Mark Hayes and Fatima Labeed

- 1:20 (412) **Electric Field Induced Particle Rotation in Microchannel;** Prashanta Dutta¹, Walid Rezanoor¹; ¹Washington State University
- 1:40 (413) **Dielectrophoresis Force Spectroscopy for Micro and Nano Particles;** H. Daniel Ou-Yang¹, S. Min-Tzo Wei¹, Jingyu Wang¹, Hyunjo Park¹, Hao Huang¹; ¹Lehigh University

Future SciX Meeting: October 8 – 13, 2017, Reno, Nevada

TECHNICAL PROGRAM – TUESDAY

Orals 1:20 – 3:00 pm

- 2:00 (414) **Contactless Dielectrophoretic Enrichment of Tumor Initiating Cells with Enhanced Viability via cell-Scale Microstructures**; Rafael V Davalos¹, Jaka Cemazar¹, Temple Douglas¹, Eva Schmelz¹; ¹Virginia Tech
- 2:20 (415) **Sample Preparation: Strengthening the Weak Link in Microfluidics Using Carbon-electrode Dielectrophoresis**; Rodrigo Martinez-Duarte¹; ¹Clemson University
- 2:40 (416) **Enhancing Dielectrophoretic Particle Manipulation**; Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology

Tuesday Afternoon, Greenway J FUSION OF LIBS WITH OTHER TECHNIQUES

Organizer and Presider: Jozef Kaiser

- 1:20 (417) **Laser Induced Breakdown Spectroscopy for Food Analysis**; Ismail Hakki Boyaci¹, Gonca Bilge¹, Banu Sezer¹, Kemal Efe Eseller², Halil Berberoglu³; ¹Department of Food Engineering, Hacettepe University; ²Department of Electrical and Electronics Engineering, Atilim University; ³Department of Physics, Gazi University
- 1:40 (418) **Use of Simultaneous Vacuum UV Plasma Spectroscopy for LIBS Improvement**; Pavel Veis¹, Jaroslav Kristof¹; ¹Comenius University, Faculty of Math., Physics and Informatics, Bratislava, Slovakia
- 2:00 (419) **Novel Analytical Application of LIBS Using External Electric and Magnetic Fields**; Prasoon Diwakar¹, Payson Dieffenbach¹, Ahmed Hassanein¹; ¹Center for Materials Under Extreme Environment, School of Nuclear Engineering, Purdue University, West Lafayette, IN
- 2:20 (420) **Utilization of Computed Tomography and Laser Spectroscopy for 3D High Resolution Mapping**; Pavel Pořízka¹, Tomáš Zikmund¹, Markéta Tesařová¹, David Prochazka¹, Jan Novotný¹, Jozef Kaiser¹; ¹Central European Institute of Technology Brno University of Technology
- 2:40 (421) **LIBS for Recognition of Natural Health Products and Process Control**; Josette El Haddad¹, Aissa Harhira¹, Mohamad Sabsabi¹, Alain Blouin¹, Camilo Martinez-Farina², Fabrice Berrué², Bob Chapman²; ¹Energy, Mining and Environment, National Research Council of Canada, Boucherville, QC, Canada; ²Aquatic and Crop Resource Development, National Research Council of Canada, Halifax, Nova Scotia, Canada

Tuesday Afternoon, Greenway B/C ION MOBILITY: NEW INSIGHTS INTO ASSEMBLY, INTERACTIONS, AND STRUCTURES

Organizer and Presider: Matthew Bush

- 1:20 (422) **Differential Metal Ion Addition, Gas-Phase Ion Chemistry, and Their Combined Potential for Distinction of Isomeric Carbohydrates by Ion Mobility Spectrometry**; Eric D. Dodds¹, Yuting Huang¹, Katherine N. Schumacher¹, Abby S. Gelb¹, Lauren M. Petrosh¹; ¹University of Nebraska - Lincoln
- 1:40 (423) **Native IM-MS of Partially Unfolded Proteins**; James Prell¹, Micah Donor¹, Jesse Wilson¹; ¹University of Oregon
- 2:00 (424) **Characterizing Trapped Ion Mobility Spectrometry (TIMS) for Transmission and Preservation of Native Analyte Structures and Their Complexes**; Christian Bleiholder¹, Samuel R. Kirk¹, F. Caroline Liu¹; ¹Florida State University

- 2:20 (425) **Analysis of Native-Like Ions Using Structures for Lossless Ion Manipulation**; Matthew Bush¹, Samuel Allen¹, Rachel Eaton¹; ¹University of Washington
- 2:40 (426) **Secondary Structure Heterogeneity Preserved into the Gas Phase**; Stephen Valentine¹, Mahdiar Khakinejad¹, Samaneh Ghassabi Kondalaji¹; ¹West Virginia University

Tuesday Afternoon, Greenway D PROCESS ANALYTICAL TECHNOLOGY IN THE BIOPHARMACEUTICAL INDUSTRIES SESSION II

Organizers: Saly Romero-Torres and Brandye Smith-Goettler;
Presider: Saly Romero-Torres

- 1:00 **SAS PAT Technical Section Business Meeting**
- 1:20 (427) **Protein Secondary Structure Prediction Using Drop Coat Deposition Confocal Raman (DCDCR) Spectroscopy**; Ravi Kalyanaraman¹, Jeremy Peters¹, Anna Luczak¹, Varsha Ganesh¹, Eugene Park¹; ¹Bristol-Myers Squibb
- 1:40 (428) **Upstream Bioprocess Characterization by Raman Spectroscopy: Trending, Quantification and Control aspects**; John Bobiak¹, Dimuthu Jayawickrama¹, Boyong Wan¹, Nobel Vale¹; ¹Bristol Myers Squibb
- 2:00 (429) **Holistic Mammalian Cell Culture Input Raw Material Characterization Strategy and its Application**; Jason Dickens¹; ¹Biogen
- 2:20 (430) **PAT Applied to Biological Manufacturing: The Next Step(s) towards Infinity and Beyond**; Steven Short¹, John Higgins¹, Douglas Richardson¹, David Pollard¹; ¹Merck
- 2:40 (431) **Best Practices for the Development of Quantitative Chemometric Models for Upstream Bioprocess PAT Applications**; Saly Romero-Torres¹, Maryann E. Cuellar², Sean J. Gilliam^{2,3}; ¹Bio-Hyperplane LLC; ²Kaiser Optical Systems

Tuesday Afternoon, Nicollet D1 SPATIALLY OFFSET RAMAN SPECTROSCOPY (SORS)

Organizer and Presider: Pavel Matousek

- 1:20 (432) **DMD-based Software-Configurable Spatially-Offset Raman Spectroscopy for Spectral Depth-Profilng of Optically Turbid Samples**; Ioan Notingher¹, Zhiyu Liao¹, Faris Sinjab¹, Graham Gibson², Miles Padgett²; ¹University of Nottingham; ²University of Glasgow
- 1:40 (433) **Axially Perpendicular Offset Raman Measurement for Direct Quantitative Analysis of Contained Samples**; Hoeil Chung¹; ¹Hanyang University
- 2:00 (434) **Line-illumination Spatially Offset Raman Spectroscopy(SORS) Coupled with Various Curve Resolution Method**; Hyung Min Kim¹; ¹Kookmin University
- 2:20 (435) **Photon Migration Assessment Inside Bones of Differing Mineral Levels Using Spatially Offset Raman Spectroscopy**; Kay Sowoidnich¹, John H. Churchwell², Kevin Buckley¹, Allen E. Goodship², Anthony W. Parker¹, Pavel Matousek¹; ¹Central Laser Facility, Research Complex at Harwell, STFC Rutherford Appleton Laboratory, Harwell Campus, UK; ²UCL Institute of Orthopaedics and Musculoskeletal Science, Royal National Orthopaedic Hospital, London, UK
- 2:40 (436) **Spatially Offset Raman Spectroscopic Probe for Through Barrier Identification**; Phillip Wilcox¹, Jason Guicheteau¹, Ashish Tripathi¹, Steven Christesen¹; ¹US Army Edgewood Chemical Biological Center

TECHNICAL PROGRAM – TUESDAY

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

Tuesday Afternoon, Lakeshore A

SERS

Organizer: Duncan Graham; Presider: Colin Campbell

- 1:20 (437) **Quantitative Investigation on pKa-SERS Relationship by "Hot Spot" Normalization;** Haoran Wei^{1,2}, Weinan Leng^{1,2}, Peter Vikesland^{1,2}; ¹Department of Civil and Environmental Engineering, Virginia Tech; ²Institute for Critical Technology and Applied Science, Virginia Tech
- 1:40 (438) **Ex vivo pH Sensing via Fibre Optic Based Surface-Enhanced Raman Scattering (SERS);** Sarah McLaughtrie¹, Michael G. Tanner², Debaditya Choudhury², Yu Fei³, Tushar Choudhary², Thomas Craven¹, Bethany Mills¹, Colin J. Campbell¹, Kevin Dhaliwal¹, Mark Bradley¹; ¹University of Edinburgh; ²Heriot-Watt University; ³University of Bath
- 2:00 (439) **Macroscale SERS Uniformity and Reproducibility Using Densely Clustered Nanopillars;** Kaiyu Wu¹, Michael Schmidt¹, Tomas Rindzevicius¹, Anil Thilsted¹, Anja Boisen¹; ¹Department of Micro- and Nanotechnology, Technical University of Denmark
- 2:20 (440) **Detecting Specific Antigens Using the Catalytic Properties of Silver Nanoparticles Combined with SER(R)S Detection;** Sian Sloan-Dennison¹, Neil C Shand², Duncan Graham¹, Karen Faulds¹; ¹University of Strathclyde; ²Defence Science and Technology Laboratory
- 2:40 (441) **Biocompatible, Liposome-Based Surface Enhanced Raman Spectroscopy (SERS) Substrates;** Laura Sagie¹, William Lum¹, Ian Bruzas¹, Sarah Unser¹; ¹University of Cincinnati

Tuesday Afternoon, Lakeshore C

BOTTOM-UP PLASMONIC NANOPARTICLES: SYNTHETIC STRATEGIES

Organizers: Amanda Haes and Jennifer Shumaker-Parry; Presider: Amanda Haes

- 1:20 (442) **A Taxonomy of the Magneto-Optical Responses of Cyclic Plasmon-Supporting Metal Oligomers;** David Masiello¹; ¹University of Washington
- 1:40 (443) **XPS Study of the Stability of Au-Nanoparticle Incorporated Oxides for Optical Sensing of H₂ at High Temperatures;** John Baltrus¹, Paul Ohodnicki¹, Gordon Holcomb¹, Joseph Tylczak¹; ¹U.S. Department of Energy - NETL
- 2:00 (444) **Self-Assembled, Free-Standing Plasmonic Nanoparticle Films as Flexible SERS Platforms;** Jennifer S. Shumaker-Parry¹; ¹University of Utah
- 2:20 (445) **Localized Surface Plasmon Resonance of Single Au-Cu alloy Nanoparticles during galvanic Replacement Reaction;** Jing Zhao¹; ¹University of Connecticut
- 2:40 (446) **Metasurface Enhanced Raman Spectroscopy;** Andrea Tao¹; ¹UC San Diego

Tuesday Afternoon, Greenway E

FRONTIERS OF FAR-AND DEEP- ULTRAVIOLET SPECTROSCOPY I

Organizers: Yukihiro Ozaki, Satoshi Kawata and Yuika Saito; Presider: Yukihiro Ozaki

- 1:20 (447) **Aluminum Film-Over-Nanosphere Substrates for Deep-UV Surface-Enhanced Resonance Raman Spectroscopy;** Richard P. Van Duyne¹; ¹Northwestern University, Chemistry Department
- 1:40 (448) **Deep UV Resonance Raman Incisive Probing of Protein and Peptide Structure and Dynamics;** David

- 2:00 Punihaole¹, Sanford Asher¹, Elizabeth M. Dahlburg¹, Ryan S. Jakubek¹, Zhenmin Hong¹; ¹University of Pittsburgh (449) **DUV Raman Spectroscopy is a Versatile Tool for Probing Protein Aggregation;** Igor Lednev¹, Tatiana Quiñones-Ruiz¹, Manuel Rosario-Alomar¹, Juan Lopez-Garriga²; ¹University at Albany, SUNY; ²University of Puerto Rico at Mayagüez
- 2:20 (450) **Deep UV Raman Microscopy: Suppression of Photo-Degradation;** Satoshi Kawata¹, Yasuaki Kumamoto²; ¹Osaka University; ²Kyoto Prefectural University of Medicine
- 2:40 (451) **Improvement of Deep-UV Photocatalytic Effect by Spectroscopic Analysis;** Yuika Saito^{1,2}, Mitsuhiro Honda³, Yasuaki Kumamoto⁴, Atsushi Taguchi¹, Satoshi Kawata¹; ¹Osaka University; ²Gakusyuin university; ³Nagoya Institute of Technology; ⁴Kyoto Prefecture University of Medicine
- 3:00 **Poster Viewing and Coffee Break, Exhibit Hall**

Tuesday Afternoon, Greenway A

CELEBRATING THE LIFE AND LEGACY OF PROFESSOR JOE CARUSO

Organizers: Steven Ray and Ken Marcus; Presider: Gary Hieftje

- 3:50 (452) **The Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD) Microplasma: An Example of What I Learned from Joe Caruso - Its More Fun Living (a little) Outside of the Box;** R. Kenneth Marcus¹; ¹Clemson University
- 4:10 (453) **Analysis of Single Muscle Cells by ICP-MS-MS to Evaluate Changes in the Ion Transport Rate of Potassium.;** Julio Landero¹, Cory Stiner¹, Tatiana Radzyukevich², Judith Heiny²; ¹University of Cincinnati, Chemistry Department; ²University of Cincinnati, Dept. of Molecular and Cellular Physiology
- 4:30 (454) **Improving Sensor Selectivity with Spectroelectrochemistry;** William Heineman¹, Samuel Bryan²; ¹University of Cincinnati; ²Pacific Northwest National Laboratory
- 4:50 (455) **Development of Cell Lysis Methods for Metalloproteomics Analysis, a Study of Histoplasma Capsulatum;** Anna Donnell¹, Stephanie Lewis¹, Julio Landero¹, George Deepe², Anne Vonderheide¹; ¹University of Cincinnati, Department of Chemistry; ²University of Cincinnati, Immunology and Infectious Diseases
- 5:10 (456) **Dr. Joe Caruso: The Scientist, Graduate Advisor, Promotor, Mentor, Career Coach and yes, Even Matchmaker;** Peter Brown¹; ¹LGC Standards

Tuesday Afternoon, Greenway G

LIPIDS AND LIPODOMICS IN HEALTH AND DISEASE

Organizer and Presider: Eric Potma

- 3:50 (457) **Tracking Lipid Dynamics following Cryolipolysis with Coherent Raman Imaging in Skin and Nerves;** Conor Evans¹, Tracy Wang¹, Yookyung Jung¹, Joshua Tam¹, Emilia Javorsky¹, Lilith Garibyan¹, Ray Jalian¹, Rox Anderson¹; ¹Wellman Center for Photomedicine, Massachusetts General Hospital
- 4:10 (458) **Using Spectral CARS to Interrogate White Matter in Health and Disease;** Peter K. Stys¹, Craig Brideau¹, Geert J. Schenk², Roel Klaver², Jeroen J.G. Geurts², Kelvin W. Poon¹; ¹University of Calgary; ²VU University Medical Centre
- 4:30 (459) **The Application of Lipid-Based Stimulated Raman Scattering Microscopy in Brain Tumor Surgery;** Daniel Orringer¹; ¹University of Michigan

TECHNICAL PROGRAM – TUESDAY

Orals 3:50 – 5:30 pm

- 4:50 (460) **Time-dependent Depth Profiles of Skin Hydration Following Treatment with Topical Products;** Fran Adar¹, Catalina David¹, Vincent Larat¹; ¹HORIBA Scientific
- 5:10 (461) **Confocal Raman Microscopy of Lectin Protein Binding to Mannose-Functionalized Supported Lipid Bilayers;** David A. Bryce¹, Jay P. Kitt¹, Joel M. Harris¹; ¹University of Utah

Tuesday Afternoon, Nicollet D2/D3 CHEMOMETRICS IN CHEMICAL AND BIOLOGICAL IMAGING: FROM MACRO- TO NANO- Organizer and Presider: Cyril Ruckebusch

- 3:50 (462) **Multiset Analysis for Hyperspectral Images;** Anna de Juan¹; ¹Universitat de Barcelona
- 4:10 (463) **Combining MALDI Spectrometric Imaging and Raman Spectroscopic Imaging: A Fruitful Marriage?!** Thomas Bocklit^{1,2}, Katharina Bräutigam^{1,2}, Günther Ernst^{2,3}, Ferdinand von Eggeling^{1,3}, Orlando Guntinas-Lichius³, Jürgen Popp^{1,2}; ¹Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Jena, Germany; ²Leibniz Institute of Photonic Technology, Jena, Germany; ³ENT Department, Jena University Hospital, Jena, Germany
- 4:30 (464) **Multivariate Analysis Strategies for Macroscopic Fluorescence Hyperspectral Imaging;** Howland Jones¹, David Haaland², Gina Stuessy³, Scott McElroy³, Gabor Kemeny³; ¹HyperImage Solutions; ²Spectral Resolutions; ³Middleton Spectral Vision
- 4:50 (465) **Analysis of single-Molecule Fluorescence 2D+t Live-Cell Images;** Cyril Ruckebusch¹, Siewert Hugelier¹, Michel Sliwa¹, Peter Dedecker³, Paul Eilers², Johan De Rooi²; ¹Université de Lille; ²Erasmus MC Rotterdam; ³KU Leuven
- 5:10 (466) **Quantum Cascade Laser Mid-Infrared Imaging and Random Forest Classification of Prostate Cancer;** Tomasz Wrobel¹, Virgilia Macias², Andre Kadjacsy-Balla², Rohit Bhargava³; ¹Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, IL; ²Department of Pathology, University of Illinois at Chicago, IL; ³Department of Bioengineering, University of Illinois at Urbana-Champaign, Urbana, IL

Tuesday Afternoon, Lakeshore B QUANTUM CASCADE LASERS - I Organizer and Presider: Bernhard Lendl

- 3:50 (467) **Noninvasive Glucose Monitoring with Mid-Infrared Quantum Cascade Laser Spectroscopy;** Alexandra Werth¹, Sabbir Liakat¹, Yezhezi Zhang¹, Anqi Dong¹; ¹Princeton University
- 4:10 (468) **MYCOSPEC: Harnessing Quantum Cascade Laser Spectroscopy for On-site Mycotoxin Analysis;** Boris Mizaikoff¹, Markus Sieger¹, Tuba Öner¹, Gregor Kos², Rudolf Krška³, Matthias Godejohann⁴; ¹Ulm University; ²McGill University; ³University of Natural Resources and Applied Life Sciences; ⁴MG Optical Solutions GmbH
- 4:30 (469) **QCL Based Liquid Sensing 2.0: A Single Chip Solution;** Benedikt Schwarz¹, Daniela Ristanic², Peter Reininger¹, Werner Schrenk², Hermann Detz^{2,3}, Tobias Zederbauer², Aaron Maxwell Andrews¹, Donald Craig MacFarland², Gottfried Strasser^{1,2}; ¹Institute for Solid State Electronics, TU Wien; ²Center for Micro- and Nanostructures, TU Wien; ³Austrian Academy of Sciences
- 4:50 (470) **Rapid and Precise Measurements of Chemical Mixtures and Isotope Ratios Using Swept External Cavity Quantum Cascade Lasers;** Mark Phillips¹,

Matthew Taubman¹, Brian Brumfield¹; ¹Pacific Northwest National Laboratory

- 5:10 (471) **Detection of Explosives with Differential Excitation Spectroscopy;** Jason Cox¹, Boyd Hunter¹, Michael Miller², Paul Harrison¹; ¹Kestrel Corporation; ²Southwest Research Institute

Tuesday Afternoon, Nicollet B/C ITP - YOUNGS SCIENTISTS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Susanne Wiedmer and Vaclav Kasicka

- 3:50 (472) **Microchip Isotachophoresis in the Analysis of the Main Pharmaceutical Components;** Jasna Hradski¹, Marina Rudašová¹, Róbert Bodor¹, Marián Masár¹; ¹Department of Analytical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Bratislava, Slovak Republic
- 4:00 (473) **Nanoparticle capillary Electrokinetic Chromatography – Evaluation of the Retention Energetics of Functionalized Carbon Nanotubes and Their Applications to the Analysis of a Wide Range of Neutral and Charged Species;** Sarah Alharthi¹, Ziad El Rassi¹; ¹Department of Chemistry, Oklahoma State University
- 4:10 (474) **Proteomic Approaches to Investigate the Salivary Glands and Ovary of the Tick Ixodes ricinus and the Relationship with the Symbiont Midichloria mitochondrii;** Monica Di Venere¹, Maddalena Cagnone¹, Marco Fumagalli², Anna Maria Floriano², Alessandra Cafiso³, Valentina Serra³, Stuart Armstrong⁴, Benjamin Makepeace⁴, Davide Sassera²; ¹Department of Molecular Medicine, University of Pavia, Italy; ²Department of Biology and Biotechnology, University of Pavia, Italy; ³Department of Veterinary Sciences, University of Milano, Italy; ⁴Institute of Infection and Global Health, University of Liverpool, UK
- 4:20 (475) **The Optimization of Pressure Cycling Technology (PCT) for Differential Extraction of Sexual Assault Casework;** Vanessa Martinez¹, Deepthi Nori¹, Bruce McCord¹; ¹Florida International University
- 4:30 (476) **In vivo Monitoring of Branched Chain Amino Acid Dynamics Using Online Microdialysis-Capillary Electrophoresis;** Megan Weisenberger¹, Michael T. Bowser¹; ¹University of Minnesota, Chemistry Dept.
- 4:40 (477) **Combination of Insulating and Conducting Posts to Create a Hybrid Dielectrophoretic Device;** Mario A. Saucedo-Espinosa¹, Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology
- 4:50 (478) **Sequence Based Separation of DNA Using Gel Electrophoresis;** Wyatt Stevens¹, Jia Zhao¹, Linda McGown¹; ¹Rensselaer Polytechnic Institute
- 5:00 (479) **Complexation of Buffer Constituents with Charged Complexation Agents;** Milan Boublík¹, Martina Riesová¹, Pavel Dubský¹; ¹Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University in Prague, Prague, Czech Republic
- 5:10 (480) **Determination of Stability Constant of Potassium-dibenzo-18-crown-6 Complex in Hydro-Organic Solvents by ACE: Evaluation of the Effect of Model Function Simplification;** Renata Konasova^{1,2}, Jana Jaklova Dytřtova^{2,3}, Vaclav Kasicka²; ¹Department of Analytical Chemistry, Faculty of Science, Charles University in Prague, Prague 2, Czech Republic; ²Institute of Organic Chemistry and Biochemistry, The Czech Academy of Science, Prague 6, Czech Republic;

TECHNICAL PROGRAM – TUESDAY

Orals 3:50 – 5:30 pm

- 5:20 (481) **Tracking Biochemical Changes Underlying Ultra-Weak Photon Emission Using Capillary Electrophoresis-Mass Spectrometry Based Metabolomics**; Rosilene Cristina Rossetto Burgos¹, Rami Ramautar¹, Eduard P. A. van Wijk², Thomas Hankemeier¹, Jan van der Greef^{1,2,3}; ¹Division of Analytical Biosciences, Leiden Academic Centre for Drug Research, Leiden University, Leiden, The Netherlands; ²Sino-Dutch Centre for Preventive and Personalized Medicine/Centre for Photonics of Living Systems, Leiden University, Leiden, The Netherlands.; ³TNO Innovation for Life, Zeist, The Netherlands.

Tuesday Afternoon, Greenway J

CLINICAL AND FORENSIC APPLICATIONS OF AMBIENT IONIZATION MASS SPECTROMETRY

Organizer and Presider: Nicholas Manicke

- 3:50 (482) **Development of a Paper Spray Cartridge with Integrated SPE to Improve Sensitivity for Drug Detection**; Chengsen Zhang¹, Nicholas Manicke¹; ¹Indiana University-Purdue University Indianapolis
- 4:10 (483) **Rapid Fingerprinting of Falsified Anti-malarial Medicines Using Ambient Plasma Ionization and Portable Mass Spectrometry Instrumentation**; Facundo M. Fernandez¹, Matthew C. Bernier¹, Joel D. Keeler¹, Stephen C. Zambrozky¹, Paul N. Newton²; ¹School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; ²Lao-Oxford-Mahosot Hospital Wellcome Trust Research Unit (LOMWRU), Laos and Centre for Tropical Medicine & Global Health, University of Oxford, UK
- 4:30 (484) **Tunable Ionization and Fragmentation with Plasma-based Ambient Ionization Sources to Expand Their Utility in Forensic Applications**; Jacob Shelley¹, Sunil Badal¹, Andrew Schwartz², Garrett MacLean¹, Courtney Walton¹, Kelsey Williams¹, Gary Hieftje²; ¹Department of Chemistry and Biochemistry, Kent State University, Kent, OH; ²Department of Chemistry, Indiana University, Bloomington, IN
- 4:50 (485) **IR-MALDESI: An Innovative Approach to Molecular Imaging**; Milad Nazari¹, Mark Bokhart¹, David Muddiman¹; ¹W. M. Keck FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC
- 5:10 (486) **A New Matrix-Assisted Ionization (MAI) Atmospheric Pressure Sampling Method Potentially Applicable for Clinical and Forensic Samples**; I-Chung Lu¹, Milan Pophristic², Charles N. McEwen^{2,3}, Sarah Trimpin^{1,2}; ¹Wayne State University, Detroit, MI; ²MSTM, Newark, DE; ³University of the Sciences, Philadelphia, PA

Tuesday Afternoon, Lakeshore C SUSTAINABLE NANOTECHNOLOGY

Organizer and Presider: Robert Hamers

- 3:50 (487) **Methods for Valid Sizing and Quantification of Engineered Nanoparticles in environmentally-Relevant Water Matrices**; Brian Mader¹, Mark Ellefson¹, Charlie Chan², Christine Loza¹, Susan Wolf¹; ¹3M Environmental Laboratory; ²3M Corporate Research Analytical Laboratory
- 4:10 (488) **Insights into Nanoparticle Interaction with Cell Surfaces from Model Systems**; Joel Pedersen¹, Eric Melby¹, Thomas Kuech¹, Arielle Mensch¹, Julianne Troiano², Arianne Vartanian³, Catherine Murphy³, Christy Haynes⁴, Franz Geiger², Robert Hamers¹; ¹University of

- Wisconsin - Madison; ²Northwestern University; ³University of Illinois Urbana Champaign; ⁴University of Minnesota
- 4:30 (489) **Using Cross-Species Comparisons to Create Sustainable Nanomaterials**; Rebecca Klaper¹; ¹University of Wisconsin-Milwaukee
- 4:50 (490) **Microbial Assays for Fast, Broad Screening of Engineered Nanoparticle Toxicity to Bacteria**; Tian (Autumn) Qiu¹, Joseph Buchman¹, Thu Nguyen², Hilena Frew², Ariane Vartanian³, Lisa Jacob³, Xi Zhang³, Catherine Murphy³, Z. Vivian Feng², Christy Haynes¹; ¹University of Minnesota; ²Augsburg College; ³University of Illinois at Urbana-Champaign
- 5:10 (491) **Investigation of Bacterial Cell Wall Components Responsible for Interactions with Nanoparticles Using B. subtilis Mutants**; Vivian Feng¹; ¹Augsburg College

Tuesday Afternoon, Greenway D

INDUSTRIAL APPLICATIONS OF VIBRATIONAL SPECTROSCOPY

Organizers and Presiders: Shawn (Xiaoyun) Chen and Mark Rickard

- 3:50 (492) **Product Development Challenges in Specialty Chemicals**; Steven Scheifers¹; ¹Stepan
- 4:10 (493) **Monitor Polymerization Reactions *in situ* with Raman Spectroscopy**; Xiaoyun Chen¹; ¹The Dow Chemical Company
- 4:30 (494) **Quantitative Near Infrared Chemical Imaging of Solid Mixtures Enables Unit Process Mass Balance for Flour Milling**; Mark Boatwright¹, David Wetzel²; ¹Department of Biochemistry & Molecular Biophysics, Kansas State University, Manhattan, KS; ²Microbeam Molecular Spectroscopy Laboratory, Kansas State University, Manhattan, KS
- 4:50 (495) **Vibrational Spectroscopy for Silicone Chemistry**; Xianghuai Wang¹, Elmer Lipp¹; ¹The Dow Chemical Company
- 5:10 (496) **Best Practices for Maintaining Calibration Models Across Multiple Instruments**; Michael Roberto¹, Randy Pell¹, Scott Ramos¹; ¹Infometrix, Inc.

Tuesday Afternoon, Greenway B/C

LOW FREQUENCY RAMAN, A PHARMACEUTICAL APPROACH

Organizer and Presider: James Carriere

- 3:50 (497) **Low Frequency Raman: Controlling the Crystallization Process**; John Wasyluk¹, Ming Huang¹, Robert Wethman¹; ¹Bristol-Myers Squibb Co.
- 4:10 (498) **Quantitative Solid-State Analysis of Amorphous and Crystalline Forms of Sulfamerazine Using THz Raman Spectrometry**; Joanna Lothian¹, Alison Nordon¹, Pol Macfhionnghaile², Keddon Powell², Paul Dallin³, John Andrews³, James Carriere⁴; ¹EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation and WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow; ²EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation University of Strathclyde, Glasgow; ³Clair Scientific Ltd, Moulton Park Industrial Estate, Northampton UK.; ⁴Ondax Incorporated, Duarte Road, Monrovia, CA
- 4:30 (499) **Applying Vibrational Spectroscopies for Quantitative Studies of Drug Recrystallization in Pharmaceutical Films**; Yi Li¹, James K. Drennen, III^{1,2}, Carl A. Anderson^{1,2}; ¹Graduate School of Pharmaceutical Sciences, Duquesne University; ²Duquesne Center of Pharmaceutical Technology, Duquesne University

TECHNICAL PROGRAM – TUESDAY

Orals 3:50 – 5:30 pm

- 4:50 (500) **Real-time Monitoring of Crystalline Compounds Using *in situ* Low Frequency Raman Probe**; Motoki Inoue¹, Hiroshi Hisada¹, Tatsuo Koide², Toshiro Fukami¹; ¹Meiji Pharmaceutical University; ²National Institute of Health Sciences
- 5:10 (501) **Raman Spectroscopy of Low Energy Phonons as a Probe of Solid State Structure of Transition Metal Dichalcogenide 2D Crystals**; David Tuschel¹; ¹HORIBA Scientific

Tuesday Afternoon, Nicollet D1

NANO-IR/NANO-RAMAN- III

Organizers: Curtis Marcott and Andrew Whitley;

Presider: Andrew Whitley

- 3:50 (502) **Tip-enhanced Raman Imaging of 2D Materials**; Dmitri Voronine¹; ¹Texas A&M University
- 4:10 (503) **Nanoscale Studies Link Amyloid Maturity with Polyglutamine Diseases Onset**; Francesco Simone Ruggeri¹, Giovanni Dietler¹, Tuomas Knowles¹; ¹University of Cambridge
- 4:30 (504) **TERS Resolution Potential - “Chemical” and Electro-Magnetic Contributions**; Volker Deckert^{1,2}, Daniel Kinzel², Stephan Kupfer², Stefanie Gräfe²; ¹IPHT; ²University of Jena
- 4:50 (505) **Chemistry at the Nanoscale: Recent Advances in Nanoscale Infrared Spectroscopy**; Miriam Unger¹, Eoghan Dillon¹, Kevin Kjoller¹, Anirban Roy¹, Qichi Hu¹, Curtis Marcott²; ¹Anasys Instruments; ²Light Light Solutions
- 5:10 (506) **Round Table Discussion**; Curtis Marcott¹, Andrew Whitley²; ¹Light Light Solutions; ²Horiba Scientific

Tuesday Afternoon, Lakeshore A

RAMAN SPECTROSCOPY FOR SECURITY AND FORENSICS PURPOSES

Organizer and Presider: Igor Lednev

- 3:50 (507) **Vibrational Spectroscopic Biosensing**; Juergen Popp^{1,2}; ¹Leibniz Institute of Photonic Technology, Jena, Germany; ²Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Jena, Germany

- 4:10 (508) **A New Capability for Explosives, Narcotics and Hazardous Materials Detection within Sealed Containers Using Spatially Offset Raman Spectroscopy (SORS)**; Robert Stokes¹; ¹Cobalt Light Systems
- 4:30 (509) **Developing Deep UV Raman Standoff Spectrometers for Trace Explosives**; Sanford Asher¹, Sergei Bykov¹, Katie Gares¹, Kyle Hufziger¹; ¹University of Pittsburgh
- 4:50 (510) **Automatic Body Fluid Differentiation by Raman Spectroscopy and Chemometrics**; Claire Muro¹, Kyle Doty¹, Luciana Fernandes¹, Igor Lednev¹; ¹University at Albany
- 5:10 (511) **SERS Sensing of Protein Targets Enabled by Polymeric Capture Agents**; Victoria Szlag¹, Matthew Styles¹, Lindsey Madison², Antonio Campos¹, Bharat Wagh¹, Dustin Sprouse¹, George Shatz², Theresa Reineke¹, Christy Haynes¹; ¹University of Minnesota; ²Northwestern University

Tuesday Afternoon, Greenway E

FRONTIERS OF FAR-AND DEEP- ULTRAVIOLET SPECTROSCOPY II

Organizers: Yukihiro Ozaki, Satoshi Kawata and Yuika Saito;

Presider: Yukihiro Ozaki

- 3:50 (512) **Generation of Coherent VUV Pulses and its Application to Laser Cooling of Hydrogen Atoms**; Takamasa Momose¹; ¹University of British Columbia
- 4:10 (513) **Two-dimensional Deep-UV Studies of (Bio)Chemical Dynamics**; Majed Chergui¹; ¹Ecole Polytechnique Fédérale de Lausanne
- 4:30 (514) **Attenuated Total Reflection Far-and Deep-Ultraviolet Spectroscopy for condensed Phase**; Yukihiro Ozaki¹; ¹Kwansei Gakuin University
- 4:50 (515) **Study of Electronic States of Molecules in the Condensed Phase by Using Attenuated Total Reflectance Far-UV Spectroscopy**; Yusuke Morisawa¹; ¹Kindai University
- 5:10 (516) **Deep-UV Surface Plasmon for Bio-imaging**; Yoshimasa Kawata¹, Masakazu Kikawada¹, Atsushi Ono¹, Wataru Ina¹; ¹Shizuoka University, Institute of Electronics

TECHNICAL PROGRAM – WEDNESDAY

Plenary Lectures, *Nicollet B/C*

Presider: **Matthieu Baudelet**



8:00 am – ANACHEM Award
(517) **Metallomembranes: Exploring the Interactions of Transition Metal Ions with Lipid Bilayers;** Paul Cremer¹; ¹Penn State University



8:30 am – Applied Spectroscopy William F. Meggers Award
(518) **Probing Reactions Using Time-Resolved Infrared Spectroscopy in Solution and in the Solid State Using Quantum Cascade Lasers;** Mike George¹, James Calladine¹, Raphael Horvath¹, Andrew Davies¹, Alisdair Wriglesworth¹, Xue-zhong Sun¹¹; ¹University of Nottingham

Orals 9:15 – 10:55 am

Wednesday Morning, *Greenway J* BIOELECTROKINETICS: BIOMOLECULES AND PARTICLES

Organizers: Roberto Gallo-Villanueva and Mark Hayes;
Presider: Mark Hayes

- 9:15 (519) **Bioelectrokinetics for Advanced Manufacturing;** Rodrigo Martinez-Duarte¹; ¹Clemson University
- 9:35 (520) **Contactless Dielectrophoresis for the Separation of Cancer Cells at Different Stages of Progression;** Rafael V Davalos¹, Temple Douglas¹, Jaka Cemazar¹, Eva Schmelz¹; ¹Virginia Tech
- 9:55 (521) **Single-microbial Monitoring by AC Electrokinetics for Tracking the Emergence of Subpopulations;** Nathan Swami¹, Yi-Hsuan Su¹, Ali Rohani¹, Cirle Warren¹; ¹University of Virginia
- 10:15 (522) **Microfluidic Multistage Integration of immunoassay for Cancer Diagnosis;** Mei He^{1,2}, Zheng Zhao¹, Kimberly Plevniak¹; ¹Kansas State University; ²Terry C. Johnson Cancer Research Center
- 10:35 (523) **Mathematical Modelling of the Electrokinetic Behavior of PEGylated Proteins Inside an Insulator-Based Dielectrophoretic Microdevice;** Roberto C. Gallo-Villanueva¹, Marco A. Mata-Gomez¹, Victor H. Perez-Gonzalez¹, Jose Gonzalez-Valdez¹, Marco Rito-Palomares¹, Sergio o. Martinez-Chapa¹; ¹Tecnologico de Monterrey

Wednesday Morning, *Greenway A* GLOW DISCHARGE SPECTROSCOPY AND RELATED TECHNIQUES

Organizer and Presider: Jorge Pisonero

- 9:15 (524) **Guiding the Development of Efficient and Durable Electrodes for Electrochemical Energy Conversion Applications through Advanced Ion Beam Analysis;** Jose Miguel Vadillo³, John Druce¹, Tatsumi Ishihara¹, John Kilner^{1,2}, Helena Tellez¹; ¹International Institute for Carbon-Neutral Energy Research (I2CNER), Kyushu University; ²Department of Materials, Imperial College London; ³University of Malaga
- 9:35 (525) **2D Mapping in Glow Discharge Mass Spectrometry;** Piotr Konarski¹, Maciej Misnik^{1,2}, Aleksander Zawada^{1,3}; ¹Institute of Tele and Radio Technology; ²Gdansk University of Technology; ³Military University of Technology (MUT) Warsaw
- 9:55 (526) **Investigation of Excitation and Ionisation Temperatures during Plasma Start-Up in GD-OES;** Arne Bengtson¹; ¹Swerea KIMAB AB
- 10:15 (527) **Elemental Analysis by Ambient Ionization Mass Spectrometry;** Paul Farnsworth¹, Wade Ellis¹; ¹Brigham Young University
- 10:35 (528) **Cross-Correlation Approach for Automated, High-Throughput Analyte-Ion Recognition, Categorization and Background Removal for Direct**

Mass-Spectral Data Analysis; Yi You¹, Sunil Badal¹, Jacob Shelley¹; ¹Department of Chemistry and Biochemistry, Kent State University

Wednesday Morning, *Greenway H/I* ANACHEM AWARD SYMPOSIUM HONORING PAUL CREMER

Organizer and Presider: Jared Anderson

- 9:15 (529) **Mobile, Oriented Proteinaceous Supported Bilayers Made Directly from Cell Plasma Membranes for Bioanalytical Assays;** Susan Daniel¹; ¹Cornell University
- 9:35 (530) **Towards Sensitive, Selective Point-Of-Care Plasmonic Diagnostic Devices;** Laura Sagale¹, Debrina Jana¹, Jie He¹, Ian Bruzas¹, Sarah Unser¹; ¹University of Cincinnati
- 9:55 (531) **Lipid-PEG-Coated Polymeric Nanoparticles for Systemic RNAi Delivery to Tumors;** Jinjun Shi¹; ¹Harvard Medical School, Brigham and Women
- 10:15 (532) **Mechano-Analytical Chemistry;** Hanbin Mao¹; ¹Kent State University
- 10:35 (533) **Phosphatidylserine-Containing Supported Lipid Bilayers as Copper-Binding Protein Filters;** Christopher Monson¹, Christopher Reynolds¹; ¹Southern Utah University

Wednesday Morning, *Greenway G* CHEMOMETRIC OPPORTUNITIES IN FORENSIC CHEMISTRY

Organizer and Presider: Stephen Morgan

- 9:15 (534) **Multivariate Analysis of Raman Spectral Data for the Identification of Body Fluid Traces;** Igor Lednev¹, Lenka Halamkova¹, Kyle Doty¹, Claire Muro¹; ¹University at Albany, SUNY
- 9:35 (535) **Analysis and Characterization of Smokeless Powders Using Multiplexed Collision-Induced Dissociation Mass Spectrometry and Chemometric Procedures;** Ruth Smith¹, Kristen L. Reese¹, A. Daniel Jones¹; ¹Michigan State University
- 9:55 (536) **Chemometric Tools for the Interpretation of Fire Debris Data;** James Harynuk¹, Lawrence Adutwum¹, Robin Abel¹; ¹University of Alberta
- 10:15 (537) **Fisher-Ratio Analysis of GC×GC-TOFMS Data for Relevant Analyte Discovery;** Robert Synovec¹; ¹University of Washington
- 10:35 (538) **To Bayes, or Not to Bayes?;** Stephen L. Morgan¹; ¹University of South Carolina

Wednesday Morning, *Lakeshore B* QUANTUM CASCADE LASERS - II

Organizer and Presider: Bernhard Lendl

- 9:15 (539) **Monolithic QCL Solutions Enabling Handheld IR Spectrometers;** Christian Pfluegl¹; ¹Pendar Technologies, LLC

TECHNICAL PROGRAM – WEDNESDAY

Orals 9:15 – 10:55 AM

- 9:35 (540) **Contactless Real-Time Identification of Chemical Substances Using External Cavity QCLs**; Marko Haertelt¹, Jan-Philip Jarvis¹, Lorenz Butschek¹, Andre Dreyhaupt², Jan Grahmann², Stefan Hugger¹, Frank Fuchs^{1,3}, Marcel Rattunde¹, Ralf Ostendorf¹, Joachim Wagner¹; ¹Fraunhofer Institute for Applied Solid State Physics, Freiburg, Germany; ²Fraunhofer Institute for Photonic Microsystems, Dresden, Germany
- 9:55 (541) **Matchbox QCL Based Analyzer for Multi-Gas Trace Detection**; Mathieu Carras¹, Mickael Brun¹, Fahem Boulila Boulila¹, Jean Guillaume Coutard¹, Gregory Maisons¹; ¹mirSense
- 10:15 (542) **Advances in LaserDirect IR Imaging**; Charles Hoke¹, Yuri Beregovski¹, Andrew Ghetler¹, Yang Han¹, Christopher Moon¹, Richard Tella¹, Zhen Zhang¹; ¹Agilent Technologies, Inc.
- 10:35 (543) **Recent Advances in Resonance Enhanced AFM-IR Spectroscopy and Imaging Using Quantum Cascade Lasers (QCL)**; Anirban Roy¹, Eoghan Dillon¹, Qichi Hu¹, Kevin Kjoller¹, Roshan Shetty¹, Craig Prater¹; ¹Anasys Instruments

Wednesday Morning, Nicollet D2/D3

ITP - METABOLOMICS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Daniel Armstrong and Carlos Garcia

- 9:15 (544) **Are We Drawing the Right Conclusions from Metabolomics Data?**; Coral Barbas¹, Danuta Dudzick¹, Joanna Godzien¹, Emily Hooper¹, Alma Villaseñor¹; ¹Universidad San Pablo CEU
- 9:55 (545) **Sheathless Capillary Electrophoresis-Mass Spectrometry for Anionic Metabolic Profiling**; Rawi Ramautar¹; ¹Leiden University
- 10:15 (546) **Metabolomic Profiling in Prostate Cancer by Hyphenated Separation Techniques and Mass Spectrometry**; Michał Markuszewski¹, Marta Kordalewska¹, Renata Bujak¹, Tomáš Kovalczuk², Agnieszka Ulanowska³; ¹Medical University of Gdansk; ²LECO Instrumente Plezen; ³LECO Poland
- 10:35 (547) **Electroextraction Strategies for Enrichment of Low-abundant Metabolites**; Peter Lindenburg^{1,2}, Amar Oedit¹, Thomas Hankemeier^{1,2}; ¹Division of Analytical Biosciences, Leiden Academic Centre for Drug Research, Leiden University, the Netherlands; ²Netherlands Metabolomics Centre, Leiden, the Netherlands

Wednesday Morning, Nicollet B/C

ITP - DNA SEQUENCING AND ELECTROPHORESIS

Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
Presiders: Nancy Stellwagen and Paolo Iadorola

- 9:15 (548) **Polymer-Based Nanosensors Using Nanoscale Electrophoresis of Mononucleotides for Single-Molecule Sequencing**; Steven Soper¹; ¹The University of Kansas
- 9:55 (549) **Unfolding of Nanochannel Confined DNA for Genomic Mapping**; Kevin Dorfman¹, Jeffery Reifenger², Han Cao²; ¹University of Minnesota; ²BioNano Genomics, Inc.
- 10:15 (550) **Monitoring Cellular Release of Chemical Messengers Using *in vitro* Microdialysis Coupled with High-Speed Capillary Electrophoresis**; Michael Bowser¹, Amy Stading^{1,2}, Rachel Harstad¹; ¹University of Minnesota
- 10:35 (551) **μ LAS, a Technological Breakthrough to Perform Quantification and Size Analysis of Plasmatic Circulating DNA Without Prior Purification**; Audrey Boutonnet¹, Comtet-Louis Andriamanampisoa¹, Aurélien

Bancaud², Jacques Favre¹, Frédéric Ginot¹, Arnaud Morin¹, Vincent Picot¹, Laure Saias¹; ¹Picometrics Technologies; ²CNRS-LAAS

Wednesday Morning, Greenway B/C

HIGH-SENSITIVITY MASS SPECTROMETRY FOR BASIC AND TRANSLATIONAL RESEARCH

Organizer and Presider: Peter Nemes

- 9:15 (552) **Exploring the Proteome of Colorectal Cancer by Mass Spectrometry**; Amanda Hummon¹; ¹University of Notre Dame
- 9:35 (553) **Mass Spectrometry-based Analysis in Genetic Disorders Related to Cholesterol Homeostasis**; Stephanie M. Colonna^{1,2}; ¹University of Illinois at Chicago; ²National Institutes of Health
- 9:55 (554) **Cell-by-cell Analysis of Protein Expression in the Frog (*Xenopus laevis*) Embryo by CE- μ ESI-HRMS**; Camille Lombard-Banek¹, Sally A. Moody², Peter Nemes¹; ¹The George Washington University Chemistry department; ²The George Washington University, Department of Anatomy & Regenerative Biology
- 10:15 (555) **Sensitivity vs. Molecular Coverage in Non-Targeted Analysis of Complex Samples**; Akos Vertes¹; ¹George Washington University
- 10:35 (556) **Mass Spectrometry Profiling of Live 3D Artificial Tumors Using the Single-Probe Device**; Wei Rao¹, Ning Pan¹, Xiang Tian¹, Zhibo Yang¹; ¹University of Oklahoma

Wednesday Morning, Lakeshore A

BIOTEMPLATE-BASED NANOMATERIALS FOR ENERGY APPLICATIONS

Organizer: Wei Zhao; Presider: Wei-Chuan Shih

- 9:15 (557) **New Photonic Materials Templated with Cellulose Nanocrystals**; Mark MacLachlan¹; ¹University of British Columbia
- 9:55 (558) **Stimuli Responsive and Reconfigurable Noble Metal Nanoparticle Biointerfaces**; Marc Knecht¹; ¹University of Miami
- 10:15 (559) **Biotemplated PZT Nanowires and 3D Printing Functional Devices**; Michael McAlpine¹; ¹University of Minnesota
- 10:35 (560) **Vertically Aligned Piezoelectric Diphenylalanine Peptide Microrods for Energy Harvesting**; Rusen Yang¹, Vu Nguyen¹, Ren Zhu¹, Kory Jenkins¹; ¹University of Minnesota

Wednesday Morning, Greenway D

ONLINE ANALYSIS OF INDUSTRIAL PROCESSES AND REACTIONS

Organizers: Anna Sandlin and JD Tate; Presider: Eric Schmidt

- 9:15 (561) **Online Analysis Using Vacuum Ultraviolet Absorption Spectroscopy**; Dale Harrison¹, Phillip Walsh¹, Jonathan Smuts¹, James Diekmann¹; ¹VUV Analytics
- 9:35 (562) **Application of On-line Process Mass Spectrometry in R&D**; Eric Schmidt¹, Derrick Flick¹, Liwei Li¹, Yujun Liu¹; ¹The Dow Chemical Company
- 9:55 (563) **Rugged in-process FTIR Using an Enhanced Sagnac interferometer**; Dan Wood¹; ¹Keit Spectrometers
- 10:15 (564) **Hard, Soft, and Circumstantial Correlations: Thinking Chemically about Motor Fuel Property Predictions by Multivariate Spectrometry**; Marcus Trygstad¹, Bradford Behr², Jeremy Linoski²; ¹Yokogawa Corporation of America; ²Tornado Spectral Systems
- 10:35 (565) **Analysis of Sulfur and Oxygenate Species in Hydrocarbon Process Streams Using a novel Ballistic GC-HPMS**; Graham Shelver¹; ¹908 Devices Inc

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

Wednesday Morning, Nicollet D1
STANDOFF RAMAN SPECTROSCOPY:
INSTRUMENTATION AND APPLICATIONS
 Organizer and Presider: Nathanie Gomer

- 9:15 (566) **Advancements in Raman Spectroscopy for Military Applications & Forensic Attribution;** Augustus Fountain¹; ¹Edgewood Chemical Biological Center
- 9:35 (567) **Scanning Standoff Raman Instruments for Large Area Hazardous Chemical Detection;** Shiv Sharma¹, Anupam Misra¹, Tayro Acosta-Maeda¹, John Porter¹; ¹University of Hawaii, HIGP/SOEST
- 9:55 (568) **Standoff Hyperspectral Raman Sensors for the Detection of Explosives;** Nathaniel Gomer¹, Charles Gardner¹, Matthew Nelson¹; ¹ChemImage Sensor Systems
- 10:15 (569) **Advances in Deep-Ultraviolet (DUV) Raman Spectroscopy for the Standoff Detection of Threat Materials;** Luisa T.M. Profeta¹, Adam J. Hopkins¹, Kenneth R. Pohl¹, Kenneth R. Pohl¹; ¹Alakai Defense Systems
- 10:35 (570) **Raman Spectroscopy of Vapor and Aerosol Chemical Warfare Agents;** Erik Emmons¹, Francis D'Amico¹, Gary Kilper², Steven Christesen¹, Aime Goad¹, David Sickenberger¹; ¹U.S. Army Edgewood Chemical Biological Center; ²Excet, Inc.

Wednesday Morning, Greenway E
THE POWER OF MANY: SUPPORTING DIVERSITY IN ANALYTICAL CHEMISTRY
 Organizers and Presiders: Anna Donnell and Ingeborg Ipping Petterson

- 9:15 (571) **Advancing Diversity in STEM Fields: Strategies and Reflections;** Colin Ingram¹; ¹Princeton Instruments
- 9:35 (572) **Gender Disparity in Scholarly Publishing;** Kristin Selinder MacDonald¹; ¹University of British Columbia/Applied Spectroscopy
- 9:55 (573) **Preparing Students with Disabilities for Graduate School: Thoughts and Experiences;** Karl Booksh¹, Sharon Rozovsky¹, Joseph Smith¹; ¹University of Delaware
- 10:15 (574) **Diversity and Inclusion in Academia;** Atcha Totachawattana¹; ¹Boston University
- 10:35 (575) **Navigating LGBT Disparities in an Industrial Workplace;** Blake Bailes¹; ¹3M

Wednesday Morning, Lakeshore C
SURFACE ANALYSIS OF BIOMATERIALS AND BIOLOGICAL MATERIALS
 Organizer and Presider: Anna Belu

- 9:15 (576) **What it is and Where it is– Super-Resolution Mass Spectrometry Imaging of Biomaterials with the New 3D nanoSIMS;** Ian Gilmore¹; ¹National Physical Laboratory
- 9:55 (577) **Single Cell Raman Spectroscopy for Understanding Freezing Damage;** Allison Hubel¹, Guanglin Yu¹; ¹University of Minnesota
- 10:15 (578) **Characterization of Surfaces and Interfaces in the Medical Device Industry;** Bill Theilacker¹, Anna Belu¹, Tony Anderson¹; ¹Medtronic, Plc
- 10:35 (579) **In situ Chemical Imaging of Biointerfaces Using Microfluidics;** Xiao-Ying Yu¹; ¹Pacific Northwest National Laboratory

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

All Wednesday posters should be put up between 9:00 – 10:00 am and removed by 3:50 pm

Chemometrics Posters

Poster Board #1

(580) **Penalized Eigendecompositions: Motivations from Domain Adaptation for Calibration Transfer and Maintenance;** Erik Andries¹; ¹Central New Mexico Community College; ²Center for Advanced Research Computing, University of New Mexico

Poster Board #2

(581) **Automated Chemical Imaging Analysis for the Identification of Drugs at Correctional Facilities;** Robert Schweitzer¹, Patrick Treado¹, Nate Gomer¹, Oksana Olkhovyk¹; ¹ChemImage Corp

Poster Board #3

(582) **Modeling and Performance Evaluation of Conformal Filter (CF) Real-Time Standoff Hazardous Materials Detection;** Arjun Bangalore¹, Mathew Nelson¹, George Ventouris¹, Patrick Treado¹; ¹ChemImage Corp.

Poster Board #4

(583) **A Case Study on NIR Online Monitoring of Blend Uniformity in Solid Dosage Form;** Jin Zhang¹, Dimuthu Jayawickrama¹, Tim Stevens¹, Jay Poorna Reddy¹, Judy Lin¹, Robert Garmise¹; ¹Bristol Myers Squibb

Poster Board #5

(584) **Reducing Spectral Analyte Prediction Error with Penalties on Interferents;** William Spence¹, John Kalivas¹; ¹Idaho State University

Poster Board #6

(585) **An Ensemble of Multiple Linear Regression Models for Easy Wavelength Selection;** Tony Lemos¹, John Kalivas¹; ¹Idaho State University

Poster Board #7

(586) **Regularization Adaption Processes with Labeled and Unlabeled Data for Multivariate Calibration Maintenance;** Anit Gurung¹, John H. Kalivas¹, Erik Andries^{2,3}; ¹Idaho State University; ²University of New Mexico; ³Central New Mexico Community College

Poster Board #8

(587) **Effect of Experimental Design and Calibration Structure on the Prediction Performance of a Near Infrared Calibration Model;** Md Anik Alam^{1,2}, Md Nayeem Hossain^{1,2}, Douglas Steinbach^{1,2}, James Drennen III^{1,2}, Carl Anderson^{1,2}; ¹Graduate School of Pharmaceutical Science, Duquesne University, Pittsburgh, PA; ²Duquesne University Center for Pharmaceutical Technology, Pittsburgh, PA

Poster Board #9

(588) **Robust Latent Variable Selection for Multiple Instrument Calibration Applications;** Douglas Steinbach¹, Anik Alam¹, Nayeem Hossain¹, Carl Anderson¹, James K Drennen¹; ¹Duquesne University Graduate School of Pharmaceutical Sciences

TECHNICAL PROGRAM – WEDNESDAY

Posters 11:00 am – 12:00 pm

Molecular Spectrometry – IR, Near IR, 2D Correlation, Imaging Posters

Poster Board #10

(589) **Improvement of Signal-To-Noise Level in 2D Asynchronous Spectra by Using Wavelet Transformation Approaches;** Yizhuang Xu¹, Anqi He¹, Xiaoyan Kang¹, Jing Chen¹, Yanjun Zhai¹, Isao Noda¹, Jinguang Wu¹; ¹Peking University

Poster Board #11

(590) **Investigation on Intermolecular Interaction between Berberine Hydrochloride and α -cyclodextrin by Using 2D Asynchronous Spectra;** Yizhuang Xu¹, Xiaoyan Kang¹, Anqi He¹, Jing Chen¹, Yanjun Zhai¹, Isao Noda¹, Jinguang Wu¹; ¹Peking University

Poster Board #12

(591) **Application of Near-infrared Spectroscopy for In-process Monitoring in Pharmaceutical Development;** Ming Huang¹, Robert Wethman¹, John Wasyluk¹; ¹BMS

Poster Board #13

(592) **Gas and Vapor Detection by Fiber-Coupled Tunable Laser Diode Absorption Spectroscopy;** Allan Chang¹, Eric Avalos¹, Michael Pocha¹, William Benett¹, Mihail Bora¹, Michael Emmons¹, Tiziana Bond¹; ¹Lawrence Livermore National Laboratory

Poster Board #14

(593) **Focal Plane Array Chemical Imaging of Heterogeneous Organic Mixtures Enables Direct Quantitative Analysis;** Mark Boatwright¹, David Wetzel²; ¹Microbeam Molecular Spectroscopy Laboratory, Kansas State University, Manhattan, KS; ²Department of Biochemistry & Molecular Biophysics, Kansas State University, Manhattan, KS

Poster Board #15

(594) **Real Time Monitoring in Cathode Material of Li-ion Battery during Electrochemical Performance Using Raman Spectroscopy;** Yeonju Park¹, Yesul Kim¹, Yujing Chen¹, Young Mee Jung¹; ¹Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University

Poster Board #16

(595) **Studies of Fertilized Fish Eggs Development by Using Near-Infrared Spectroscopy and Imaging;** Paralee Puangchit¹, Mika Ishigaki¹, Yasui Yui¹, Yukihiro Ozaki¹; ¹School of Science and Technology, Kwansei Gakuin University

Poster Board #17

(596) **Near Infrared Spectroscopy for Measuring Moisture Levels in Solvents and Monomers;** Caleb Brian¹; ¹3M

Poster Board #18

(597) **Real-Time Composition of Liquid and Gas Phase Hydrocarbons with a MEMS Widely Tunable Laser Based Near Infrared Spectrometer;** Steven Minehhan, Paul Little¹; ¹JP3 Measurement; ²Axsun Technologies

Poster Board #19

(598) **In vivo Monitoring for Growth and Abnormality of Fish Egg by Near-Infrared Spectroscopy and Imaging;** Yui Yasui¹, Mika Ishigaki¹, Paralee Puangchit¹, Yukihiro Ozaki¹; ¹Department of Chemistry, Graduate School of Science and Technology, Kwansei Gakuin University

Mass Spectrometry Posters

Poster Board #21

(600) **Near-field Laser Ablation Sampling for Proteomics and Genomics;** Kermit Murray¹, Fan Cao¹, Fabrizio Donnarumma¹; ¹Louisiana State University

Poster Board #22

(601) **MALDI-TOFMS Determination of Copper and Mercury in Food Related Matrices Using Bi(III) as Internal Standard and sodium Diethyldithiocarbamate for Complexation;** Manuel Méndez García¹, Kazimierz Wrobel¹, Armando Alcázar Magaña¹, Alma Rosa Corrales Escobosa¹, Francisco Javier Acevedo Aguilar¹, Katarzyna Wrobel¹; ¹University of Guanajuato

Poster Board #23

(602) **Metabolite Profiling in Helianthus Annuus Hydroponically Grown under Exposure to Cr(VI);** Alan Alexander González Ibarra¹, Katarzyna Wrobel¹, Alma Rosa Corrales Escobosa¹, Félix Gutiérrez Corona¹, Víctor Manuel Mondragón Olguín², Kazimierz Wrobel¹; ¹University of Guanajuato; ²Center of Excellence, Agilent Technologies, Mexico

Poster Board #24

(603) **Metabolomics of Hepatocytes and Human Serum by Laser Desorption Ionization Mass Spectrometry from Silicon Nanopost Arrays;** Andrew Korte¹, Akos Vertes¹; ¹The George Washington University

Poster Board #25

(604) **Transportable Linear Ion Trap Mass Spectrometer with Continuous Atmospheric Pressure Inlet;** Yang Cui, Michael Volny¹, Lynn Chandler¹, William Yang¹; ¹BaySpec Inc.

Poster Board #26

(605) **Analytical-Tool for the Automatic Determination of Trace Metals Contained in Organic Media: Coupling of in-Syringe Magnetic Stirring-Assisted Liquid-Liquid Microextraction to ICP-OES Total Sample Consumption;** José Luis Todolí¹, Raquel Sánchez¹, Burkhard Horstkotte^{2,3}, Salvador Maestre¹, Manuel Miró^{2,3}; ¹University of Alicante; ²Charles University; ³University of the Balearic Islands

Poster Board #27

(606) **Comparison of High Resolution Quadrupole-Time-of-Flight and Orbitrap Mass Spectrometers for the Analysis of Small Hydrophobic Molecules;** Marzieh Ramezani¹, Lee Parsons¹, Edgar Arriaga¹; ¹University of Minnesota

Poster Board #28

(607) **Comparison of Dissociation Characteristics of Oligosaccharides and Glycoconjugates via Collision-Induced Dissociation and Surface-Induced Dissociation;** Forouzan Aboufazel¹, Eric D. Dodds¹; ¹University of Nebraska–Lincoln

Poster Board #29

(608) **Single Cell Elemental Analysis of Human Cells Using Droplet Injection ICP-AES/MS;** Shunsuke Hosoda¹, Satoshi Kohno¹, Aida Mari¹, Ken Kakegawa¹, Tomoko Miyake¹, Takahiro Iwai², Hidekazu Miyahara¹, Mikio Shimada³, Yoshihisa Matsumoto³, Akitoshi Okino¹; ¹FIRST, Tokyo Institute of Technology; ²Department of Applied Chemistry for Environment, Kwansei Gakuin University; ³Institute of Innovative Research, Tokyo Institute of Technology

TECHNICAL PROGRAM – WEDNESDAY

Posters 11:00 am – 12:00 pm

Nanotechnology Posters

Poster Board #30

(609) **Oligonucleotide Modified Nanoparticles for Harmful Algal Bloom Detection**; Claire Lenehan¹, Karen Bruce¹, Amanda Ellis¹, Sophie Leterme¹; ¹Flinders University

Poster Board #31

(610) **Enhanced Ferromagnetism in Nanoscale Transition Metal-Doped TiO₂**; Swati Naik¹; ¹Central Michigan University

Poster Board #32

(611) **One-Pot Growth of 3D Reduced Graphene Oxide Foams Embedded with NiFe Oxide Nanocatalysts for Oxygen Evolution Reaction**; Daoyuan Wang¹, Wei Zhao¹; ¹Department of Chemistry, University of Arkansas at Little Rock

Poster Board #33

(612) **Laser induced Fluorescence System with Error Compensator for Sandwich-Type Immunoassay Using Nanoparticles**; Heung Bin Lim¹, Yeunghyun Kim¹; ¹Dankook University

Poster Board #34

(613) **Environmental Toxicity Assessment of Industrially Relevant Nanomaterials Using Bacteria Model**; Sunipa Pramanik¹, Jeslin Wu¹, Shreyashi Ganguly¹, Bryce Williams¹, Eray Aydil¹, Uwe Kortshagen¹, Christy Haynes¹; ¹University of Minnesota

Poster Board #35

(614) **Novel tris(2-aminoethyl)amine Functionalized Magnetic Iron Oxide Nanoparticles for Curcumin Delivery**; Emily Czapiewski¹, Anselm Omoike¹; ¹University of South Carolina Upstate

Raman – SERS/TERS Posters

Poster Board #36

(615) **New Directions in Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy with Molecular-Resolution Scanning Tunneling Microscopy**; Philip Whiteman¹, Zachary Porach¹, Nan Jiang¹; ¹University of Illinois at Chicago

Poster Board #37

(616) **Effect of Substituents on Surface Equilibria of Thiophenols and Isoquinolines on Gold Substrates Studied Using Surface-Enhanced Raman Spectroscopy**; Erik Emmons¹, Ashish Tripathi¹, Augustus Fountain III¹, Steven Christesen¹, Jason Guicheteau¹; ¹U.S. Army Edgewood Chemical Biological Center

Poster Board #38

(617) **Vibrational Nanoscopy with Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy (UHV-TERS)**; Naihao Chiang¹, Guillaume Goubert¹, Eric A. Pozzi¹, Nan Jiang², Tamar Seideman¹, Mark C. Hersam¹, Richard P. Van Duyne¹; ¹Northwestern University; ²University of Illinois at Chicago

Poster Board #39

(618) **Development of Plasmonic Platforms for Multispectral Surface-enhanced Spectroscopies**; Gregory Wallace¹, Mohammadali Tabatabaei¹, Renjie Hou¹, Matthew Coady¹, Peter Norton¹, Todd Simpson², Scott Rosendahl³, Alexandre Merlen⁴, François Lagugné-Labarthe¹; ¹Western University; ²Western Nanofabrication Facility; ³Canadian Light Source; ⁴Université de Toulon

Poster Board #40

(619) **Using Stark Shifts to Understand the Driving Forces in Plasmonic Catalysis**; Darby Nelson¹, Zachary Schultz¹; ¹University of Notre Dame

Poster Board #41

(620) **Single Molecule Surface-Enhanced Raman Spectroscopy: Towards Reliable Proof Methodology and Nonresonant Detection**; Nolan Wong¹, Alyssa Zrimsek¹, Richard Van Duyne¹; ¹Northwestern University

Poster Board #42

(621) **Graphene-plasmonic Hybrid Nanocomposite for surface Enhanced Raman Scattering (SERS) Aptasensing**; Ahmed Mahmoud^{1,2}, Mark McDermott^{1,2}; ¹Department of Chemistry, University of Alberta; ²National Institute for Nanotechnology

Poster Board #43

(622) **Tip-Enhanced Raman Spectroscopy for Studying Single-Molecule Electrochemistry**; Michael Mattei¹, Xu Chen¹, Gyeongwon Kang¹, Guillaume Goubert¹, Richard P. Van Duyne¹; ¹Northwestern Univ

Poster Board #44

(623) **Investigating Single, Heterogeneous One-Electron Transfer Reactions with EC-SERS**; M. Fernanda Cardinal¹, Zaleski Stephanie¹, Chulhai Dhabih², Jordan M. Klingsporn¹, Lasse Jensen², Richard P. Van Duyne¹; ¹Northwestern University, Department of Chemistry, Evanston, IL; ²Pennsylvania State University, Department of Chemistry, University Park, PA

Poster Board #45

(624) **Plasmon-Driven Hot Electron Chemistry in Isotopically Edited 4,4'-Bipyridine Gold Nanoantennas**; Emily Sprague-Klein, Michael McAnally¹, Dmitry Zhdanov¹, Alyssa Zrimsek¹, Vartkess Apkarian², George Schatz¹, Tamar Seideman¹, Richard Van Duyne¹; ¹Northwestern University; ²Univ of California at Irvine

Surface Plasmon Resonance and Surface Science Posters

Poster Board #46

(625) **Nanoparticle Enhanced SPRI as a Diagnostic Platform for the Early Detection of Acute Kidney Injury**; Kristy S. McKeating¹, Samuel S. Hinman¹, Siqi Li², Zhiguo Zhou², Quan Cheng¹; ¹University of California, Riverside; ²Luna Innovations Inc

Poster Board #47

(626) **Investigation of Far-and Deep-Ultraviolet Surface Plasmon Resonance Depending on Refractive Indices and Absorbance on Al Film**; Koji Watari¹, Ichiro Tanabe², Yoshito Tanaka³, Takeyoshi Goto¹, Wataru Inami⁴, Yoshimasa Kawata⁴, Yukihiko Ozaki¹; ¹Kwansei Gakuin Univ.; ²Osaka Univ.; ³Tokyo Univ.; ⁴Shizuoka Univ.

Poster Board #48

(627) **Bioconjugation Strategy to Increase Stability of Protein Modified Gold Nanoparticles for use in Light Scattering Immunoassays**; Seth Filbrun¹, Alex Mandl¹, Kirk Eichenberg¹, Francis Lovato¹, Jeremy Driskell¹; ¹Illinois State University

Poster Board #49

(628) **Storing Matter technique in Secondary Ion Mass Spectrometry: Application for Depth Profiling**; Maciej Miśnik^{1,2}, Aleksander Zawada^{1,3}, Piotr Konarski^{1,3}; ¹Institute of Tele and Radio Technology, Warszawa, Poland; ²Gdańsk University of Technology, Gdańsk, Poland; ³Military University of Technology, Warszawa, Poland

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 #50

(629) **Plasmonic Graded Gratings for Hyperspectral - Infrared Sensing and Imaging**; Arthur Montazeri¹, Hoi-Ying Holman¹; ¹Lawrence Berkeley National Laboratory

11:40AM – 1:10 PM

WHAT'S HOT VENDOR PRESENTATIONS, *Exhibit Hall*

Presider: Brian Dable, *Arete Associates*

Free lunch available in exhibit hall for all conferees, ticket required

- 11:40 **LECO** “What’s Hot at LECO”
- 11:50 **Metrohm** “Metrohm Spectroscopy – Solutions from the Lab to the Line”
- 12:00 **Princeton Instruments** “Lever Your Genius with the New Fergie Spectroscopy System”
- 12:10 **Ondax** “Process Analysis with Low Frequency Raman”
- 12:20 **BaySpec** “Bring High Performance Spectrometers out of Laboratory to Samples: Novel Transportable Field Mass Spectrometers and Miniaturized Hyperspectral Imagers for Airborne Remote Sensing”
- 12:30 **Applied Spectra** “J200 Tandem LA – LIBS: Landmark LA Innovation for Measuring Every Elements in the Periodic Table with Laser Pulses”
- 12:40 **PD-LD**
- 12:50 **Brightspec** “A new implementation of an old tool: FT-MRR gets rotational spectroscopy solving problems in the lab”
- 1:00 **HORIBA** “DiP, Direct Thickness Measurement along with Elemental Depth Profiling”

Wednesday Afternoon, *Nicollet D2/D3*

RSC-ACS SYMPOSIUM - SOLVING GLOBAL HEALTH CHALLENGES: MOLECULAR TECHNIQUES TOWARDS DIAGNOSTICS AND DETECTION

Organizers: Philippa Hughes and Douglas Duckworth;

Presider: Philippa Hughes

- 1:20 (630) **Electrochemical Insights into Neurodegenerative Diseases: Using *Drosophila* Models to Understand Parkinson Disease**; B. Jill Venton¹, Eve Privman¹, Ryan Borman¹, Poojan Pyakurel¹, Danielle Wolin¹, Leah Ostendorf¹, Subrahata Sanyal², Nathan Dolenson²; ¹University of Virginia; ²Bioden Idec
- 1:40 (631) **Multiplexed, Photonic Sensor Arrays for Informative Disease Diagnosis**; Ryan Bailey^{1,2}; ¹University of Michigan; ²University of Illinois at Urbana-Champaign
- 2:00 (632) **Does Raman Spectroscopy Offers a Solution to currently Unmet Medical Needs!?**; Juergen Popp^{1,2}; ¹Leibniz Institute of Photonic Technology, Jena, Germany; ²Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Jena, Germany
- 2:20 (633) **Detection and Diagnosis of Malignancies Using Raman Spectroscopic Techniques**; Nick Stone¹; ¹University of Exeter; ²STFC Rutherford Appleton Laboratory; ³Cranfield University
- 2:40 (634) **Label-free Diagnosis and Detection Using Molecular Vibrational Fingerprints**; Ji-Xin Cheng¹; ¹Purdue University

Wednesday Afternoon, *Greenway J*

MICRO- AND NANOFUIDICS FOR PREPARATION, SEPARATION AND DETECTION OF BIOMOLECULES AND CELLS

Organizers and Presiders: Noritada Kaji and Kazuma Mawatari

- 1:20 (635) **Microscale Analysis of Heterogeneous Circulating Tumor Cells**; Reza Mohamadi¹, Shana Kelley¹; ¹University of Toronto

- 1:40 (636) **Label-free Electrical Detection of Enzymatic Reactions in 2-D Nanochannels**; Chuanhua Duan¹; ¹Boston University
- 2:00 (637) **Single Cell and Single Molecule Analytical Devices Utilizing Nanofluidic Technology**; Kazuma Mawatari¹, Takehiko Kitamori¹; ¹The University of Tokyo
- 2:20 (638) **Microfluidic Platform for Bilayer Experimentation**; S  verine Le Gac¹; ¹University of Twente
- 2:40 (639) **Electrical Detection and Discrimination of Bacteria and Cells in Microfluidic Devices**; Noritada Kaji¹, Hirotoshi Yasaki¹, Mamiko Sano¹, Takao Yasui¹, Yoshinobu Baba^{1,2}; ¹Nagoya University; ²National Institute of Advanced Industrial Science and Technology

Wednesday Afternoon, *Greenway A*

ICPMS: FUNDAMENTALS AND APPLICATIONS

Organizer and Presider: Martin Resano

- 1:20 (640) **High-Precision Isotopic Analysis of Essential Transition Metals in human Body Fluids for Medical Diagnosis, Prognosis & Monitoring**; Frank Vanhaecke¹, Yulia Anoshkina¹, Marta Costas-Rodr  guez¹, Maria del Rosario Florez¹, Sara Lauwens¹, Hans Van Vlierberghe², Marijn Speekkaert³, Joris Delanghe⁴; ¹Ghent University, Department of Analytical Chemistry; ²Ghent University Hospital, Department of Gastroenterology and Hepatology; ³Ghent University Hospital, Department of Nephrology; ⁴Ghent University Hospital, Department of Clinical Chemistry
- 1:40 (641) **Asymmetrical Flow Field-Flow Fractionation Coupled to Inductively Coupled Plasma Mass Spectrometry for Assessment of the Quality of Functionalized Quantum Dots**; Jose Manuel Costa-Fernandez¹, Diego Bouzas Ramos¹, Mario Menendez Miranda¹, Jorge Ruiz Encinar¹, Alfredo Sanz-Medel¹; ¹University of Oviedo
- 2:00 (642) **Analysis of Whole Blood through ICP-MS Equipped with a High Temperature Total Sample Consumption System**; Jos  -Luis Todol  ¹,   gueda Ca  abate¹, Esperanza Garc  a-Ruiz², Mart  n Resano²; ¹University of Alicante; ²University of Zaragoza
- 2:20 (643) **Monitoring of Molecular Species for Elemental and Isotopic Analysis**; Mart  n Resano¹, Esperanza Garc  a-Ruiz¹, Maite Aramend  a^{1,2}, Ananda Guarda¹, Diego Leite¹; ¹University of Zaragoza; ²Centro Universitario de la Defensa, Zaragoza
- 2:40 (644) **Nanoparticle Detection in Environmentally Relevant Matrices Using Differential Mobility Analysis-Inductively Coupled Plasma Mass Spectrometry**; Qilin Chan¹, Mark Ellefson¹, Christine Loza¹, Brian Mader¹, Susan Wolf¹; ¹3M

Wednesday Afternoon, *Greenway H/I*

MEGERS AWARD SYMPOSIUM HONORING MIKE GEORGE

Organizer and Presider: Mike George

- 1:20 (645) **Transient Raman Spectroscopy of Ruthenium(II) Complexes with Electron Donor ligands**; Keith Gordon¹, Georgina Shillito¹; ¹University of Otago
- 1:40 (646) **Time-resolved Vibrational Spectroscopy of Photoexcited States**; Terry Gustafson; ¹The Ohio State University
- 2:00 (647) **What We See by time-Resolving in Near-IR**; Koichi Iwata¹; ¹Gakushuin University

TECHNICAL PROGRAM – WEDNESDAY

Orals 1:20 – 3:00 pm

- 2:20 (648) **Mechanistic Studies into the Light Driven Production of H₂ from a Biomimetic of the Active Site of [NiFe] Hydrogenase**; Peter Summers^{1,2}, James Calladine², Fabio Ghiotto², Jonathan McMaster², Martin Schröder^{2,3}, Michael George^{1,2}; ¹Department of Chemical and Environmental Engineering, The University of Nottingham Ningbo China, Ningbo, China; ²School of Chemistry, The University of Nottingham, University Park, Nottingham, UK; ³School of Chemistry, University of Manchester, Manchester, UK
- 2:40 (649) **Slow Time-Resolved Measurements Raman Measurements in Industry**; Paul Pudney; ¹Unilever Discover

Wednesday Afternoon, Greenway G
CLIRSPEC BIOMEDICAL APPLICATIONS OF NEAR-FIELD INFRARED SPECTROSCOPY
 Organizer and Presider: Kathleen Gough

- 1:20 (650) **Plasmon-assisted Infrared-structured Illumination Microscopy of Living Cells**; Liang Chen¹, Hoi-Ying Holman¹, Arthur Montazeri^{1,2}, Giuseppe Calafiore^{1,4}, Giovanni Birarda^{1,3}, Alexksandr Polyakov¹, Nazir Kherani², Stefano Cabrini¹; ¹Lawrence Berkeley National Laboratory, University of California, Berkeley, CA; ²University of Toronto, Toronto, Ontario, Canada; ³Elettra – Sincrotrone Trieste, Basovizza, Trieste Italy; ⁴Polytechnic University of Turin, Torino, Italy
- 1:40 (651) **AFM-IR Technique: A New Outlook for Biomedical Studies**; Alexandre Dazzi¹, Jérémie Mathurin¹, Ariane Deniset-Besseau¹; ¹Université Paris-Sud
- 2:00 (652) **Synchrotron IR Nanospectroscopy at Diamond Light Source**; Chris Kelley¹, Paul Donaldson^{1,3}, Jacob Filik^{1,2}, Mark Frogley¹, Ann Fitzpatrick¹, Katia Wehbe¹, Gianfelice Cinque¹; ¹MIRIAM - Beamline B22 - Diamond Light Source, UK; ²Scientific Computing Group - Diamond Light Source, UK; ³Central Laser Facility, UK
- 2:20 (653) **Contact Resonance Drifts in PTIR? Solved.**; Georg Ramer^{1,2,3}, Florian Reisenbauer², Anna Balbekova², Andreas Schwaighofer², Bernhard Lendl²; ¹Center for Nanoscale Science and Technology, National Institute of Standards and Technology; ²Institute for Chemical Technologies and Analytics, TU Wien, Austria; ³Maryland Nanocenter, University of Maryland
- 2:40 (654) **Nanoscale Infrared Spectroscopy and Imaging of Control and Overload-Damaged Tendon**; Kathleen Gough¹, Richard Wiens¹, Catherine Findlay¹, Daisy Ma¹, Samuel Baldwin², Laurent Kreplak²; ¹University of Manitoba; ²Dalhousie University

Wednesday Afternoon, Lakeshore B
CLIRSPEC: CLINICAL APPLICATIONS OF IR SPECTROSCOPY AND IMAGING
 Organizer and Presider: Matthew Baker

- 1:20 (655) **Exploring Breast Cancer Prognosis Specific Tissue Microenvironment Changes through Infrared Spectroscopy**; Saumya Tiwari¹, Sarah Holton¹, Tiziana Triulzi², Elda Tagliabue²; ¹University of Illinois at Urbana Champaign; ²Molecular Targeting Unit, Fondazione IRCCS Istituto Nazionale dei Tumori

- 1:40 (656) **Fourier Transform Infrared (FTIR) Spectroscopic Imaging Driven Histopathological Assessment of Epithelial Misplacement versus Polyp Cancer in the Colon**; Jayakrupakar Nallala¹, Rebecca Griggs², Gavin Lloyd², Timothy Cook³, Catherine Kendall², Hugh Barr^{2,3}, Neil Shepherd^{2,4}, Nick Stone¹; ¹College of Engineering, Mathematics and Physical Sciences, University of Exeter, UK; ²Biophotonics Research Unit, Gloucestershire Hospitals NHS Foundation Trust, Gloucester, UK; ³Department of Surgery, Gloucestershire Hospitals NHS Foundation Trust, Gloucester, UK; ⁴Department of Cellular Pathology, Gloucestershire Hospitals NHS Foundation Trust, Cheltenham, UK
- 2:00 (657) **Vibrational Spectroscopy in the Management of Cancer. Aren't We There Yet?**; Abigail Rutter¹, Josep Sulé-Suso¹; ¹Keele University
- 2:20 (658) **Chemical Imaging of Amyloid- β Plaques**; Francesca Palombo¹, Francesco Tamagnini¹; ¹University of Exeter
- 2:40 (659) **Detecting Biochemical Changes in Liver Fibrosis Using Quantum Cascade Laser Infrared Spectroscopic Imaging**; Michael Walsh¹, Vishal Varma¹, Hari Sreedhar¹, Grace Guzman¹; ¹University of Illinois at Chicago

Wednesday Afternoon, Nicollet B/C
ITP CLOSING KEYNOTE LECTURES I
 Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
 Presiders: Steven Soper and Kevin Dorfman

- 1:20 (660) **Analysis of Drug-Protein Interactions Using High-Performance Affinity Microcolumns: Recent Developments for Clinical Samples and Personalized Medicine**; David Hage¹; ¹University of Nebraska-Lincoln
- 1:45 (661) **Partially Filling Affinity Capillary Electrophoresis - Complementary or Alternative Technique for Biosensors in Biomolecular Interaction Studies?**; Marja-Liisa Riekkola¹, Joanna Witos¹, Katriina Lipponen¹, Jörgen Samuelsson², Torgny Fornstedt², Katriina Öörni³, Matti Jauhiainen⁴; ¹Department of Chemistry, University of Helsinki, Finland; ²Department of Engineering and Chemical Sciences, Karlstad University, Sweden; ³Wihuri Research Institute, Helsinki, Finland; ⁴National Institute for Health and Welfare, Genomics and Biomarkers Unit, Biomedicum, Helsinki, Finland
- 2:10 (662) **Affinity Capillary Electrophoresis: A Valuable Contribution to Ligand Binding Assay platforms**; Hermann Wätzig¹, Imke Oltmann-Norden¹, Mona Mozafari¹, Hassan AlHazmi^{1,4}, Markus Nachbar¹, Deia Abd El-Hady^{2,3}, Sami El Deeb¹; ¹TU Braunschweig, Institute for Medicinal and Pharmaceutical Chemistry; ²Chemistry Department, Faculty of Science, University of Jeddah, Jeddah, Saudi Arabia; ³Chemistry Department, Faculty of Science, Assiut University, Egypt; ⁴Jazan University, Jazan, Saudi Arabia
- 2:35 (663) **Glycohistopathology of Formalin Fixed – Paraffin Embedded (FFPE) Samples**; Andras Guttman^{1,2}, Boglarka Donczó^{1,2}, Marton Szigeti¹, Bryan Fonslow²; ¹Horvath Csaba Memorial Institute of Bioanalytical Research; ²Sciex

TECHNICAL PROGRAM – WEDNESDAY
Orals 1:20 – 3:00 pm and ITP Closing Plenary 3:05 pm

Wednesday Afternoon, Calhoun
ITP CLOSING KEYNOTE LECTURES II
 Organizers: Blanca Lapizco-Encinas and Ziad El Rassi;
 Presiders: Jorg Kutter and Marian Masar

- 1:20 (664) **Monolithic Columns with Incorporated Bare and Surface Bonded Silica Nanoparticles for Hydrophilic Interaction Liquid Chromatography**; Ziad El Rassi¹, Nisansala Ganewatta¹; ¹Oklahoma State University
- 1:45 (665) **Nanobiodevice-based Separations of Single Biomolecule, Exosome, and Cell for Medical Innovations**; Yoshinobu Baba¹; ¹Nagoya University
- 2:10 (666) **Our Recent Studies on Enantiomer Separation Mechanisms in Capillary Electrophoresis**; Bezhn Chankvetadze¹; ¹Tbilisi State University
- 2:35 (667) **HILIC-MS of Intact Glycoproteins**; Govert W. Somsen¹, Elena Dominguez Vega¹, Jordy van Angeren¹, Klara Petru², Sara Tengattini³, Rob Haselberg¹; ¹Vrije Universiteit Amsterdam; ²Charles University Prague; ³University of Pavia

Wednesday Afternoon, Nicollet B/C
ITP CLOSING PLENARY AND CLOSING REMARKS
 Organizers and Presiders: Blanca Lapizco-Encinas and Ziad El Rassi

- 3:05 (668) **Practice and Ramifications of Ultra Fast Chiral and Chiral Separations**; Daniel Armstrong¹; ¹University of Texas at Arlington
- 3:35 **ITP Closing Remarks**

Wednesday Afternoon, Greenway B/C
FUNDAMENTALS OF LIBS FOR ENHANCED ANALYTICAL PERFORMANCE
 Organizer and Presider: Alessandro De Giacomo

- 1:20 (669) **Femtosecond Filaments in Remote Isotope Analysis**; Vassilia Zorba¹, George C.-Y. Chan¹, Huaming Hou², Xianglei Mao¹, Richard Russo¹; ¹Lawrence Berkeley National Laboratory; ²The Peac Institute of Multiscale Sciences, Chengdu, China
- 1:40 (670) **Real Time Isomer Fingerprinting with LIBS**; Ishan Barman¹; ¹Johns Hopkins University
- 2:00 (671) **Elemental Imaging by LIBS: Present and Potential Future**; Vincent Motto-Ros¹, Frédéric Pelascini²; ¹Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Villeurbanne, France; ²CRIT Matériaux Alsace, Schiltigheim, France
- 2:20 (672) **Nanoparticle Enhanced Laser Induced Breakdown Spectroscopy Applications**; Alessandro De Giacomo^{1,2}, Marcella Dell², Rosalba Gaudioso¹, Can Koral¹, Gabriele Valenza¹; ¹University of Bari, Department of Chemistry; ²CNR-Nanotec
- 2:40 (673) **Modeling and Diagnostics of Molecules in Laser Induced Plasma**; Igor Gornushkin¹, Sergei Shabanov², Reto Glaus¹, Ulrich Panne^{1,3}; ¹BAM, Federal Institute for Material Research and Testing; ²University of Florida; ³Humboldt University Berlin

Wednesday Afternoon, Greenway D
ADVANCES IN ON-LINE PROCESS ANALYSIS
 Organizer and Presider: Alison Nordon

- 1:20 (674) **Towards Hyperpolarised Benchtop NMR Spectroscopy for Industrial Process Monitoring and Control**; Meghan Halse¹, Simon Duckett¹, Alison Nordon², Andrew Parrott², Peter Richardson¹, Olga Semenova¹; ¹Centre for Hyperpolarisation in Magnetic Resonance, Department of Chemistry, University of York, UK; ²Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow, UK

- 1:40 (675) **X-Ray Imaging for Design of Gas Nozzles in Large Scale Fluidised Bed Reactors**; Massimiliano Materazzi¹, Paola Lettieri¹, Jonathan Dodds², Andrew Milliken³; ¹University College London (UCL); ²National Nuclear Laboratory (NNL); ³Sellafield Ltd
- 2:00 (676) **The Monitoring of Secondary Processes Using Process Analytical Technologies**; Joanna Lothian¹, Alison Nordon¹, Peter Hamilton², Richard Elkes²; ¹EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Crystallisation and WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow; ²GlaxoSmithKline, GSK, Gunnels Wood Road, Stevenage Herts
- 2:20 (677) **Online LC/MS Monitoring of a Continuous Process with a Portable Single-Quadrupole Mass Spectrometer: low Level Impurity Monitoring and Impurity Identification**; Bradley Campbell¹, Mindy Forst¹, Todd Maloney¹; ¹Eli Lilly and Company
- 2:40 (678) **LifeCycle Management of Raman Spectroscopy of the Active Content of an Oral Dosage Form**; Md Nayeem Hossain¹, Benoît Igne², Md Anik Alam¹, Carl Anderson¹, James Drennen¹; ¹Duquesne University Center for Pharmaceutical Technology; ²GlaxoSmithKline, PA

Wednesday Afternoon, Lakeshore C
NOVEL APPROACHES TO BIOPHARMACEUTICAL ANALYSIS
 Organizer and Presider: Rina Dukor

- 1:20 (679) **Probing Higher-Order Structure in Biopharmaceuticals Using Raman and Raman Optical Activity**; Laurence Nafie^{1,2}, Rina Dukor², Carolina Carballo², Juanita Sanchez²; ¹Syracuse University; ²BioTools, Inc.; ³BioTools, Inc.; ⁴BioTools, Inc.
- 1:40 (680) **Spectroscopic Characterization of Protein-Based Pharmaceuticals**; John Wasyluk¹, Rose Soskind¹, Michaela Raglione¹, Mary Krause¹, Daniel Faschana¹; ¹Bristol-Myers Squibb Co.
- 2:00 (681) **Chemically Modified Oligonucleotides Target the SERCA/PLN Complex**; Kailey J. Soller¹, Jing Yang¹, Raffaello Verardi², Gianluigi Veglia², Michael Bowser¹; ¹University of Minnesota, Department of Chemistry; ²University of Minnesota, Department of Biochemistry, Molecular Biology and Biophysics
- 2:20 (682) **A Multiscale Analysis of the Mechanical Properties of the fibrous Proteins of the Extracellular Matrix Using Brillouin Light Scattering Spectroscopy**; Ryan Edginton¹, Francesca Palombo¹, Ellen Green¹, C. Peter Winlove¹; ¹University of Exeter
- 2:40 (683) **Molecular Structure and Thermal Behavior of Biodegradable Poly(3-hydroxybutyrate- co-3-hydroxyhexanoate) /Polyethylene Glycol Blends**; Yujing Chen¹, Yeonju Park¹, Isao Noda^{2,3}, Young Mee Jung¹; ¹Department of Chemistry, Kangwon National University, Korea; ²Department of Materials Science and Engineering, University of Delaware, Newark, DE; ³MHG, Inc., Bainbridge, GA

Wednesday Afternoon, Nicollet D1
RAMAN SPECTROSCOPIC SENSING
 Organizer and Presider: Torsten Frosch

- 1:20 (684) **Ultrasound Enhanced In-Line Raman Sensing of Particles in Suspensions**; Bernhard Lendl¹, Stefan Radel¹, Stefan Tauber¹; ¹Technische Universität Wien

TECHNICAL PROGRAM – WEDNESDAY

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

- 1:40 (685) **Detection of β -sheet-rich Insulin Oligomers and Organic Dyes Using Surface-Enhanced Raman Spectroscopy (SERS). A New Approach in Neurodegenerative Diseases and Forensics;** Dmitry Kurouski^{1,1}; ¹Boehringer-Ingelheim Pharmaceuticals
- 2:00 (686) **Raman Spectroscopy with Broadband Light Sources;** Johannes Kiefer^{1,1}; ¹Universitaet Bremen
- 2:20 (687) **Raman Spectroscopy of Cellular Defence Responses;** Alison J. Hobro¹, Nicholas I. Smith¹; ¹Immunology Frontier Research Center, Osaka University, Japan.
- 2:40 (688) **Fiber and Cavity Based Raman Sensing;** Torsten Frosch^{1,2}, Di Yan¹, Tobias Jochum¹, Jürgen Popp^{1,2}; ¹Leibniz Institute of Photonic Technology; ²Friedrich Schiller University Jena

Wednesday Afternoon, Lakeshore A PHARMACEUTICAL RAMAN Organizer and Presider: Ian Lewis

- 1:20 (689) **Evaluation of Specialized Vibrational Spectroscopic Techniques for Chiral Purity Analysis;** Sergey Arzhantsev¹; ¹US Food and Drug Administration
- 1:40 (690) **Application of Back-scatter Raman Spectroscopy to Fluidized Bed Coating Process;** Hanzhou Feng¹, James Drennen¹, Carl Anderson¹; ¹Duquesne University, Graduate School of Pharmaceutical Sciences
- 2:00 (691) **A Comparative Study between Near-infrared and Raman Calibration Methods for Quantitative Analysis of Tablets Containing Multiple APIs;** Md Anik Alam^{1,2}, Md Nayeem Hossain^{1,2}, Douglas Steinbach^{1,2}, James Drennen^{1,2}, Carl Anderson^{1,2}; ¹Graduate School of Pharmaceutical Science, Duquesne University, Pittsburgh, PA; ²Duquesne University Center for Pharmaceutical Technology, Pittsburgh, PA
- 2:20 (692) **Towards a Universal Model for Bioprocess Monitoring;** Joana Murtinheira Faustino¹, Adrian Stacey², Linda Harvey¹, Brian McNeil¹; ¹University of Strathclyde; ²TAP Biosystems
- 2:40 (693) **Impact of Chemical and Thermal Stresses on Monoclonal Antibody Secondary Structure by Deep UV Resonance Raman Spectroscopy;** Sergey Arzhantsev¹, Chen Qiu¹; ¹US Food and Drug Administration

Wednesday Afternoon, Greenway E MAKING THE LEAP: PATHWAYS FROM GRADUATE SCHOOL TO A PERMANENT POSITION -PANEL DISCUSSION- Organizer and Presider: Anthony Stender

- 1:20 (694) **Making the Leap: Pathways from Graduate School to a Permanent Position;** Anthony Stender¹, Carrie Lendon⁵, Lisa Brown⁷, Deanna O'Donnell², Jared Anderson³, Matt Meyer⁶, Sam Alvarado⁴; ¹Rice University; ²Hamline University; ³Iowa State University; ⁴University of Wisconsin - River Falls; ⁵Cargill; ⁶Thermo Fisher; ⁷3M
- 3:00 **Poster Viewing and Coffee Break, Exhibit Hall**

Wednesday Afternoon, Greenway J NANOSCOPIC POROUS SENSORS

Organizers and Presiders: Joseph Robertson and Joseph Reiner

- 3:50 (695) **Cluster-enhanced Single Molecule Nanopore Spectrometry (SMNS): Towards Optimal Detection of Peptides;** Joseph Reiner¹, Nuwan Kothalawala², Amy Chavis¹; ¹Virginia Commonwealth University; ²University of Mississippi
- 4:10 (696) **Polymers and Peptides Characterization in Confined Space;** Abdelghani Oukhaled¹; ¹Laboratoire LAMBE University of Cergy-Pontoise

- 4:30 (697) **A New Methodology for Monitoring Phase Behaviour inside Nano-Channels.;** Mike George¹; ¹University of Nottingham
- 4:50 (698) **Thin-film Nanofluidic Devices for Single-Molecule Science;** Jason Dwyer¹; ¹University of Rhode Island
- 5:10 (699) **Democratizing Nanopore-based Single-Molecule Research;** Vincent Tabard-Cossa¹; ¹University of Ottawa

Wednesday Afternoon, Greenway A ATOMIC SPECTROMETRY WITH GLOW DISCHARGES AT ATMOSPHERIC PRESSURE Organizer and Presider: Jose Broekaert

- 3:50 (700) **Investigations of Sample Introduction for a Glow Discharge at Atmospheric Pressure;** José Broekaert¹; ¹University of Hamburg - Department of Chemistry
- 4:10 (701) **From Soft Ionization to Element Excitation with a Dielectric Barrier Discharge;** Joachim Franzke¹, Sebastian Bandt¹, Alexander Schütz¹, David Klute¹, Antje Michels¹, Vlasta Horvatic², Cedo Vadla²; ¹ISAS - Leibniz-Institut für Analytische Wissenschaften, Dortmund, Germany; ²Institute of Physics, Zagreb, Croatia, Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia,
- 4:30 (702) **Microwave-Sustained, Inductively Coupled, Atmospheric-Pressure Plasma (MICAP): An Attractive Alternative to the Inductively Coupled Plasma (ICP);** Cera Cissna¹, Andrew Schwartz¹, Gary Hieftje¹; ¹Indiana University
- 4:50 (703) **Comprehensive Elemental/Isotopic Analysis with LS-APGD-MS/OES;** R. Kenneth Marcus¹, Edward Hoegg¹, Htoo Paing¹; ¹Clemson University
- 5:10 (704) **How Can Battery-Operated Microplasmas On-Chips be Used for Elemental Analysis of Solid Microsamples?;** Vassili Karanassios¹; ¹University of Waterloo

Wednesday Afternoon, Greenway G CLINICAL BIOMEDICAL IMAGING Organizer and Presider: Rohith Reddy

- 3:50 (705) **Label-Free Biological Imaging below the Diffraction Limit Using Stimulated Raman Spectroscopy;** Christian Graefe¹, W. Ruchira Silva¹, Renee Frontiera¹; ¹University of Minnesota
- 4:10 (706) **Histopathological Analysis of Melanocytic Lesions Using Pump-probe Microscopy can Improve Melanoma Diagnosis and Staging;** Francisco Robles^{1,2}; ¹Georgia Institute of Technology; ²Emory University
- 4:30 (707) **Quantitative, Comparable Broadband Coherent Anti-Stokes Raman Scattering Microspectroscopy for High-Speed Cell and Tissue Imaging;** Charles Camp Jr¹, Young Jong Lee¹, Marcus Cicerone¹; ¹National Institute of Standards and Technology
- 4:50 (708) **Quantum Cascade Laser Infrared Spectroscopic Imaging: Predicting Transplant Outcome;** Michael Walsh¹, Vishal Varma¹, Hari Sreedhar¹, Imran Uraizee², Aliya Husain², Suman Setty¹; ¹University of Illinois at Chicago; ²University of Chicago
- 5:10 (709) **In vivo Imaging of Endocrine Tissue for Intra-Operative Guidance;** Anita Mahadevan-Jansen¹, Melanie McWade¹, Giju Thomas¹, Melinda Sanders², Carmen Solarzano²; ¹Vanderbilt University; ²Vanderbilt University Medical Center

TECHNICAL PROGRAM – WEDNESDAY

3:50 – 5:30 pm

Wednesday Afternoon, Nicollet D2/D3

RETHINKING CALIBRATION

Organizer and Presider: John Kalivas

- 3:50 (710) **Deep Semi-Supervised Generative Models for Spectroscopic Data**; Ian Gemp¹, Darby Dyar², Mario Parente¹, Arun Saranath¹; ¹University of Massachusetts Amherst; ²Mount Holyoke College
- 4:10 (711) **Joint Modeling of Calibration and Inference in the Statistical Analysis of Spectroscopy Data**; Timothy Randolph¹, Jaroslaw Harezlak²; ¹Fred Hutchinson Cancer Research Center; ²Indiana University
- 4:30 (712) **Big Data for Extraterrestrial Spectroscopy**; Thomas Boucher¹, Darby Dyar²; ¹University of Massachusetts; ²Mount Holyoke College
- 4:50 (713) **Rethinking Local Calibration Using Local Adaptive Fusion Regression**; Rachel Emerson¹, John Kalivas²; ¹Idaho National Laboratory; ²Idaho State University
- 5:10 (714) **Integration of Chemometric Methods with Total Synchronous Fluorescence Spectroscopy**; Keshav Kumar¹; ¹Department of Molecular Biology, Umea University, Sweden

Wednesday Afternoon, Greenway D

FORENSIC ANALYSIS: FROM THE LAB TO THE CRIME SCENE

Organizer and Presider: Igor Lednev

- 3:50 (715) **Forensic Science R&D Funding Program at the National Institute of Justice: Opportunities in Analytical Chemistry, Applied Spectroscopy and Bioanalysis**; Minh Nguyen¹, Gregory Dutton¹; ¹National Institute of Justice
- 4:10 (716) **From the Lab to the Field: Taking Mass Spectrometry out of Its Element and into the Harsh Environment**; Guido Verbeck¹, Kenneth Wright²; ¹University of North Texas; ²Inficon
- 4:30 (717) **Pioneering Uses of Headspace Analysis for the Rapid Identification of Objects of Forensic Interest in the Field**; Howard Holness^{1,2}, Lauren Colon-Crespo^{1,2}, Adhly Huertas^{1,2}, Vanquilla Shellman^{1,2}, Rodolfo Mesa^{1,2}, Abuzar Kabir^{1,2}, Kenneth G. Furton^{1,2}; ¹Florida International University; ²International Forensic Research Institute
- 4:50 (718) **A Raman ‘Spectroscopic Clock’ for Bloodstain Age Determination**; Kyle C. Doty¹, Gregory McLaughlin¹, Igor K. Lednev¹; ¹Department of Chemistry, University at Albany, SUNY
- 5:10 (719) **Identification of Surface Deposited Bacteria Using Vibrational Spectroscopy**; Claire Pickering^{1,4}, Elaine Perkins², William Sellors², Roy Goodacre³, Matthew Baker^{1,4}; ¹WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde, Technology and Innovation Centre, Glasgow, UK; ²DSTL, Porton Down, Salisbury, Wiltshire, UK; ³School of Chemistry, Manchester Institute of Biotechnology, The University of Manchester, Manchester, UK; ⁴Centre for Forensic Science, Department of Pure and Applied Chemistry, University of Strathclyde, Thomas Graham Building, Glasgow

Wednesday Afternoon, Lakeshore B

DECODING CIRCULATING BIOMARKERS WITH SPECTROSCOPY: NEXT GENERATION ASSAYS

Organizer and Presider: Ishan Barman

- 3:50 (720) **Illuminating Membrane Receptor Recognition Using Plasmonic Enhancements**; Zachary Schultz¹; ¹University of Notre Dame
- 4:10 (721) **Implantable Materials that Enable Noninvasive Metabolic Monitoring**; Mike McShane¹; ¹Texas A&M University
- 4:30 (722) **Development of a Microfluidic Device for Drug Detection**; Neal Kline¹, Ashish Tripathi², Rustin Mirsafavi³, Chrysafis Andreou³, Martin Moskovits³, Carl D. Meinhart³, Jason Guicheteau², Steven D. Christesen², Augustus W. Fountain III²; ¹Oak Ridge Institute for Science and Education; ²Research and Technology Directorate, Edgewood Chemical Biological Center, Aberdeen Proving Ground, MD; ³University of California Santa Barbara
- 4:50 (723) **Towards a Rapid and Selective Solution Assay for Biopharmaceutical Glycosylation Analysis Using Lectin-Coated Nanoparticles and SERS**; Craig Ward¹, Daniel Bracewell², Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde; ²University College London
- 5:10 (724) **Development of a 3D Cell Culture Model for Drug Discovery Studies Using Surface Enhance Raman Spectroscopy**; Mustafa Culha¹, Mine Altunbek¹; ¹Yeditepe University

Wednesday Afternoon, Greenway B/C

RECENT ADVANCES IN SPRAY IONIZATION MASS SPECTROMETRY

Organizer and Presider: Andre Venter

- 3:50 (725) **Electrospray Characterization by Pulsed Field Ion Mobility Mass Spectrometry**; Kaveh Jorabchi¹, William McMahon¹, Carina Minardi¹, Arjuna Subramanian¹; ¹Georgetown University
- 4:10 (726) **Quantitative Analysis of Live Single Cells Using Single-probe Mass Spectrometry Techniques**; Zhibo Yang¹, Ning Pan¹, Haiqing Yu¹, Wei Rao¹; ¹University of Oklahoma
- 4:30 (727) **Desorption Electro-Flow Focusing Ionization and In-Source Collision Induced Dissociation for Trace Detection and Chemical Imaging of Military-Grade and Homemade Explosives**; Thomas Forbes¹, Edward Sisco¹, Greg Gillen¹; ¹NIST
- 4:50 (728) **Enhancement from Vacuum-assisted Plasma Ionization on Surface Acoustic Wave Nebulization**; Matthew C. Bernier¹, Stephen C. Zambrzycki¹, Joel D. Keelor¹, Facundo M. Fernandez¹; ¹School of Chemistry and Biochemistry, Georgia Inst of Technology, Atlanta, GA
- 5:10 (729) **Delayed Desorption to Improve Protein Analysis by Desorption Electrospray Ionization Mass Spectrometry**; Andre Venter¹, Wisam Alisai¹, Elahe Honarvar¹; ¹Western Michigan University

Wednesday Afternoon, Nicollet D1

INFRARED AND RAMAN SPECTROSCOPY GROUP

Organizer and Presider: Karen Faulds

- 3:50 (730) **Nanoparticle Aggregates Protected in Swellable Polymers as “Smart” Materials for SERS**; Steven Bell¹, Wendy Lee¹, Yen Cheng Ho¹, Ryan Donnelly¹, Colin McCoy¹, Louise Jones¹, Victoria Silversen¹; ¹Queen
- 4:10 (731) **Brilliant Brillouin and Waves. New Approaches in Biomedicine**; Francesca Palombo¹, Ryan S. Edginton¹, C. Peter Winlove¹, Nick Stone¹, Daniele Fioretto²; ¹University of Exeter; ²University of Perugia

TECHNICAL PROGRAM – WEDNESDAY

Orals 3:50 – 5:30 pm

- 4:30 (732) **In-field Detection and Identification of Threat Materials**; Neil Shand¹, Clare Nixon¹, Terry Clark¹; ¹Defence Science and Technology Laboratory, Porton Down, Salisbury, UK
- 4:50 (733) **Raman Spectroscopy for Cytopathology: Label Free Identification of cervical Pre-Cancer**; Fiona Lyng¹; ¹Dublin Institute of Technology
- 5:10 (734) **Towards a Standardized Characterization of Solution Phase Protein Structure Using Raman Optical Activity**; Carl Mensch^{1,2}, Christian Johannessen¹; ¹University of Antwerp; ²University of Ghent

Wednesday Afternoon, Lakeshore A NANO-RAMAN

Organizers and Presiders: Volker Deckert and Francois Lagugne

- 3:50 (735) **Single Molecule Sensitivity in Ambient AFM-based gap-mode TERS**; Marc Chaigneau¹, Dmitry Evplov², Vasily Gavriluk², Andrey Krayev², Ophélie Lancry¹, Vladimir Zhizhimontov², Sergey Saunin²; ¹HORIBA Scientific; ²AIST-NT
- 4:10 (736) **Negative Image Contrast in Tip-Enhanced Raman Spectroscopy**; Andreas Ruediger¹, Julien Plathier¹, Chahinez Dab¹, Jiawei Zhang¹, Gitanjali Kolhatkar¹; ¹INRS-EMT; ²Department of Electrical Engineering, University of Sherbrooke
- 4:30 (737) **Two Mechanisms of Tip Enhancement of Raman Scattering by Protein Aggregates**; Igor Lednev¹, Valentin Sereda¹; ¹University at Albany, SUNY
- 4:50 (738) **TERS of Amyloid beta at Neuronal Spines**; François Lagugné-Labarthe¹, Mohammadali Tabatabaei¹; ¹Western University
- 5:10 (739) **TERS Investigation of Explosive Mixtures**; Volker Deckert^{1,2}, Tanja Deckert-Gaudig¹, Vincent Pichot³, Denis Spitzer³; ¹IPHT; ²University of Jena; ³NS3E «Nanomatériaux pour les Systèmes Sous Sollicitations Extrêmes», UMR ISL/CNRS/UNISTRA, French-German Research Institute of Saint-Louis,

Wednesday Afternoon, Greenway H/I CHEMISTRY IN ART AND ARCHAEOLOGY

Organizer and Presider: Mary Kate Donais

- 3:50 (740) **Modern Imaging Technologies in Historical Studies**; Roger Easton¹, Gregory Heyworth², Keith Knox³, Kenneth Boydston³, Brent Seales⁴; ¹Chester F. Carlson Center for Imaging Science, Rochester Institute of Technology; ²University of Mississippi; ³Early Manuscripts Electronic Library; ⁴University of Kentucky
- 4:10 (741) **Chemical Mapping of Pigments by Visible and Near-Infrared Multispectral Imaging**; Jana Striova¹; ¹INO-CNR, Florence, Italy
- 4:30 (742) **Characterization of Late 17th Century Artists' Pigment from the Childhood home of Henri Toulouse-Lautrec**; Aaron Shugar¹; ¹SUNY - Buffalo State
- 4:50 (743) **Mobile Raman Spectroscopy in Archaeometry**; Peter Vandenabeele¹; ¹Ghent University
- 5:10 (744) **Identification of Pigments in Art Paintings Using Mid IR to THz Spectroscopy**; Sergey Shilov¹; ¹Bruker Optics

Wednesday Afternoon, Greenway E RECENT DEVELOPMENTS ON MASS CYTOMETRIC ANALYSIS

Organizer and Presider: Edgar Arriaga

- 3:50 (745) **Understanding Biological Heterogeneity through Mass Cytometry**; Jennifer Frahm¹, Olga Ornatsky², Dmitry Bandura², Vladimir Baranov², Scott Tanner², Gary Impey², Ashton Breikreutz²; ¹Fluidigm Corporation; ²Fluidigm Canada Inc.
- 4:10 (746) **Organotellurium Probes for Mass Cytometry – Chemical Biology at the Bottom of the Periodic Table**; Mark Nitz¹, Landon Edgar¹, Ravi Vellanki², Brad Wouters², David Headly²; ¹University of Toronto; ²Princess Margaret Cancer Centre
- 4:30 (747) **Reproducibility and Robustness in Mass Cytometry Assays**; Michael Leipold¹, Holden Maecker¹; ¹Stanford University
- 4:50 (748) **Mass Cytometry for the Quantification of Autophagy in Individual Cells**; Heather Grundhofer¹, Edgar Arriaga¹, Michelle Kuhns¹; ¹University of Minnesota
- 5:10 (749) **Single-cell Analysis Reveals Molecular Mechanisms of Leukemia Stem Cell Self-Renewal in a Murine Model of AML**; Zohar Sachs¹, Rebecca LaRue¹, Klara Noble¹, Conner Hansen¹, Ngoc Ha¹, David Largaespada¹; ¹University of Minnesota

Wednesday Afternoon, Lakeshore C BIOANALYTICAL APPLICATIONS OF PLASMONICS

Organizer: Jean-Francois Masson; Presider: Emilie Ringe

- 3:50 (750) **Morphology-based Plasmonic Sensors**; Jennifer Chen¹; ¹York University
- 4:10 (751) **Signal Enhancement at Lipid Bilayer Interface for SPR Imaging**; Quan Cheng¹, Samuel Hinman¹; ¹University of California Riverside
- 4:30 (752) **Challenges and Successes of Plasmonic Sensing in Clinical Samples**; Jean-Francois Masson¹, Alexandra Aubé¹, Julien Breault-Turcot¹, David Charbonneau¹, Joelle Pelletier¹; ¹Université de Montréal
- 4:50 (753) **Novel Bimodal SPRI/SERS Biochip Reader Instrument and Optimization of Associated Plasmonic Substrate Structures**; Michael Canva^{1,2}; ¹CNRS - Inst. d; ²LN2/LCF
- 5:10 (754) **Integration of Quantum Dots with SPRI for Enhanced Sensitivity**; Marinella Sandros^{1,2}; ¹HORIBA Scientific; ²University of North Carolina at Greensboro

TECHNICAL PROGRAM – THURSDAY

Plenary Lectures, *Nicollet B/C*

President: **Matthieu Baudelet**



8:00 am – Lester W. Strock Award
(755) **Spectroscopy as an Important Key for Understanding Martian Paleoclimates**; Raymond Arvidson¹; ¹Washington University in Saint Louis



8:30 am – AES Mid Career Award
(756) **Electrophoretic Cytometry: Targeted Proteomics in Single Cells**; Amy Herr¹; ¹University of California, Berkeley

Orals 9:15 – 10:55 am

Thursday Morning, *Greenway J* **CAPILLARY ELECTROPHORESIS-MASS SPECTROMETRY FOR ULTRASENSITIVE BIOANALYSES**

Organizer and President: Roza Wojcik

- 9:15 (757) **Capillary Zone Electrophoresis-Mass Spectrometry for Ultrasensitive Proteomic Analysis**; Norman Dovichi¹, Liangliang Sun¹, Emily Amenson¹; ¹University of Notre Dame
- 9:35 (758) **Capillary elCapillary Electrophoresis-Mass Spectrometry for the Characterization of Intact Proteoforms**; Govert Somsen¹, Elena Dominguez Vega¹, Jordy van Angeren¹, Klara Petru², Sara Tengattini³, Rob Haselberg¹; ¹Vrije Universiteit Amsterdam; ²Charles University Prague; ³University of Pavia
- 9:55 (759) **Limit of Detection for Capillary Electrophoresis Mass Spectrometry**; David Chen¹; ¹University of British Columbia
- 10:15 (760) **Capabilities and Challenges Using Capillary Electrophoresis-ICP-MS to Characterize Engineered Nanoparticles**; Shi Jiao¹, John Olesik¹; ¹The Ohio State University
- 10:35 (761) **Dielectrophoretic Sorting of Plasmid and Genomic DNA**; Paul Jones¹, Gabe Salmon¹, Alexandra Ros¹; ¹Arizona State University

Thursday Morning, *Greenway A* **DEVELOPMENT AND APPLICATIONS OF ATMOSPHERIC PRESSURE GLOW DISCHARGES**

Organizer and President: Arne Bengtson

- 9:15 (762) **SCGD – a Technique for Online Analysis of Liquids**; David Malmström¹, Peter Lundin¹, Arne Bengtson¹; ¹Swerea KIMAB
- 9:55 (763) **The Solution Cathode Glow Discharge: A Source for Antithetical Applications?**; Steven Ray¹, Jaime Ibanez-Orejas¹; ¹State University of New York at Buffalo
- 10:15 (764) **Method for Flagging Matrix Effects in Solution-Cathode Glow Discharge Emission Spectrometry**; Gina Roesch¹, Andrew Schwartz¹, Gary Hieftje¹; ¹Indiana University
- 10:35 (765) **Optimization of a Dielectric Barrier Discharge for soft Ionization or Excitation of Dissociated Molecules**; Felix David Klute¹, Antje Michels¹, Sebastian Brandt¹, Alexander Schütz¹, Joachim Franzke¹; ¹Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V.

Thursday Morning, *Greenway H/I* **LESTER STROCK AWARD SYMPOSIUM HONORING RAYMOND ARVIDSON**

Organizer and President: Raymond Arvidson

- 9:15 (766) **Mercury: Reflectance Spectroscopy of a Reduced, Volatile-rich Planet**; Scott Murchie¹; ¹Applied Physics Laboratory
- 9:35 (767) **Europa: Exploring an Ocean World Using Reflectance Spectroscopy**; Diana Blaney¹; ¹NASA Jet Propulsion Laboratory, California Institute of Technology

- 9:55 (768) **Mapping Mineralogy at Gale Crater with Reflectance Spectroscopy**; Abigail Fraeman¹; ¹Jet Propulsion Laboratory, California Institute of Technology
- 10:15 (769) **Martian Surface Mineralogy from Rovers with Spirit, Opportunity, and Curiosity**; Richard Morris¹; ¹NASA Johnson Space Center
- 10:35 (770) **Mars: Early Aqueous Alteration from Orbital Infrared and *in situ* Spectroscopies**; Bethany Ehlmann^{1,2}; ¹Division of Geological & Planetary Sciences, California Institute of Technology; ²Jet Propulsion Laboratory, California Institute of Technology

Thursday Morning, *Greenway G* **NOVEL BIOMEDICAL TECHNOLOGIES**

Organizer: Bradford Clay; President: Karen Esmonde-White

- 9:15 (771) **Raman Spectroscopy for Bone Quality Assessment: From Bench to Bedside**; Xiaohong Bi¹, Hao Ding¹; ¹University of Texas Health Science Center at Houston
- 9:35 (772) **Sensing the Body through Garment-Integrated Technologies**; Lucy Dunne¹; ¹University of Minnesota
- 9:55 (773) **Multiplex Measurements of Glucose, Lactate and Antibody through Single-Use Biocontainer Films Using Raman Spectroscopy**; Mekhala Spencer¹, Yun Xu¹, Katherine A. Hollywood^{1,2}, Lorna Ashton^{1,4}, John Welsh³, Peter Levison³, Alan Dickson², Royston Goodacre¹; ¹Manchester Institute of Biotechnology, University of Manchester; ²Faculty of Life Sciences, University of Manchester; ³Pall Life Sciences, Portsmouth; ⁴Dept of Chemistry, Lancaster University
- 10:15 (774) **Molecular Imaging of Chemically Communicating Bacterial Communities of the Opportunistic Human Pathogen *Pseudomonas aeruginosa***; Nameera Baig¹, Sage Dunham², Sneha Polisetti¹, Nydia Morales-Soto¹, Joshua Shrout¹, Jonathan Sweedler², Paul Bohn¹; ¹University of Notre Dame; ²University of Illinois at Urbana-Champaign
- 10:35 (775) **The Role of Lipopolysaccharides in the Toxicity of Nanoparticles to Gram-negative Bacteria**; Joseph Buchman¹, Emily Caudill², Ariane Vartanian³, Lisa Jacob³, Xi Zhang³, Catherine Murphy³, Joel Pedersen², Christy Haynes¹; ¹University of Minnesota; ²University of Wisconsin-Madison; ³University of Illinois at Urbana-Champaign

Thursday Morning, *Nicollet D2/D3* **METABOLITE PATTERN RECOGNITION: THE KEY TO AUTHENTICATION**

Organizers: Pei Chen and Mengliang Zhang; President: Pei Chen

- 9:15 (776) **Validating Multivariate Methods for Pattern Recognition**; Richard Brereton¹; ¹University of Bristol
- 9:55 (777) **Flow-injection Mass Spectrometric Fingerprinting - A Powerful Tool for Authentication Plant Materials**; Pei Chen¹, Jianghao Sun¹, James M. Harnly¹; ¹FCMDL, BHNRC, ARS, USDA

TECHNICAL PROGRAM – THURSDAY

Orals 9:15 – 10:55 am

- 10:15 (778) **Instantaneous Determination of Food Authenticity by Rapid Evaporative Ionisation Mass Spectrometry**; Sara Stead¹, Emrys Jones¹, Mike Wilson¹, Julia Balog¹, Zoltan Takats², Lorraine Kay¹; ¹Waters Corporation; ²Imperial College London
- 10:35 (779) **A Generic Tool for Flow Injection Mass Spectrometric Fingerprinting**; Mengliang Zhang¹, Jianghao Sun¹, Pei Chen¹; ¹Food Composition and Methods Development Laboratory, Beltsville Human Nutrition Research Center, Agricultural Research Service, U.S. Department of Agriculture, Beltsville, MD

Thursday Morning, Lakeshore B TWO-DIMENSIONAL CORRELATION ANALYSIS - I

Organizer: Isao Noda; Presider: Young Mee Jung

- 9:15 (780) **Evolution of Two-Dimensional Correlation Spectroscopy Techniques**; Isao Noda¹; ¹University of Delaware
- 9:35 (781) **Comparability is Assessed for Monoclonal Antibody Fragments Using 2D IR and Co-distribution correlation Spectroscopy**; Belinda Pastrana¹; ¹Protein Dynamic Solutions, LLC
- 9:55 (782) **A Method to Estimate the Strength of Intermolecular Interaction between Two Solutes Dissolved in the Same Solutions Based on the DAOSD Approach**; Yizhuang Xu¹, Ran Guo¹, Anqi He¹, Jing Chen¹, Zhanlan Yang¹, Isao Noda¹, Jinguang Wu¹; ¹Peking University
- 10:15 (783) **2D Chemiluminescence Correlation Spectroscopy for Polymers**; Hideyuki Shinzawa¹, Junji Mizukado²; ¹Hideyuki Shinzawa; ²Junji Mizukado
- 10:35 (784) **Analysis of Thin Films on Silicon by p-Polarized Multiple Angle Incidence Resolution Spectrometry (pMAIRS)**; David Drapcho¹, Richard Murdey², Nobutaka Shioya², Takeshi Hasegawa²; ¹Thermo Fisher Scientific; ²Kyoto University, Institute for Chemical Research

Thursday Morning, Greenway B/C MASS SPECTROMETRY-BASED METABOLOMICS

Organizer and Presider: Erin Carlson

- 9:15 (785) **A Global View of Streptomyces coelicolor: Transcriptomic, Proteomic, and Metabolomic Analysis of the Life Cycle of a Model Antibiotic-Producing Organism**; Andrew Johnson², Erin Carlson¹; ¹University of Minnesota; ²Indiana University
- 9:35 (786) **Mapping Specialized Bacterial Metabolite Pathways via Pathway-Targeted Molecular Networking**; Jason Crawford¹, Hyun Bong Park¹, Corey Perez¹; ¹Yale University
- 9:55 (787) **Metabolomics and Marine Bacteria: Tools to Stimulate Antibiotic Discovery**; Tim Bugni¹, Fan Zhang¹, Navid Adnani¹, Doug Braun¹, Chris Thomas¹, Yan Zhang¹; ¹University of Wisconsin-Madison
- 10:15 (788) **Exploring the Master Regulators of Microbial Behavior**; Erin Carlson¹; ¹University of Minnesota
- 10:35 (789) **Metabolomic Tracking of Cell Differentiation in the Cleavage-stage Xenopus Embryo**; Peter Nemes¹, Erika P. Portero¹, Rosemary M. Onjiko¹, Sally A. Moody²; ¹Department of Chemistry, The George Washington University; ²Department of Anatomy and Regenerative Bioogy, The George Washington University

Thursday Morning, Lakeshore C TOPICS IN NANOTECHNOLOGY

Organizer: Alexandra Ros; Presider: Rusen Yang

- 9:15 (790) **Raman Spectroscopy of Optical Phonons Confined in TiO₂ Nanopowders**; Sergey Mamedov¹; ¹Horiba Scientific
- 9:35 (791) **Synthesis and Characterization of Strained GexSn1-x Alloy Nanocrystals and IV/II-VI Core-Shell Nanocrystals Showing Enhanced Photoluminescence**; Brett W. Boote^{1,2}, Long Men^{1,2}, Ujjal Bhattacharjee^{1,2}, Jacob W. Petrich^{1,2}, Javier Vela^{1,2}, Emily A. Smith^{1,2}; ¹Iowa State University; ²Ames Laboratory
- 9:55 (792) **Mesoporous Silica-Coated Nanoparticles as a SERS Sensing Platform**; Zhe Gao¹, Nathan Burrows, Nicholas A. Valley, George C. Schatz, Catherine J. Murphy, Christy L. Haynes¹; ¹University of Minnesota
- 10:15 (793) **Highly Fluorescent Carbon Nitride Nanoparticles for Optosensing of Mercury Ions and Bisphenol A**; Yong-Ill Lee¹, Bui The Huy¹, Nguyen Thi Thu Thuy¹; ¹Changwon National University
- 10:35 (794) **Mechanisms of Reduction of Silver Metal Ion to Silver Nanoparticles by atmospheric Pressure Plasma Jets**; Urvashi Gangal¹, V.S. Santosh K Kondeti¹, Peter Bruggeman¹; ¹Department of Mechanical Engineering, University of Minnesota

Thursday Morning, Greenway E PAT: FLOW CHEMISTRY AND CONTINUOUS MANUFACTURING MONITORING

Organizer and Presider: Jim Rydzak

- 9:15 (795) **Developing Process Control for Flow Chemical Reactions: Applications of Sampling, Sensing and Data Handling**; Brian Marquardt^{1,2}, Mark Weller¹, Natasha Hippler¹, Dave Veltkamp¹, Michael Roberto³; ¹MarqMetrix Inc.; ²University of Washington APL; ³Infometrix, Inc.
- 9:35 (796) **Streamlining Pharmaceutical Processes into Continuous Operations**; Frank Gupton¹; ¹Virginia Commonwealth University
- 9:55 (797) **In situ Analytics: A Technological Shift in Continuous Processing**; Dominique Hebrault¹; ¹Mettler Toledo Autochem
- 10:15 (798) **Developing Chemometric Models to Support Continuous Drug Product Manufacturing**; John-David McElderry¹, Chunsheng Cai¹, Justin Pritchard¹, Kelly Swinney¹; ¹Vertex Pharmaceuticals
- 10:35 (799) **Modeling and Monitoring of Batch Processes in Relative Time**; Heather Brooke¹; ¹CAMO Software

Thursday Morning, Nicollet B/C CHIRALITY IN PHARMA

Organizer: Rina Dukor; Presider: Don Pivonka

- 9:15 (800) **Automating Workflow to Determine Absolute Configuration by Integrating VCD, OR, CD Spectroscopy with QM Calculations**; Oliver McConnell¹, Jano Jusuf¹, Viral Vyas¹, Atsu Apedo¹, Yan He¹, Daniel Cheney¹, Malcolm Davis¹; ¹Bristol-Myers Squibb
- 9:35 (801) **Chiral Separation Mechanism on Macrocyclic Antibiotics Stationary Phases: a Spectroscopic and Chromatographic Study**; Nelu Grinberg¹, Ling Wu¹, Shengli Ma⁴, Heewon Lee¹, Sherry Shen³, Frank Roschangar¹, Chris Senanayake¹, David Bell²; ¹Boehringer Ingelheim Pharmaceuticals; ²Millipore Sigma; ³FDA; ⁴Genetech

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

- 9:55 (802) **Application of Fourier Transform Molecular Rotational Resonance Spectroscopy for Chiral Purity Characterization**; Linda H. Kidder¹, Justin L. Neill¹, Matthew T. Muckle¹, Brent J. Harris¹, Brooks H. Pate²; ¹BrightSpec, Inc.; ²University of Virginia
- 10:15 (803) **Characterization of Ciprofloxacin Tablets Using Near-Infrared Spectroscopy and Chemometric Modeling**; Nathan Fuenffinger¹, Connie Gryniewicz-Ruzicka¹; ¹FDA, Division of Pharmaceutical Analysis, St. Louis, MO
- 10:35 (804) **Analytical Applications of Copolymerized Silica Nanoparticles**; Gabor Patonay¹, Maged Henary¹, Walid Abdelwahab¹, Gala Chapman¹; ¹Georgia State University

Thursday Morning, Nicollet D1
BIOMEDICAL RAMAN SPECTROSCOPY (CLIRSPEC)
Organizer and Presider: Nick Stone

- 9:15 (805) **Integrated Multimodal Spectral Imaging for Margin Assessment during Breast Conserving Surgery**; Ioan Notingher¹; ¹University of Nottingham
- 9:35 (806) **Tracking Pregnancy and Labor *in vivo* with Raman Spectroscopy**; Anita Mahadevan-Jansen¹, Christine O'Brien¹, Katherine Cochran¹, Kelly Bennett², J Michael Newton²; ¹Vanderbilt University; ²Vanderbilt University Medical Center
- 9:55 (807) **Development of SERS Active Photothermal and Magnetothermal Nanoparticles for the Diagnosis and Therapeutic Treatment of Atherosclerotic Plaques**; Samuel Mabbott¹, Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde
- 10:15 (808) **Keeping Your Hair Up: Understanding the Behaviour of a Complex Keratin Based Biomaterial Using Raman Spectroscopy**; Paul Pudney¹, David David Tiemessen¹, Christopher Marsh¹; ¹Unilever Discover
- 10:35 (809) **Species of Interest Recovery in Raman Spectra of Heterotopic Ossification**; Katherin Cilwa^{1,2}, Ammar Qureshi^{1,2}; ¹Naval Medical Research Center, Regenerative Medicine; ²The Henry M. Jackson Foundation for the Advancement of Military Medicine

Thursday Morning, Lakeshore A
BIO RAMAN
Organizer: Pavel Matousek; Presider: Bhavya Sharma

- 9:15 (810) ***In vitro* Monitoring of Adverse Outcomes Pathways in Aminated Nanoparticle Exposed Cells by Using Raman Spectroscopy**; Esen Efeoglu^{1,2}, Alan

- Casey^{1,2}, Hugh J. Byrne^{1,2}; ¹Dublin Institute of Technology; ²Focas Research Institute
- 9:35 (811) **Monitoring Isoxazole Induced Differentiation in Pancreatic Cell Lines Using Raman Spectroscopy**; Katherine Hollywood¹, Saba Khan¹, Karen Cosgrove¹, Mark Dunne¹, Nicholas Lockyer¹, Alex Henderson¹, Alan Dickson¹, Roy Goodacre¹; ¹Faculty of Life Sciences, University of Manchester
- 9:55 (812) **Confocal Raman Microscopy for Characterizing Interactions of Cytochrome C with Cardiolipin-Containing Membranes of Individual, Optically-Trapped Phospholipid Vesicles**; Jay Kitt¹, David Bryce¹, Joel Harris¹; ¹University of Utah
- 10:15 (813) **The Development and Applications of Surface Enhanced Spatially Offset Raman Spectroscopy**; Fay Nicolson¹, Neil Shand², Duncan Graham¹, Karen Faulds¹; ¹University of Strathclyde; ²Defence Science and Technology Laboratory
- 10:35 (814) **Encapsulated SERS Nanosensors – Fibre-based pH Sensing**; Holly Fleming¹, Sarah McLaughtrie¹, Mike Tanner², Debaditya Choudhury², Colin Campbell¹, Mark Bradley¹; ¹University of Edinburgh; ²Heriot Watt University

Thursday Morning, Greenway D
APPLICATION OF PHOTOELECTRON SPECTROSCOPY TECHNIQUES TO ANALYSIS OF NANOMATERIALS AND DEVICES
Organizer and Presider: Franklin Tao

- 9:15 (815) **Membrane Based Approach in Ambient Pressure Photoelectron Spectromicroscopy**; Andrei Kolmakov¹; ¹Center for Nanoscale Science and Technology, NIST
- 9:55 (816) **Operando XPS Studies of Electrocatalysis**; Hirohito Ogasawara¹; ¹SLAC National Accelerator Laboratory
- 10:15 (817) **Bridging the Gap – *In situ* Study of Surface Chemistry Using Ambient Pressure X-ray Photoelectron Spectroscopy**; Iradwikanari Waluyo¹; ¹National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY
- 10:35 (818) **Chemically Modified Antibodies to Form Stable Gold Nanoparticle Conjugates for Use in Light Scattering Immunoassays**; Jeremy Driskell¹, Seth Filbrun¹, Francis Lovato¹, Alexandra Mandl¹; ¹Illinois State University

Thursday Poster Session
11:00 am – 12:00 pm
Nicollet A

All Thursday posters should be put up between 9:00 – 10:00 am and removed by 4:30 pm

Electrokinetics - AES Posters

Poster Board #1

- (819) **Free solution Protein Separation via Microchip Electrophoretic Exclusion**; Fanyi Zhu¹, Mark Hayes¹; ¹Arizona State University

Poster Board #2

- (820) **The Evaluation of Cationic Latex Nanoparticles as Pseudostationary Phases for Electrokinetic Chromatography**; Julie McGettrick¹, Chris Palmer¹, Adam Sutton², Emily Hilder²; ¹University of Montana; ²University of South Australia

Poster Board #3

- (821) **Exploring the Role and Impact of Faradaic Reactions on Hemolysis in Non-Uniform AC Electric Fields**; Sanaz Habibi¹, Hector Moncada-Hernandez¹, Adrienne Minerick¹; ¹Department of Chemical Engineering, Michigan Technological University

Poster Board #4

- (822) **Quantitative Comparison of a Laser and Light-Emitting Diode for Fluorescence Detection with Capillary Electrophoresis**; Thu Nguyen¹, S. Douglass Gilman¹; ¹Louisiana State University

Poster Board #5

- (823) **Fluoride Treatment of Silica Capillary Surfaces**; Christopher Harrison¹, Charles Lumba¹; ¹San Diego State University

TECHNICAL PROGRAM – THURSDAY

Posters 11:00 am – 12:00 pm

Poster Board #6

(824) Separation of Complex Biological Mixtures Using Asymmetric Posts and Electric Fields; Mario Saucedo-Espinosa¹, Blanca Lapizco-Encinas¹; ¹Rochester Institute of Technology

Poster Board #7

(825) A Proposed cDEP Device Design for Improved Device Reusability and Range of Applied Voltage; Cynthia Hanson¹, Elizabeth Vargis¹; ¹Utah State University

Atomic Spectroscopy Posters

Poster Board #8

(826) Pharmaceutical Atomic Spectroscopy: Not Just the Metals Lab; Lydia Breckenridge¹; ¹Bristol-Myers Squibb

Poster Board #9

(827) Comprehensive Laser Plasma Characterization Through the Combination of Emission and Absorption Spectroscopy; Nicole LaHaye¹, Sivanandan Harilal¹, Mark Phillips¹; ¹Pacific Northwest National Laboratory

Poster Board #10

(828) Analysis of Cedar from Western North Carolina for Aluminum, Calcium, and Magnesium; David Butcher¹; ¹Western Carolina University

Poster Board #11

(829) Determination of Inorganic Arsenic by Off-Line Solid Phase Extraction - Hydride Generation - Microwave Plasma Atomic Emission Spectrometry (HG-MP-AES); Moisés Guerrero Esperanza¹, Katarzyna Wrobel¹, Eunice Yáñez Barrientos¹, Alma Rosa Corrales Escobosa¹, Francisco Javier Acevedo Aguilar¹, Kazimierz Wrobel¹; ¹University of Guanajuato

Poster Board #12

(830) Bioavailability and Quantification of Heavy Metals in Consumable Fish of Lakes and Local Supermarkets by Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES); M Abdul Mottaleb¹, Daniel R. Johnson¹, Musavvir Arafat Mottaleb¹, Kurt Nagel¹; ¹Northwest Missouri State University

Poster Board #13

(831) Performance Analysis of Regularized MLM Hyperspectral Imaging for Mars Reconnaissance Orbiter CRISM Along-Track Oversampled data; Linyun He¹, Daniel Politte¹, Joseph O¹, Raymond Arvidson²; ¹Department of Electrical and Systems Engineering, Washington University in Saint Louis; ²Department of Earth and Planetary Sciences, Washington University in Saint Louis

Poster Board #14

(832) Development of an Innovative Interface for the Analysis of Gaseous Compounds Using Pulsed Radiofrequency Glow Discharge Time of Flight Mass Spectrometry; Jorge Pisonero¹, Jonatan Fandiño¹, Marcos Bouzas², Alfredo Sanz-Medel², Nerea Bodel¹; ¹Department of Physics, University of Oviedo; ²Department of Physical and Analytical Chemistry, University of Oviedo

Poster Board #15

(833) Spectroscopy of Laser-Produced Plasmas for Nuclear Forensics and Verification; Kyle Hartig^{1,2}, Nicole Lahaye², Sivanandan Harilal², Mark Phillips², Igor Jovanovic³; ¹The Pennsylvania State University; ²Pacific Northwest National Laboratory; ³University of Michigan

Poster Board #16

(834) High-resolution Continuum Source Graphite Furnace Atomic Absorption Spectrometry for the Monitoring of Au Nanoparticles; Esperanza Garcia-Ruiz¹, Raul Garde¹, Martin Resano¹; ¹Universidad de Zaragoza

Poster Board #17

(835) Investigation of Ambient Gas Heating and Hydrodynamics of Laser-Induced Sparks; Patrick J Skrodzki^{1,2}, Alex Miloshevsky¹, Brian E Brumfield¹, Mark C Phillips¹, Sivanandan S Harilal¹; ¹Pacific Northwest National Laboratory, Richland WA; ²University of Michigan, Ann Arbor MI

Poster Board #18

(836) Use of CaF Molecular Emission Bands for Improving the F Quantification Capabilities in Atmospheric Air LIBS; Jorge Pisonero¹, Cesar Alvarez-Llamas¹, Nerea Bodel¹; ¹University of Oviedo

Poster Board #19

(837) Development of a XRF Detection Unit for Capillary Electrophoresis; Inger Marie Tyssebotn¹, Ursula Fittschen¹; ¹Department of Chemistry, Washington State University

Biomedical and Bioanalytical Sciences Posters

Poster Board #20

(838) Discovery of G-quadruplex Aptamers Using a Genome-Inspired Reverse Selection Approach; Kathleen Morrissey¹, Christina Albanese¹, Linda B. McGown¹; ¹Rensselaer Polytechnic Institute

Poster Board #21

(839) Longitudinal Determination of Vitamin Concentrations in Tears and Blood Serum of Infants and Parents; Maryam Khaksari¹, Lynn Mazzoleni¹, Adrienne Minerick¹; ¹Michigan Technological University

Poster Board #22

(840) A Novel Growth-Based Bacterial Viability Assay for High-Throughput Nanoparticle Toxicity Screening; Tian (Autumn) Qiu¹, Thu Nguyen², Hilena Frew², Ariane Vartanian³, Lisa Jacob³, Catherine Murphy³, Z. Vivian Feng², Christy Haynes¹; ¹University of Minnesota; ²Augsburg College; ³University of Illinois at Urbana-Champaign; ⁴

Poster Board #23

(841) Electrochemical Sensors for the Rapid Detection of *Pseudomonas aeruginosa* in Human Wound Exudate; Edgar Goluch¹, Hunter Sismaet¹, Anirban Banerjee², Sean McNish², Yongwook Choi³, Manolito Torralba³, Sarah Lucas³, Agnes Chan³, Victoria Shanmugam²; ¹Northeastern University; ²George Washington University; ³J Craig Venter Institute

Poster Board #24

(842) Dual Functioning Reporter+Probe Biosensors to Visualize Absence or Presence of microRNA; Nicholas E. Larkey¹, Sean M. Burrows¹; ¹Oregon State University

Poster Board #25

(843) Influence of Experimental Conditions on Equilibrium Constant Determination for the Thrombin-Binding DNA Aptamers: Benchmarking the Model System; Rebecca Whelan¹, Kepler Mears¹, Daniel Markus¹; ¹Oberlin College

Poster Board #26

(844) Toxicity of Chromium in Zebrafish Embryos; Jacqueline Arroyo¹, Rodney Dale¹, Mark Malham¹, Martina Schmeline¹; ¹Loyola University Chicago

TECHNICAL PROGRAM – THURSDAY

Posters 11:00 am – 12:00 pm

Poster Board #27

(845) **Identification of Proteins in Tetrahymena thermophila Using LC-MS/MS**; Mary Beth Dahl¹, Zach Turner¹, Douglas Beussman¹; ¹St. Olaf College

Poster Board #28

(846) **Enhancing the Spatial Resolution of far-field FTIR Spectromicroscopy via Laterally Structured Illumination**; Liang Chen¹, Giovanni Birada^{1,2}, Antoine Masson¹, Hans Bechtel¹, Hoi-Ying Holman¹; ¹Lawrence Berkeley National Laboratory, University of California, Berkeley, CA; ²Elettra – Sincrotrone Trieste, Basovizza, Trieste, Italy

Poster Board #29

(847) **Co-Localized Excitation-Emission Resolution (CLEER) of Multiple Fluorophores**; C. Kyle Almlie¹, Sean M. Burrows¹; ¹Oregon State University, Corvallis, OR

Poster Board #30

(848) **A Method to Automate ABCDE Law Applied in Melanocytic Nevii**; Jorge Castro-Ramos¹, Adriana May-Salazar², Diana Antonieta Sen-Salinas¹, Francisco Gutiérrez-Delgado³, Reimer Romero- Hernández⁴; ¹INAOE, Instituto Nacional de Astrofísica Óptica y Electrónica; ²IMSS, Instituto Mexicano del Seguro Social; ³CEPREC, Centro para la prevención del cáncer; ⁴Universidad de Carabobo. Departamento de Física, Facultad de Ciencias y Tecnología

Chromatography Posters

Poster Board #31

(849) **Using Copper Oxide as an Interface for HPLC-FTIR Analysis**; Yizhuang Xu¹, Yan LI¹, Ran Guo¹, Yaping Huang¹, Jing Chen¹, Isao Noda¹, Jinguang Wu¹; ¹Peking University

Poster Board #32

(850) **Advantages and Challenges Associated with Automated Sample Preparation for Arsenic Speciation Analytical Method**; Rebecca Hunt¹, Nolan Hilliard¹, Cynthia Ward¹, Kathleen Caldwell¹, Robert Jones¹; ¹Centers for Disease Control and Prevention

Poster Board #33

(851) **Determination of Dimethyl Trisulfide in Rabbit Blood Using Stir Bar Sorptive Extraction Gas Chromatography-Mass Spectrometry**; Erica Manandhar¹, Ilona Petrikovics², Gary Rockwood³, Brian Logue¹; ¹South Dakota State University; ²Sam Houston State University; ³US Army Medical Research Institute of Chemical Defense

Poster Board #34

(852) **Analysis of Chemical Markers in Adulterated Fuels Using a Transportable Ultrafast Micro Gas Chromatograph**; Jeremy Reyes¹, Winniford Bill¹, Jazdzewski Brian², Smith Warren², Asif Zahid², Crandall John³, Roques Ned³, Parker Spencer³, Perron Joe³, Holliday Matt³; ¹Analytical Sciences, The Dow Chemical Company, Freeport, TX; ²Dow Industrial Solutions, The Dow Chemical Company, Freeport, TX; ³Falcon Analytical Systems & Technology, LLC, Lewisburg, WV

Environmental and Oceanographic Posters

Poster Board #35

(853) **Arduino Controlled Synchronous Light Scattering by Phytoplankton for use in a Multivariate Optical Computing Instrument**; Stefan Faulkner¹, Camron Rekully¹, Shawna Tazik¹, Tim Shaw¹, Tammi Richardson², Michael Myrick¹; ¹University of South Carolina

Department of Chemistry and Biochemistry; ²University of South Carolina Department of Biological Sciences

Poster Board #36

(854) **Taxonomic Classification of Phytoplankton with Multivariate Optical Computing: Instrument Improvements and Community Characterization Strategies**; Cameron Rekully¹, Stefan Faulkner¹, Shawna Tazik¹, Tammi Richardson², Timothy Shaw¹, Michael Myrick¹; ¹University of South Carolina Department of Chemistry and Biochemistry; ²University of South Carolina Department of Biological Sciences

Poster Board #37

(855) **Verifying Sub-sampling and Preparation of Laboratory Samples for the Elemental Analysis of Grains**; Anja Richter¹; ¹Canadian Grain Commission

Poster Board #38

(856) **pH Quantification Capability of Solution-Phase Tetrakis(4-carboxyphenyl)porphyrin**; Matthew Clark¹, Anselm Omoike¹; ¹University of South Carolina- Upstate

Poster Board #39

(857) **Degradation of Dimethyl Trisulfide Using Slow Releasing Manganese Oxide Coated Potassium Permanganate Particles**; Dustin Harmon, Anselm Omoike¹; ¹University of South Carolina- Upstate

Poster Board #40

(858) **Trace Aqueous Lead Sensing Using Silicon-on-Insulator Ring Resonators**; Xiaowei Wu¹, Hao Chen¹, Sogol Borjian¹, John Saunders¹, Cathleen M. Crudden¹, Hans-Peter Loock¹, Dan-xia Xu²; ¹Department of Chemistry, Queen's University, Kingston, ON; ²Information and Communication Technologies, National Research Council Canada, Ottawa, Ontario, Canada

Poster Board #41

(859) **Study of BPA Removal from Water in the Presence of Normal Organic Matter Using Magnetic Nanoparticles Coated with Manganese Oxide**; James Blume¹, Anselm Omoike¹; ¹University of South Carolina Upstate

Poster Board #42

(860) **Novel Materials from Clay and Functionalized Clay Nanoparticles: Application in Remediation of Lead, Cadmium and Pentachlorophenol from Water**; Wanyika Harrison¹, David Mutegi Marikah¹, Erastus Gatebe²; ¹Jomo Kenyatta University of Agriculture and Technology; ²Kenya Industrial Research and Development Institute

LIBS Posters

Poster Board #43

(861) **Quantitative Analysis of Laser Induced Breakdown Spectroscopy of Rock Powders Doped with Cr, Mn, Ni, Zn and Co**; Kate Lepore¹, Caleb Fassett¹, Elly Breves¹, Stephen Giguere², Thomas Boucher², J. Michael Rhodes², Michael Vollinger², Chloe Anderson³, Richard Murray³, M. Darby Dyar¹; ¹Mt. Holyoke College; ²University of Massachusetts Amherst; ³Boston University

Poster Board #44

(862) **Baseline Removal versus Feature Selection in LIBS**; Darby Dyar¹, Stephen Giguere², CJ Carey², Thomas Boucher², Ian Gemp²; ¹Mount Holyoke College; ²University of Massachusetts

TECHNICAL PROGRAM – THURSDAY

Posters 11:00 am – 12:00 pm

Poster Board #45

(863) **Self-Absorption Study of Copper Resonant Lines in Laser-Induced Plasmas Using a Photomultiplier Tube;** Yangting Fu^{1,2}, Richard Warren³, Tobias Guenther¹, Willis Jones¹, Benjamin Smith¹, Nicolo Omenetto¹;
¹Department of Chemistry, University of Florida; ²State Key Lab of Power System, Tsinghua University;
³Environmental and Bioassay Laboratory, Savannah River Site

Poster Board #46

(864) **Detection of Chlorine in Concrete Using Laser Ablation and CaCl Emission in Ambient Air and He Environments;** Will Jones¹, Tobias Guenther¹, Yangting Fu^{1,2}, Benjamin Smith¹, Nicolo Omenetto¹; ¹Department of Chemistry, University of Florida; ²State Key Lab of Power System, Tsinghua University

Poster Board #47

(865) **Pseudocontinuum Source Atomic Absorption Spectroscopy in Transient Plasmas;** Jonathan Merten¹, Alex Goff¹; ¹Arkansas State University

Poster Board #48

(866) **LIBS analysis of Soils from New Caledonia to Evaluate the Environmental Impact of the Extraction of Nickel Ore;** Bruno Bousquet¹, Julian Guezencoc¹, Camille Pasquet², Peggy Gunkel-Grillon², Lena Bassel¹;
¹University of Bordeaux; ²University of New Caledonia

Poster Board #49

(867) **Effects of Laser Wavelength on Aluminum Plasma in Transverse Magnetic Fields;** Payson Dieffenbach¹, Carolyn Borkowski¹, Michael Marino¹, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Purdue University

Poster Board #50

(868) **Spot Size Effects on Plume Hydrodynamics of Laser-Produced Plasmas in Transverse Magnetic Fields;** Payson Dieffenbach¹, Carolyn Borkowski¹, Michael Marino¹, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Purdue University

Poster Board #51

(869) **Ion Emission Mechanisms during Ultrashort Laser Ablation of Solid Targets;** Ahmed Elsieid¹, Nicholas Termini¹, Prasoon Diwakar¹, Ahmed Hassanein¹;
¹Center for Materials under Extreme Environment (CMUXE), School of Nuclear Engineering Purdue University, West Lafayette, IN

Poster Board #52

(870) **Optimizing Spark- and Laser-Induced Breakdown Spectroscopy in Ambient Gas Conditions;** Carolyn Borkowski¹, Payson Dieffenbach¹, Arianna Avellan^{1,2}, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center for Materials Under eXtreme Environment, School of Nuclear Engineering, Purdue University, West Lafayette, IN; ²Department of Materials Science and Engineering, College of Engineering, University of Maryland, College Park, MD

Poster Board #53

(871) **Plume Propagation and Emission Dynamics of Two Colliding Plasmas;** John Oliver¹, Tatyana Sizyuk¹, Prasoon Diwakar¹, Ahmed Hassanein¹; ¹Center for Materials Under eXtreme Environment (CMUXE), School of Nuclear Engineering, Purdue University, West Lafayette, IN

Poster Board #54

(872) **Determination of the LOD Using PLSR of 10B & 11B Boric Acid Mixtures via Laser Ablation Molecular Isotopic Spectroscopy (LAMIS);** Candace Harris¹, Codjo A. Akpovo¹, Lewis Johnson¹, Luisa Profeta¹;
¹Florida Agriculture and Mechanic University; ²Alakai Defense Systems Inc.

Microscopy and Materials Characterization Posters

Poster Board #55

(873) **Monitoring the Catalyzed Reduction of Nitrite with Fluorescence Techniques;** Anthony Stender¹, Emilie Ringe¹; ¹Rice University

Poster Board #56

(874) **Interactive Simulation of Broadband Imaging Using Mie Theory on Symmetric Samples;** Sebastian Berisha¹, P. Scott Carney², David Mayerich¹; ¹University of Houston; ²University of Illinois at Urbana-Champaign

Poster Board #57

(875) **Multiresonant Coherent Multidimensional Spectroscopy in Semiconductor Systems;** Blaise Thompson¹, Daniel Kohler¹, Kyle Czech¹, John Wright¹;
¹University of Wisconsin-Madison

Poster Board #58

(876) **Linear Photothermal Imaging in the Mid-Infrared with Sub-Diffraction Limited Resolution;** Atcha Totachawattana¹, Casey A. Biederman¹, Karl Muench¹, Mi K. Hong³, Shyamsunder Erramilli^{3,4}, Michelle Y. Sander^{1,2}; ¹Department of Electrical and Computer Engineering, Photonics Center, Boston University; ²Division of Materials Science and Engineering, Boston University; ³Department of Physics, Boston University; ⁴Department of Biomedical Engineering, Boston University

Process Analytical Technology Posters

Poster Board #59

(877) **High Throughput Virtual Slit (HTVS) Technology's Performance Impact on Raman Limit of Detection Applications;** Jeremy Linoski¹, Art Hamfeldt¹, Bradford Behr¹, Sharon Deram¹; ¹Tornado Spectral Systems

Poster Board #60

(878) **Using PLS-DA to Evaluate the Quality of Spore Inoculum to Optimize Biotechnological Process Control;** Karin Wieland¹, Cosima Koch¹, Julia Kuligowski², Johannes Ofner¹, Daniela Ehgartner³, Christoph Herwig³, Bernhard Lendl¹; ¹Institute of Chemical Technologies and Analytics; ²Health Research Institute Hospital La Fe; ³Institute of Chemical Engineering

Poster Board #61

(879) **Ultrasound-Enhanced In-line Raman Sensing of Solid Samples in Liquid Matrices;** Karin Wieland¹, Stefan Tauber¹, Stefan Radel², Bernhard Lendl¹; ¹Institute of Chemical Technologies and Analytics; ²Institute of Applied Physics

Pharmaceutical Analysis Posters

Poster Board #62

(880) **Screening of Kratom Products for Mitragynine Using Ion Mobility Spectrometry;** Connie Gryniiewicz-Ruzicka¹, Nathan Fuenffinger¹, Melissa Ritchie¹, Ashley Gucinski-Ruth¹; ¹US Food and Drug Administration

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

Poster Board #63

(881) **Efficient Near-infrared Calibration Set Development for Quantitative Analysis of Tablets Containing Multiple APIs**; Md Anik Alam^{1,2}, James Drennen^{1,2}, Carl Anderson^{1,2}; ¹Graduate School of Pharmaceutical Science, Duquesne University, Pittsburgh, PA; ²Duquesne University Center for Pharmaceutical Technology, Pittsburgh, PA

Poster Board #64

(882) **Melamine Detection Using Surface Enhanced Raman Spectroscopy (SERS) & 1064 nm Handheld Raman Spectrophotometer**; Joseph Stoltz¹, Jonas Sacros¹; ¹Pfizer Inc.

Poster Board #65

(883) **Develop an Effective Quality Control Approach to Determine Polymorph Content in a Pharmaceutical Formulation Using Raman Spectroscopy**; Hanzhou Feng¹, Yi Li¹, James Drennen^{1,2}, Carl Anderson^{1,2}; ¹Duquesne University, Graduate School of Pharmaceutical Sciences; ²Duquesne Center for Pharmaceutical Technology

Thursday Afternoon, Greenway H/I
AES MID-CAREER AWARD SYMPOSIUM HONORING
AMY HERR

Organizer and Presider: Rodrigo Martinez-Duarte

- 1:20 (884) **Quantitative Biology with Single cells and Single Animals**; Hang Lu¹; ¹Georgia Institute of Technology
- 1:40 (885) **Droplet Microfluidic Platform for High Throughput Enzyme Screening and Synthetic Biology Applications**; Anup Singh¹; ¹Sandia National Laboratories; ²Joint BioEnergy Institute
- 2:00 (886) **Mainstreaming Microfluidics: Keys to Navigating Commercialization**; Josh Molho¹; ¹ProteinSimple
- 2:20 (887) **Genetic and Functional analysis of CTCs and Tumor Microvesicles**; Brian Kirby¹; ¹Cornell University
- 2:40 (888) **Micro-Assays for the Single Cell**; Nancy Allbritton^{1,2}; ¹University of North Carolina; ²North Carolina State University

Thursday Afternoon, Greenway G
CLINICAL VIBRATIONAL SPECTROSCOPY

Organizer and Presider: Katherine Cilwa

- 1:20 (889) **Applications of Raman Spectroscopy in Monitoring Human Mesenchymal Stem Cell Development into Bone**; Ryan Kane¹, Katherine Lau², Duncan Graham¹, Karen Faulds¹, Matthew Dalby³, Carol-Anne Smith³; ¹University of Strathclyde; ²Renishaw PLC; ³University of Glasgow
- 1:40 (890) **Monitoring Combat Wound Healing by IR Hyperspectral Imaging**; Ehsan Gazi¹, Chris Howle¹, Abigail Spear¹, Nicole Crane^{2,3}; ¹Defence Science and Technology Laboratory; ²Naval Medical Research Center; ³Uniformed Services University of Health Sciences
- 2:00 (891) **Endoscopic Raman Spectroscopy for Characterization of Inflammatory Bowel Disease**; Isaac Pence¹, Dawn Borromeo Beaulieu², Sarah Horst², David Schwartz², M. Kay Washington³, Alan Herline⁴, Anita Mahadevan-Jansen¹; ¹Vanderbilt University; ²Vanderbilt University Medical Center, Division of Gastroenterology, Hepatology and Nutrition; ³Vanderbilt University Medical Center, Department of Pathology, Microbiology, and Immunology; ⁴Medical College of Georgia Department of Surgery
- 2:20 (892) **Comprehensive Breast Tissue Characterization and Model Comparisons Using High Definition (HD)**

Infrared Spectroscopic Imaging; Shachi Mittal^{1,2}, Tomasz P. Wrobel¹, L. Suzanne Leslie^{1,2}, Andre Kadajcsy Balla^{3,4}, Rohit Bhargava^{1,2,4}; ¹Beckman Institute for Advanced Science and Technology, Urbana, IL; ²Department of Bioengineering, University of Illinois at Urbana-Champaign, Urbana, IL; ³Department of Pathology, University of Illinois at Chicago, IL; ⁴University of Illinois Cancer Center

2:40

(893) **Development of a Label-free Raman Imaging Technique for Differentiation of Infected & Non-Infected Malaria Tissue**; Laura Frame¹, James Brewer², Paul Garside², Gianluca Grassia², Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde; ²University of Glasgow

Thursday Afternoon, Nicollet D2/D3
THE GOOD, THE BAD AND THE UGLY: FINDING THE
HELPFUL VARIABLES AND REMOVING THE HARMFUL
VARIABLES IN DATA

Organizer and Presider: Barry Lavine

- 1:20 (894) **An "Elastic" Variable Selection Approach for Calibration**; Steven Brown¹, Cannon Giglio¹; ¹University of Delaware
- 1:40 (895) **A Few Variables More: Feature Selection in Spectral Library Matching**; Barry Lavine¹, Collin White¹, Matthew Allen¹, Tao Ding¹; ¹Department of Chemistry, Oklahoma State University, Stillwater, OK
- 2:00 (896) **Adaptive Regression via Subspace Elimination: Novel Algorithm for Predicting in the Presence of Uncalibrated Chemical Constituents**; Karl Booksh¹, Joshua Ottaway¹; ¹University of Delaware
- 2:40 (897) **Multiway PLS Method for Estimating the Strain Hardening Modulus in Polyethylene Resins**; Paul DesLauriers¹, Nathan Cole¹, Collin White², Barry Lavine²; ¹Chevron Phillips; ²Oklahoma State University

Thursday Afternoon, Lakeshore C
CBRNE DETECTION

Organizer and Presider: Edita Botonjin-Sehic

- 1:20 (898) **Improving Sensitivity and Source Attribution of Homemade Explosives with Low Frequency/THz-Raman® Spectroscopy**; James Carriere¹, Anjan Roy¹, Randy Heyler¹; ¹Ondax, Inc.
- 1:40 (899) **Challenging Real World Samples for Handheld Raman**; Katherine Bakeev¹, Kristen Frano¹, Thomas Padlo¹, Philip Zhou¹, Jun Zhao¹, Dawn Yang¹; ¹B&W Tek Newark, DE
- 2:00 (900) **Advancing Basic Science for Countering Weapons of Mass Destruction**; Cathie Condrón¹; ¹Defense Threat Reduction Agency
- 2:20 (901) **Through-barrier Explosives and Hazardous Material Detection Using a Handheld Spatially Offset Raman Spectrometer**; Matthew Bloomfield¹; ¹Cobalt Light Systems Inc
- 2:40 (902) **Driving Medicine Quality Assurance through Effective and Appropriate Utilization of Surveillance and screening Technologies**; Lukas Roth¹; ¹U.S. Pharmacopeial Convention

Thursday Afternoon, Lakeshore B
TWO-DIMENSIONAL CORRELATION ANALYSIS - II

Organizer: Isao Noda; Presider: Hideyuki Shinzawa

- 1:20 (903) **2D Correlation Study of Cathode Materials of Lithium Ion Battery**; Young Mee Jung¹, Yeonju Park¹, Yeseul Kim¹, Isao Noda²; ¹Kangwon National University; ²University of Delaware

TECHNICAL PROGRAM – THURSDAY

Orals 1:20 – 3:00 pm

- 1:40 (904) **2D Correlation Analysis of Time/Temperature-Resolved Infrared Spectra to Probe Structure Development of a Bio-Based, Biodegradable Polymer and Its Thermally Reversible Gel**; Brian Sobieski¹, Isao Noda^{1,2}, Liang Gong¹, John Rabolt¹, Bruce Chase¹; ¹University of Delaware; ²MHG Biopolymers
- 2:00 (905) **Raman Analysis of Phase Transitions of Alkanes and Polyethylene by Moving-Window 2DCOS**; Young Jong Lee¹, Ying Jin¹, Anthony P. Kotula², Angela R. Hight Walker³, Kalman B. Migler²; ¹Biosystems and Biomaterials Division, National Institute of Standards and Technology; ²Materials Science & Engineering Division, National Institute of Standards and Technology; ³Engineering Physics Division, National Institute of Standards and Technology
- 2:20 (906) **Structural Changes of Bread under External Perturbations: A 2DCOS Analysis of NIR-Spectroscopic Data**; Heinz Siesler², Tine Ringsted¹, Soren Engelsen¹, Frank Pfeifer²; ¹Department of Food Science, University of Copenhagen, Rolighedsvej 26, 1958 Frederiksberg, Denmark; ²Department of Physical Chemistry, University of Duisburg-Essen, Schuetzenbahn 70, D 45117 Essen, Germany
- 2:40 (907) **Baseline Removal Using Manifold Optimization**; Stephen Giguere¹, Darby Dyar², Sridhar Mahadevan¹, CJ Carey¹, Thomas Boucher¹; ¹University of Massachusetts, College of Information and Computer Sciences; ²Mount Holyoke College

Thursday Afternoon, Greenway D

LIBS FOR FORENSIC ANALYSIS

Organizer and Presider: Matthieu Baudelet

- 1:20 (908) **LIBS for Forensic Anthropology**; Matthieu Baudelet¹; ¹University of Central Florida
- 1:40 (909) **Trace Analysis of Uranium and Its Isotopic Ratio Determination with Laser Plasma Spectrochemistry**; George Chan¹, Xianglei Mao¹, Inhee Choi¹, Vassilia Zorba¹, Richard Russo¹; ¹Lawrence Berkeley National Laboratory
- 2:00 (910) **Laser-Induced Breakdown Spectroscopy for the Rapid Detection of Lead-Free Gunshot Residues**; Lashaundra Fambro¹, Deidre Vandenbos¹, Matthew Rosenberg¹, Ethan Miller^{1,2}, Christopher Dockery¹; ¹Kennesaw State University; ²Berry College
- 2:20 (911) **Study of Matrix Effects for Reproducible LIBS Analysis of Powders**; Sudeep Jung Pandey¹, Richard Locke¹, Mauro Martinez⁴, Romain Gaume^{1,2,3}, Matthieu Baudelet^{1,4}; ¹CREOL, UCF; ²Department of Materials Science and Engineering, UCF; ³Nanoscience Technology Center, UCF; ⁴NCFS/Chemistry Department, UCF
- 2:40 (912) **Simultaneous Laser Absorption-Emission Spectroscopy of Laser Ablation Plumes**; Sivanandan Harilal¹, Nicole LaHaye¹, Mark Phillips¹; ¹Pacific Northwest National Laboratory

Thursday Afternoon, Greenway J

RAPID TESTING USING FIELD-DEPLOYABLE SPECTROMETERS

Organizer and Presider: Jason Rodriguez

- 1:20 (913) **Asymptotically Approaching Usability for Stacked, Mutually Rotated Gratings and Shallow Well CMOS Camera Visible Spectrometry**; Alexander Scheeline¹; ¹SpectroClick Inc.
- 1:40 (914) **A Novel Spectral Identification Method by Means of Variable Reduction and Multivariate Statistics**; Jun Zhao¹; ¹B&W Tek, Inc.

- 2:00 (915) **Portable Raman with Visible Excitation: Breaking Analysis Speed and Accuracy Limitations**; Aleksandr Mikhonin¹, Rina Dukor¹, Laurence Nafie^{1,2}; ¹BioTools Inc., Jupiter, FL; ²Department of Chemistry, Syracuse University, Syracuse, NY
- 2:20 (916) **Rapid Testing Using Field-Deployable Raman Spectrometers**; Latevi Lawson¹, Chelliah Navin¹, Jason Rodriguez¹; ¹FDA Division of Pharmaceutical Analysis
- 2:40 (917) **Quantitative Analysis of Injectable Drug Products Using Non-invasive Wideband Raman Technology**; Bei Ma¹, Roman Galeev², Anatolyi Saveliev³, Arislanov Ilshat²; ¹The U.S. Pharmacopeial Convention (USP); ²Kazan City Institute for Drug Control, Russian Federation Drug Administration; ³Kazan Federal University

Thursday Afternoon, Nicollet D1

PHARMACEUTICAL APPLICATIONS OF TRANSMISSION RAMAN SPECTROSCOPY

Organizer and Presider: Mark Mabry

- 1:20 (918) **Fast Nondestructive Detection of Low Level Crystalline Forms in Amorphous Spray Dried Dispersion Using Transmission Raman Spectroscopy and Comparison to Existing technologies**; Archana Kumar¹, Joseph Lubach¹, Julia Griffen², Matthew Bloomfield², Pavel Matousek³, Larry Wigman¹; ¹Genentech Inc.; ²Cobalt Light Systems; ³Central Laser Facility, Research Complex at Harwell
- 1:40 (919) **Analysis of Polyethylene Oxide in Sintered Pharmaceutical Tablets by Transmission Raman**; Heather Boyce¹, Stephen W. Hoag¹; ¹University Maryland Baltimore, School of Pharmacy
- 2:00 (920) **Quantifying Phase Changes in High Throughput Excipient Compatibility Studies Using Transmission Raman Spectroscopy**; Nicole Canfield¹, Timothy Rhodes¹, Matthew Lamm¹; ¹Merck & Co, Inc
- 2:20 (921) **Comparison of Transmission Raman and NIR Spectroscopies for the Effects of Tablet Physical Properties**; Bruce Thompson¹, Brandye Smith-Goettler¹, Gregory Troup¹, Colleen Neu¹, Manoharan Ramasamy¹, Cindy Starbuck¹; ¹Merck
- 2:40 (922) **Rheo-Raman Microscopy: Gaining Insight to Chemical, Conformational, Mechanical, and Microstructural Properties of Soft Materials**; Matthew Meyer¹, Anthony Kotula², Jan Plog¹, Kalman Migler², Angela Hight Walker²; ¹Thermo Fisher Scientific, Madison, Wisconsin 53711; ²Materials Science & Engineering Division, NIST, Gaithersburg, Maryland 20899

Thursday Afternoon, Greenway E

ANALYTICAL CHEMISTS EASING WORLD POVERTY

Organizer and Presider: Rebecca Airmet

- 1:20 (923) **Frugal Science: Building Low-Cost Scientific Tools for Global Explorations in Chemistry, Ecology and Health-Care**; Saad Bhamla¹, James Cybulski¹, George Korir¹, Manu Prakash¹; ¹Stanford University
- 2:00 (924) **Merging Business, Science, and Culture in East Africa**; Merlin Bicking¹; ¹ACCTA, Inc.
- 2:20 (925) **The Role of a Woman in Science in Poverty Reduction – “An African Perspective”**; Simiso Dube¹; ¹University of South Africa

TECHNICAL PROGRAM – THURSDAY

Orals 1:20 – 3:00 pm

Thursday Afternoon, Lakeshore A HANDHELD AND PORTABLE SPECTROSCOPY APPLICATIONS

Organizer: Alexandra Ros; Presider: Amy Bauer

- 1:20 (926) **Hand-held LIBS for Provenance of Ammunition Cartridges**; Amy Bauer¹, Robert Robinsky¹, Kellen Sorauf², Greg Petersen¹, Markus Gaelli¹; ¹TSI, Incorporated; ²Regis University
- 1:40 (927) **From Multispectral Fiber Systems to Spectral Sensors**; Viacheslav Artyushenko¹, Igor Nazarov¹; ¹art photonics GmbH
- 2:00 (928) **LIBS Analysis of Agricultural Soils : Accurate Control of a Portable LIBS Instrument to Assess the Analytical Ability of the Method**; Bruno Bousquet², Julian Guezenoc¹, Clement Melkebeke², Lena Bassel², Anne Gallet-Budynek¹; ¹INRA; ²University of Bordeaux
- 2:20 (929) **Evolution of Handheld LIBS: Recent Developments in 2nd Generation Analyzers**; David Day¹, Brendan Connors¹; ¹SCIAPS

Thursday Afternoon, Nicollet B/C TOPICS IN MICROFLUIDICS

Organizer: Alexandra Ros; Presider: Adam Woolley

- 1:20 (930) **Frequency Dependent Dielectrophoretic Signatures of ABO-Rh Red Blood cells**; Hector Moncada-Hernandez^{1,2}, Min Wang¹, Rob Minerick², Adrienne Minerick^{1,2}; ¹Chemical Engineering, Michigan Technological University; ²Microdevice Engineering, LLC
- 1:40 (931) **3D Printed Micro Free-Flow Electrophoresis Device**; Sarah Anciaux¹, Michael Bowser¹; ¹University of Minnesota
- 2:00 (932) **Challenges to Using Dielectrophoretic Diagnostic Devices in Low-Resource Settings**; Shannon Huey Hilton¹, Mark A. Hayes¹; ¹Arizona State University
- 2:20 (933) **Electrically Driven, pH-Mediated Solid-Phase Extraction and Preconcentration on Monoliths in Microfluidic Devices**; Adam Woolley¹, Mukul Sonker¹, Radim Knob¹, Vishal Sahore¹; ¹Brigham Young University
- 2:40 (934) **Dielectrophoretic Response of Condensed DNA Clusters in AC fields**; Paul Jones¹, Seunghyun Lee¹, Gabe Salmon¹, Alexandra Ros¹; ¹Arizona State University

Thursday Afternoon, Greenway B/C TOPICS IN CHROMATOGRAPHY

Organizer: Alexandra Ros; Presider: TBD

- 1:20 (935) **Effect of Temperature on the Shelf-Life of AITC in Horseradish Using Headspace-Solid-Phase Microextraction-Gas Chromatography-Mass Spectrometry (HS-SPME-GC-MS)**; Sonali Pandey¹; ¹South Dakota State University
- 1:40 (936) **Characterizing Volatile Polymer Degradation Components Using Frontier Pyrolysis and Thermogravimetric Analysis**; Renee Cline¹, Joan Schroeder¹; ¹3M
- 2:00 (937) **GC-FTIR for Source Emission Measurements of BTEX**; Allan Bohlke¹, Martin Spartz¹, Peter Behnke¹; ¹Prism Analytical Technologies Inc.
- 2:20 (938) **Mass Spectrometry for comprehensive Assessment of Toxic and Nutritional Elements in Dietary Supplement Kelp**; Lee Yu¹, Rolf Zeisler¹, Rabia Oflaz¹, Rick Paul¹, Karen Murphy¹, George Caceres¹, Brittany Kassim¹, Stephen Long¹, Clay Davis¹, Michael Ellis¹; ¹NIST

Thursday Afternoon, Greenway A SCANNING PROBE METHODS FOR SURFACE SCIENCE PROBLEMS

Organizer and Presider: Melissa Hines

- 1:20 (939) **Challenges and Solutions to Achieving Robust, High-resolution Multi-property Imaging**; Eric Altman^{1,2}, Omur Dagdeviren^{1,3}, Mehmet Baykara⁴, Udo Schwarz^{1,2,3}; ¹Yale University, Center for Research on Interface Structures and Phenomena; ²Yale University, Department of Chemical and Environmental Engineering; ³Yale University, Department of Mechanical Engineering and Materials Science; ⁴Bilkent University, Department of Mechanical Engineering and Institute of Materials Science and Nanotechnology
- 1:40 (940) **One Dimensional Metallic Grain Boundaries in Two Dimensional Semiconductors**; Matthias Batzill¹; ¹University of South Florida
- 2:00 (941) **Imaging Water Reactions with Reduced, Stoichiometric, and Oxidized RuO₂(110) Surfaces**; Zdenek Dohnalek¹; ¹Fundamental and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory
- 2:20 (942) **Analysis of Redox-Active Metal-Organic Chemistry at Surfaces by Combinations of Scanning Probe Microscopies and Surface-sensitive Spectroscopies**; Steven Tait¹; ¹Indiana University
- 2:40 (943) **STM Reveals the Spontaneous Formation of Self-Assembled Monolayers on TiO₂ in Air and Solution**; Melissa Hines¹, Erik Skibinski¹, Anqi Song¹, William DeBenedetti¹, Amnon Ortoll-Bloch¹; ¹Cornell University
- 3:00 **Poster Viewing and Coffee Break, Nicollet A**

Thursday Afternoon, Nicollet B/C FACSS INNOVATION AWARD

Organizer and Presider: Matthieu Baudelet

- 3:50 (944) **Nanowell Sample Preparation Combined with Ultrasensitive LC- and CE-MS towards Single Cell Omics**; Ryan Kelly¹, Ying Zhu¹, Yongzheng Cong¹, Richard Smith¹; ¹Pacific Northwest National Laboratory
- 4:10 (945) **An Inexpensive Medical Device for Barrett's Esophagus Screening**; Rohith Reddy^{1,2}, Michalina Gora^{1,2}, Jing Dong^{1,2}, Matthew Beatty², Wolfgang Trasischker^{1,2}, Kanwarpal Singh^{1,2}, Amna Soomro², Catriona Grant², Mireille Rosenberg², Guillermo Tearney^{1,2}; ¹Harvard Medical School; ²Massachusetts General Hospital
- 4:30 (946) **Innovative Environmental Monitoring of Inorganic Compounds by means of 'Microalgae Sensors'**; Frank Vogt¹, Zachary Ogburn¹; ¹University of Tennessee
- 4:50 (947) **Combining Functionalised Nanoparticles and SERS for the Detection of miRNA Biomarkers Related to Type 2 Diabetes**; Laila Al Maqbali¹, Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde

FRIDAY MORNING CLOSING SESSION

Lakeshore A

7:30 – 8:00 am Continental Breakfast

8:00 **Announcement of Innovation Award Winner**

8:15 – 10:15 am

SCIENCE BEYOND BORDERS

Organizers and Presiders: Alexandra Ros and Mary Kate Donais

- 8:15 (948) **Meeting Healthcare Needs across the Globe through Non-Invasive Molecular Diagnostics**; Barbara S. Smith¹; ¹Arizona State University
- 8:45 (949) **Science With Purpose**; Maureen Tholen¹; ¹3M
- 9:15 (950) **Opportunities and Challenges for Women Scientists as Practitioners in Improving the Quality of Life in Africa**; Simiso Dube¹; ¹University of South Africa
- 9:45 (951) **Things Scientists Can Learn From Science Journalists: A Talk About How to Talk About Your Work**; Maggie Koerth-Baker¹; ¹FiveThirtyEight
- 10:15 Preview of 2017 Conference
- Adjourn

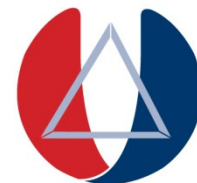
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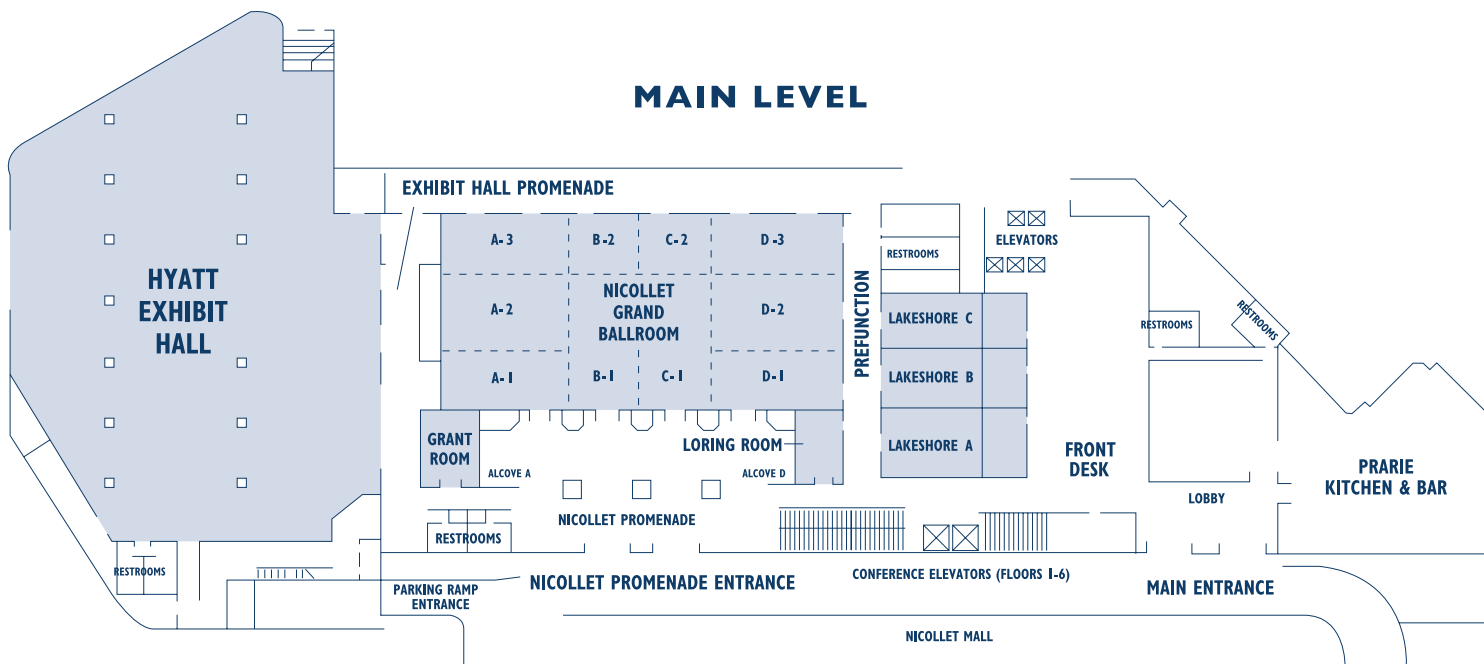
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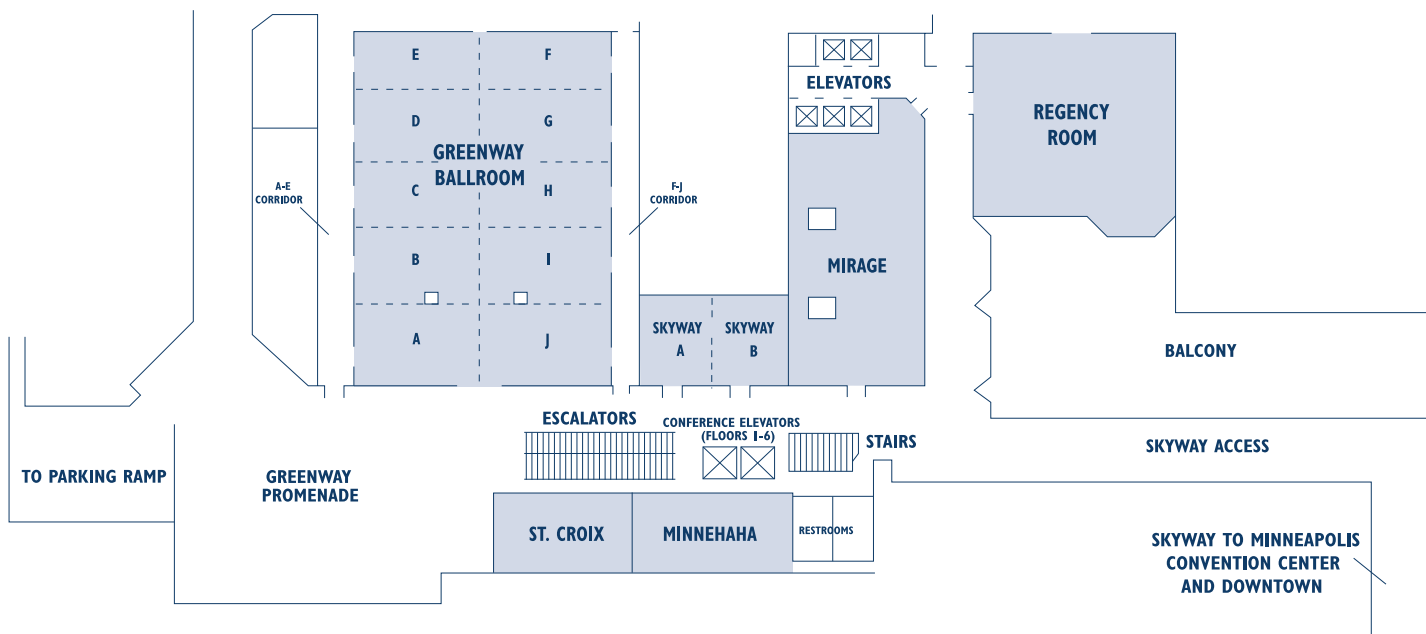
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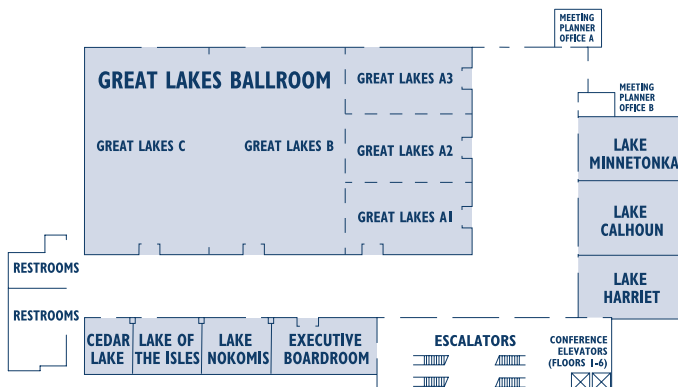
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SECOND LEVEL



FOURTH FLOOR



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