FACSS PRESENTS

SCIX2022

National Meeting

AES Electrophoresis Society

The Coblentz Society

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

Society for Applied Spectroscopy (SAS)

FINAL PROGRAM

OCTOBER 2–7

Northern Kentucky Convention Center - Covington, KY

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Attention Presenters: *Find your name in the index to locate your talk date/time/room or poster number. Check the mobile app and registration desk for any recent changes, or if you need assistance.*

SciX Conference and FACSS International Office
19 Mantua Road, Mount Royal, New Jersey 08061
(856) 224-4266 | facss@facss.org | scix@scixconference.org | www.scixconference.org | www.facss.org

WELCOME TO SciX 2022

On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS), it is our pleasure to welcome you to SciX 2022. This year, we explore a new city for our conference, Covington, KY, a location with a strong local scientific and industrial community. The SciX organizing team has worked tremendously hard to offer what we know to be the favorite week of the year for many of us. With the dedicated support and experience of the FACSS Governing Board Chair, Mike Carrabba, Talley Management Group, and our Marketing Chair, Tina Gong, we present you an amazing journey through analytical chemistry and spectroscopy like no other, with a fresh design to make the trip even more enjoyable and rewarding.

Our Program Chair, Robert Lascola, assembled a scientific program highlighting the Analytical Chemistry of Space Exploration. Sunday's Keynote Lecture by Dr. Amanda Hendrix of the Planetary Science Institute is "The Future of Space Exploration: Earth-Based, Deep Space-Based, Robotic, and Human". She will share her view as a principal investigator of observing programs with the Hubble Telescope, a co-chair of the National Academy of Sciences Committee on Planetary Protection, and co-author of the book "Beyond Earth – Our Path to a New Home in the Planets". There are additional space-themed sessions in vibrational spectroscopy, LIBS, mass spectrometry, and electrophoresis, and a special session on Friday morning to close out the conference.

Programming on cutting-edge analytical science includes: numerous sessions on the interaction of artificial intelligence and machine learning with imaging, spectroscopy, and biomedical applications; an analytical imaging symposium supported by the NSF Chemical Measurements and Imaging Program; a symposium on coherent multidimensional spectroscopy that ties into the Lippincott Award symposium; sessions highlighting academic and industrial chemistry in the Ohio/Kentucky region; and sessions honoring Peter Griffiths and Stanley Crouch, among many, many others. Oral sessions begin on Sunday afternoon, providing non-stop scientific knowledge until Friday morning with more than 120 oral sessions, plus posters Sunday through Wednesday.

The fourteen FACSS member societies will delight us with plenary talks from their new awardees. Organized by Awards Chair Karen Faulds, this section will see its highlight with the FACSS Innovation Award finalist presentations on Thursday morning. This internationally recognized award is our recognition of work being done in analytical chemistry and its application to all aspects of measurement science. In keeping with tradition, this session stands alone to maximize the opportunity to see spectacular new work.

The scientific program would not be complete without continuous education provided by our member societies, industrial sponsors, and Workshops Chair, Annie Dowgiallo. Courses target career advice to technical skills and applications. It is not too late to register onsite! In this transformed economy, providing our attendees and societies members with new career opportunities is crucial. We have organized a Career Fair, under the supervision of Robert Chimenti, on Wednesday morning. We are excited to offer this service free to the community after more than two years of primarily virtual networking. We are also presenting several technical sessions on career development and guidance, as well as highlighting the research achievements of our student and early career attendees.

Exhibits Chair Scott Rudder has organized a stellar exhibits experience. The Tuesday Happy Hour is back, networking while overlooking the Ohio River and downtown Cincinnati. Wednesday afternoon is our Exhibits Only closing event: with no technical sessions, the floor should be packed for an exhibits send-off. That evening, a Pub Crawl will explore Covington's eclectic nightlife.

The culmination of our social program – the SciX Gala – is on a new day, Thursday evening. After a full week of Space Science, it will be time to beat back Space Invaders at the SciX Arcade! From console games like Pac Man, Galaga, and Daytona Racing to old favorites like air hockey and shuffleboard, get ready to have fun, cheer on your friends, and compete for prizes like never before at SciX. Don't forget to dress up as your favorite game-themed character. The night is yours to create new memories!

SciX 2022 is the "Right Size, Right Science, Right Conference", with an even more exciting feel. Organizers, professors, post-docs, students, and exhibitors, we make Analytical Chemistry stronger every year during this SciX week. Welcome to your conference!

Matthieu Baudelet
SciX 2022 General Chair

SciX 2022 General Chair
Matthieu Baudelet
University of Central Florida

SciX 2022 Program Chair
Robert Lascola
Savannah River National Laboratory

SciX 2022 Exhibits Chair
Scott Rudder
OptoSigma Corporation

FACSS & SciX Marketing Chair
Tina Gong
Perkin Elmer

SciX 2022 Awards Chair
Karen Faulds
University of Strathclyde

SciX 2022 Short Courses Chair
Annie Dowgiallo
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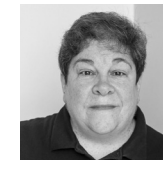

SciX 2022 Local Chair
Gloria Story
P&G

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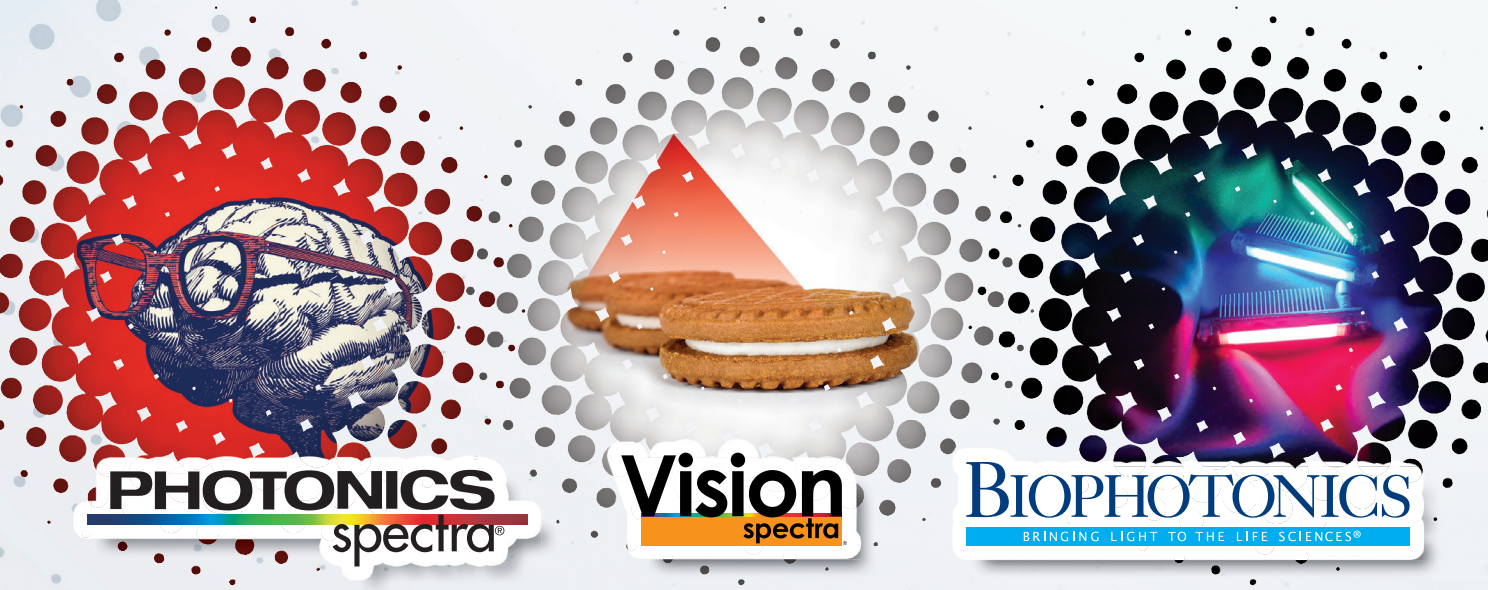

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FACSS AND SciX CONFERENCE ORGANIZATION

FACSS Member Organizations

American Chemical Society Division of Analytical Chemistry
AES Electrophoresis Society
ANACHEM
Austrian Society of Analytical Chemistry
CLIRSPEC
The Coblentz Society
Council for Near Infrared Spectroscopy
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
Society for Archaeological Sciences
Spectroscopical Society of Japan

2022 FACSS Executive Committee

Governing Board Chair: Mike Carrabba
Droplet Measurement Technologies

Governing Board Chair Elect: Karen Esmonde-White, *Endress+Hauser*

Past Governing Board Chair: Christopher Palmer, *University of Montana*

Secretary: Gary Brewer, *ISA Analysis Division West Virginia*

Treasurer: Ian Lewis, *Endress+Hauser*

Marketing Chair: Tina Gong, *Perkin Elmer*

SciX 2022 Section Chairs

2022 PROGRAM CHAIR
Robert Lascola
Savannah River National Laboratory

2022 AWARDS CHAIR and 2023 PROGRAM CHAIR
Karen Faulds
University of Strathclyde Glasgow

AES ELECTROPHORESIS
Chris Harrison
San Diego State University

ART & ARCHAEOLOGY
Mary Kate Donais
Saint Anselm College

ATOMIC SPECTROSCOPY
Derrick Quarles Jr.
Elemental Scientific

Benjamin Manard
Oak Ridge National Laboratory

BIOMEDICAL & BIOANALYTICAL
Fay Nicolson
Dana-Farber Cancer Institute & Harvard Medical School

Juergen Popp
Leibniz Institute of Photonic Technology e.V. Jena

CHEMOMETRICS
Peter Harrington
Ohio University

CONTEMPORARY ISSUES & EARLY CAREER RESEARCHERS
Karen Esmonde-White
Endress+Hauser

FORENSICS AND SECURITY
Betsy Jean Yakes
U.S. Food and Drug Administration

MASS SPECTROMETRY
Kaveh Jorabchi
Georgetown University

Jacob Shelley
Rensselaer Polytechnic Institute

MOLECULAR SPECTROSCOPY (IR)
Curt Marcott
Light Light Solutions

Michael George
University of Nottingham

Bernhard Lendl
TU Wien

NASLIBS
Vincent Motto-Ross
Universite Claude Bernard Lyon 1

Noureddine Melekechi
UMass Lowell

PHARMACEUTICAL ANALYSIS
John Wasylyk
Bristol-Myers Squibb

Katherine Hollywood
The University of Manchester

PROCESS ANALYTICAL TECHNOLOGY
Shawn Chen
Dow Chemical

Edita Botonjic-Sehic
Pall Corporation

RAMAN SPECTROSCOPY
Ian Lewis
Endress+Hauser

Duncan Graham
University of Strathclyde

Pavel Matousek
Rutherford Appleton Laboratory

SPECIAL SESSIONS
Robert Lascola
Savannah River National Laboratory

SPSJ - SPECTROSCOPICAL SOCIETY OF JAPAN
Yukihiro Ozaki
Kwansei Gakuin University

SURFACE PLASMON RESONANCE (PLASMONICS)
Amanda Haes
University of Iowa

Emilee Ringe
University of Cambridge

GENERAL INFORMATION

LOCATION of all plenaries, symposia, workshops/short courses, and exhibits are the Northern Kentucky Convention Center and the Marriott RiverCenter.

CONFERENCE REGISTRATION / INFORMATION DESK is located on the 1st Floor of the Northern Kentucky Convention Center.

Sunday	3:00 pm – 7:30 pm
Monday	8:00 am – 5:30 pm
Tuesday	8:00 am – 5:00 pm
Wednesday	8:00 am – 5:30 pm
Thursday	7:30 am – 4:45 pm

INTERNET ACCESS is available in all meeting areas. Verify connectivity details at the registration desk.

PRESENTERS should check the online program to verify the schedule of your talk or poster. Bring your slides to your session room on a USB flash drive 30 minutes prior to the session start. Format should be PowerPoint to run on a PC with Office 2019 and slide resolution should be 16:9. Speakers may NOT present from their own laptop. See the registration desk if you need to preview your slides.

POSTER SESSIONS

Sunday, *Ballroom B*
7:15 pm – 9:15 pm SAS Student Poster Session
Poster set up 5:30 pm – 6:00 pm, remove at 9:00 pm

For SciX poster sessions: Poster presenters are required to attend their poster at BOTH the morning and afternoon sessions on their designated days. This will extend the time for discussion and judging for student awards.

Posters must remain up all day on your designated day - early removal is not permitted. Posters not removed by 4 pm will be placed at the registration desk and discarded if not claimed by the end of the conference.

EXHIBITS

Tuesday, October 4 – 10:00 am – 5:00 pm

Coffee break/poster viewing	10:10 am – 10:45 am
Plenary Session (in exhibit hall)	10:45 am – 12:00 pm
Lunch included/seating in hall	12:00 pm – 1:30 pm
Break/poster viewing	3:10 pm – 3:50 pm
Exhibitor hosted Happy Hour (outside exhibit hall)	5:30 pm – 7:30 pm

Wednesday, October 5 –10:00 am – 6:00 pm

Coffee break/poster viewing	10:15 am – 10:45 am
Plenary Session (in exhibit hall)	10:45 am – 12:00 pm
Lunch included/seating in hall	12:00 pm – 1:30 pm
Break, poster viewing	3:10 pm – 3:50 pm
Exhibits Closing Reception	3:50 pm – 5:45 pm

LUNCH is on-own on Monday and Thursday. A lunch ticket will be provided for a boxed lunch in the exhibit hall on Tuesday and Wednesday.

WORKSHOPS offer introductory and fundamental topics. Onsite registration is available at the registration desk – space permitting. See page 31 for all course offerings.

SPECIAL EVENTS included with registration (badge required for all events).

Welcome Mixer and SAS Sponsored Student Poster Session
Sunday, 7:15 pm, Ballroom B

FACSS SciX Social Hour
Monday, 5:30 pm, RiverCenter Lobby

Exhibitor-Hosted Happy Hour
Tuesday, 5:30 pm, Riverview Ballroom (Marriott)

SciX Career Fair
Wednesday, 8:00 am, Kentucky Room (Marriott)

Exhibit Closing Reception
Wednesday, 3:50 pm, Event Center

SciX 2022 Gala
Thursday, 7:00 pm, Ballroom B&C

COMPANION REGISTRATION includes the Sunday Evening Welcome Mixer, Monday FACSS SciX Social, Wednesday Exhibit Closing Reception and Thursday Gala. Cost is $125 and companions may be added at registration.

MOBILE APP includes the most current program information and is updated as changes happen. Scan the QR code below to download the "eventScribe" app from the Apple App Store or the Google Play Store. Install and open the app, then search for "SciX" to locate the SciX Conference.

SOCIETY AND COMMITTEE MEETINGS

FACSS/SciX

Sunday, October 2

1:00 pm – 3:00 pm SciX 2023 Sparks/Reno: Budget/General Planning/Program *Kentucky Room (Marriott)*
3:00 pm – 4:15 pm FACSS Long Range Planning Meeting (Federation) *Kentucky Room (Marriott)*
4:15 pm – 5:30 pm SciX Long Range Planning Meeting (Conference) *Kentucky Room (Marriott)*

Monday, October 3

12:15 pm – 1:30 pm SciX 2024 General Planning K*entucky Room (Marriott)*

Tuesday, October 4

12:30 pm – 1:30 pm FACSS Budget Committee and Finance Committee *Kentucky Room (Marriott)*

Wednesday, October 5

7:00 am – 8:30 am Executive Committee Meeting (for the Executive Committee only) *Kentucky Room (Marriott)*

Thursday, October 6

12:30 pm – 2:00 pm Governing Board Meeting *Kentucky Room (Marriott)*

COBLENTZ SOCIETY

Sunday, October 2

4:30 pm – 5:30 pm "How to Make Connections: Student Networking at Conferences" *Meeting Room 6 (NKYCC)*
7:15 pm – 9:15 pm Coblentz Society Student Award Presentations at SAS Student Poster Session *Ballroom B*

Monday, October 3

7:00 am – 8:30 am Coblentz Annual Member Meeting and Breakfast *Covington 1&2 (Marriott)*
12:00 pm – 1:30 pm Coblentz Speed Mentoring Session *Covington 1&2 (Marriott)*

The Coblentz Society is 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.

Wednesday, October 5

12:00 pm – 3:00 pm Headshots in Exhibit Hall *Booth 323 Event Center (NKYCC)*
7:00 pm – 9:00 pm Coblentz Reception: *Stop by the Coblentz booth for details!*

SOCIETY FOR APPLIED SPECTROSCOPY

Sunday, October 2

7:15 pm – 9:15 pm SAS Student Poster Session *Ballroom B (NKYCC)*

Monday, October 3

8:00 pm SAS Student Event *Offsite: Molly Malones*
8:00 pm SAS Early Career Event *Offsite: Smoke Justis*

Tuesday, October 4

12:00 pm SAS Governing Board Luncheon *Location TBD*
7:30 pm – 8:30 pm SAS Award Presentations *Covington 3 (Marriott)*
8:30 pm – 11:00 pm SAS Members' Wine and Cheese Reception *Covington 1&2 (Marriott)*

NASLIBS

Wednesday, October 5

12:00 pm – 1:00 pm NASLIBS Member Meeting *Kentucky Room (Marriott)*

NASLIBS

Wednesday, October 5

4:00 pm – 5:30 pm AES Member Meeting *Kentucky Room (Marriott)*

CONFERENCE CODE OF CONDUCT

The Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) and the SciX Conference organizers are dedicated to providing a professional, pleasant and harassment-free conference experience for everyone, regardless of gender, gender identity, gender expression, sexual orientation, disability, physical appearance, race, ethnicity, nationality, age, religion or any other basis prohibited by law. We do not tolerate unprofessional behavior or harassment of conference participants in any form. Language or behavior that is offensive or unwelcoming to others is not appropriate at any FACSS-sponsored event. Disruptive or unprofessional behavior, including talking, use of cell phones, and unsanctioned photography/video/screen recording or any other form of digital capture is not permitted in any sessions or anywhere in a virtual conference interface. Conference participants violating these rules may be sanctioned or expelled from the conference without a refund at the discretion of the conference organizers.

General:

- An official name badge must be visible at all times.
- No smoking, including the use of e-cigarettes, in any conference areas.
- Participants at FACSS or SciX networking events where alcoholic beverages are served must drink responsibly.
- Participants must not be under the influence of illegal drugs or other unauthorized, mind-altering or intoxicating substances while attending FACSS or SciX events. This policy does not prohibit the possession and proper use of lawfully prescribed drugs taken in accordance with the prescription.
- No advertising materials or organized marketing efforts are permitted outside of the Exhibit Hall without the express authorization of the conference management, Exhibits Chair or Workshops Chair. Only official exhibitors may display in the Exhibit Hall. No instrument demonstrations or distribution of any type of literature outside the Exhibit Hall without the express authorization of the conference management, Exhibits Chair or Workshops Chair.
- In virtual settings where participants have a platform to be heard and/or seen by other attendees, advertising and organized marketing efforts are prohibited unless arranged and/or authorized by conference management, Exhibits Chair or Workshops Chair.
- No touching/opening/reverse engineering of exhibitor equipment without their express permission.
- No unauthorized removal of exhibitors' materials or promotional items from the exhibit hall.

While in oral or poster sessions and award ceremonies:

- All devices including cell phones must be silenced.
- Do not talk or otherwise interrupt the presenter.
- Do not take photographs or videos of PowerPoint presentations or posters, or use screen recording or any other form of digital capture.
- Do not distribute product literature or literature promoting other conferences.
- Do not demonstrate products (by presenters or attendees).
- Do not use powered or operational instruments.
- Do not use compressed gases or flammable/toxic chemicals.

Expected Behavior throughout the Conference:

- Respectfulness and consideration of others and of the facilities

Unacceptable Behavior:

- Physical or verbal abuse of anyone attending or involved with the conference
- Harassment, intimidation or discrimination in any form; Examples of harassment are provided below

Harassment includes, but is not limited to:

- Unwelcome or inappropriate verbal comments related to gender, gender identity and expression, sexual orientation, disability, physical appearance, race, age, or religion
- Sexual images in public spaces
- Deliberate intimidation, stalking, or following
- Unwelcome photography or recording
- Sustained disruption of talks or other events
- Inappropriate physical contact
- Unwelcome sexual attention
- Advocating for, or encouraging, any of the above behavior

Exhibitors, sponsor or vendor booths, or similar activities are also held to the community standards described in this Code of Conduct. In particular, exhibitors should not use sexualized images, activities, or other material.

Enforcement

Participants must follow this Code of Conduct at all physical and virtual conference venues and conference-related social activities. Participants asked to stop any behavior in violation of this Code of Conduct must comply immediately. If a participant engages in behavior in violation of this Code of Conduct, conference organizers retain the right to take any actions to keep the event a professional and welcoming environment for all participants. This includes warning the offender or expulsion of the offender from the conference without a refund. Conference organizers may take action to redress anything designed to, or with the clear impact of, disrupting an event or making the environment hostile for any participants.

Reporting
FACSS/SciX are actively engaging in developing guidance for leadership, volunteers and staff to help monitor for behavior in violation of this code of conduct and to intervene as appropriate. That said, there must also be a mechanism for attendees to report such behavior. If you experience or observe unprofessional conduct, harassment, or other Code of Conduct violations, please report it as soon as possible. Make a report during regular conference and event hours:

- In person: Contact a volunteer in t-shirt or leaders and staff with ribbons on badges.
- Via email: report@scixconference.org
- Voice or Text: +1 (856) 494-6418

To ensure your report is managed properly, volunteers and staff will alert the FACSS Governing Board Chair and the FACSS Account Executive (or their designees), who will arrange to receive the details of your report in a safe environment where you cannot be overheard. Once safe, you will be asked to state what happened. This can be upsetting, but will be handled as respectfully as possible, and you may bring someone to support you. You won't be asked to confront anyone, and no one will be told who you are. The FACSS/SciX team can help you contact hotel/venue security, local law enforcement, or local support services; provide escorts; or otherwise assist you to feel safe for the duration of the conference. If you are not comfortable reporting, anonymous reporting is also possible. While this limits our ability to follow-up, we still encourage anonymous reporting over not reporting an issue at all.

Emergency Contacts
If you feel you are in danger, observe someone else or are yourself considering harm to yourself or someone else, or if it is after hours and you do not receive a response via one of the reporting mechanisms above, you should contact local law enforcement, hotel or event center security, local hotlines, or emergency services as appropriate. FACSS/SciX officers and staff are not available at all hours and are not equipped or trained to respond to emergencies or situations involving violence or other physical altercations.

- Emergencies: 9-1-1
- National Suicide Prevention Lifeline: 8-1-1
- National Domestic Violence Hotline: 1 (800) 799- 7233
- Crisistextline.org: Text HOME to 741741

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Coblentz Society – *Award, Molecular/IR*

Cytorecovery – *AES*

Elemental Scientific – *Atomic*

Elemental Scientific Lasers – *Atomic*

Fortis Life Sciences – *Atomic*

Glass Expansion – *Atomic*

Hamamatsu – *Forensics*

Harrington Center for Intelligent Instruments – *Chemometrics*

Leco – *Atomic*

Lightigo – *LIBS*

Meinhard/Elemental Scientific – *Atomic*

Nu Instruments – *Atomic*

PerkinElmer Inc. – *Atomic*

RedWave Technology – *Special*

Royal Society of Chemistry – *Atomic*

SAS Chemometrics Section – *Chemometrics*

Si-Ware – *Forensics*

Society for Archeological Sciences – *Art and Archaeology*

TOFWERK – *Atomic*

VIAVI Solutions – *Process Analytical Technology*

Wasatch Photonics – *Forensics*

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Separations

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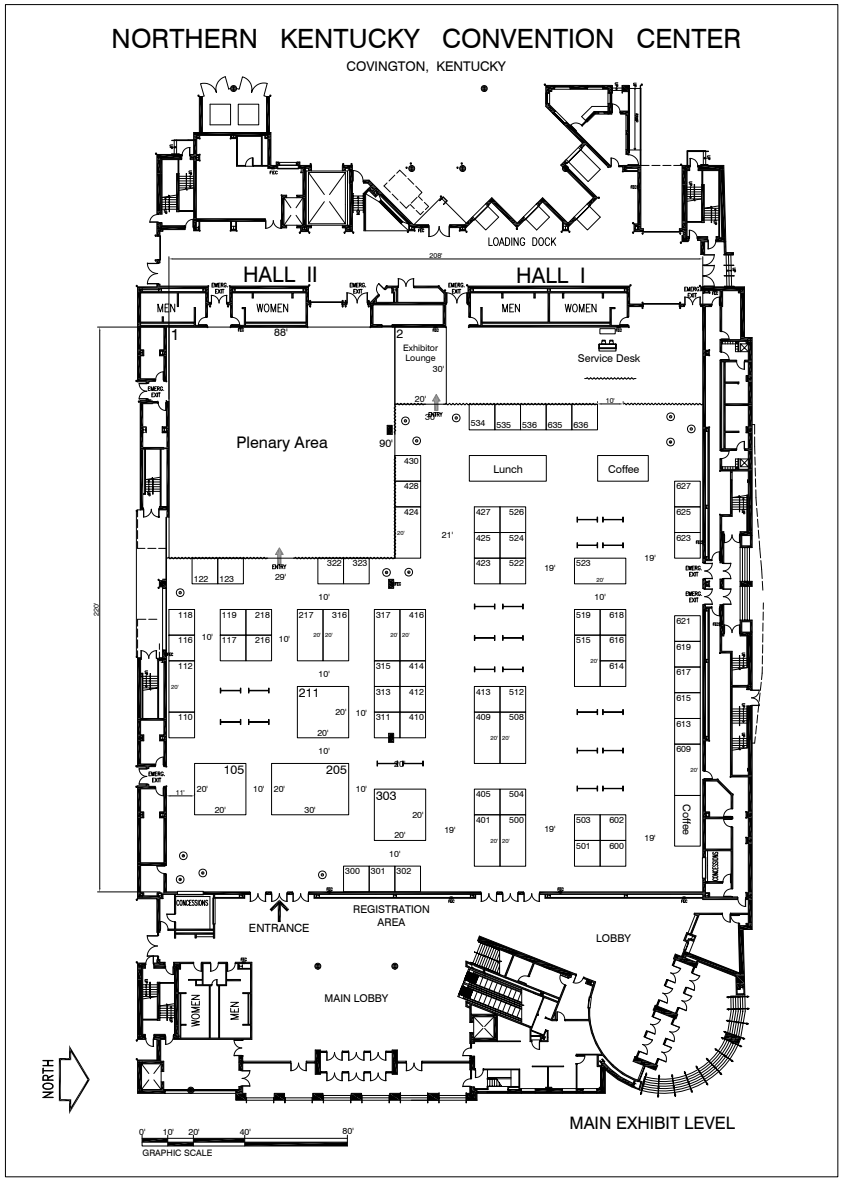
As of September 9, 2022



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PREVIOUS FACSS BOARD AND MEETING CHAIRS

1973		
	Jeannette Grasselli	Governing Board Chair
1974 - Atlantic City		
	James White	Governing Board Chair
	George Heinz	General
	James White	Program
	Edward Ruffing	Exhibit
1975 - Indianapolis		
	James Holcombe	Governing Board Chair
	Gerald Wallace	General
	James Holcomb	Program
	Edward Ruffing	Exhibit
1976 - Philadelphia		
	Edward Brame	Governing Board Chair and General
	Edward Dunlap	Program
	Douglas Robinson	Arrangements
	Edward Ruffing	Exhibit
1977 - Detroit		
	Edgar Peck	Governing Board Chair
	Mitch Kapron and James Burns	General
	Jeannette Grasselli	Program
	L. Felix Schneider	Arrangements
	Edward Ruffing	Exhibit
1978 - Boston		
	James Williamson	Governing Board Chair
	Paul Lublin	General
	James Cosgrove	Program
	James Cornwell	Arrangements
	Edward Ruffing	Exhibit
1979 - Philadelphia		
	Peter Keliher	Governing Board Chair
	Douglas Robinson	General
	Philip LeFleur	Program
	Sydney Fleming	Arrangements
	Edward Ruffing	Exhibit
1980 - Philadelphia		
	L. Felix Schneider	Governing Board Chair
	Sydney Fleming	General
	Theodore Rains	Program
	Robert Barford	Arrangements
	Edward Ruffing	Exhibit
1981 - Philadelphia		
	Jack Katon	Governing Board Chair
	Robert Barford	General
	Mary Kaiser	Program
	James Cavanaugh	Arrangements
	Peter Keliher	Exhibit
1982 - Philadelphia		
	Sydney Fleming	Governing Board Chair
	James Cavanaugh	General
	Andrew Zander	Program
	Matthew O'Brien	Arrangements
	Peter Keliher	Exhibit
1983 - Philadelphia		
	Mary Kaiser	Governing Board Chair
	Matthew O'Brien	General
	John Lephardt	Program
	D. Bruce Chase	Arrangements
	Peter Keliher	Exhibit
1984 - Philadelphia		
	Theodore Rains	Governing Board Chair
	D. Bruce Chase	General
	Patricia Rouse Coleman	Program
	Fred Corcoran	Arrangements
	Peter Keliher	Exhibit
1985 - Philadelphia		
	Robert Barford	Governing Board Chair
	Fred Corcoran	General
	Matthew Klee	Program
	Marshall Fishman	Arrangements
	Peter Keliher	Exhibit
1986 - St. Louis		
	Ronald Schroeder	Governing Board Chair
	Marshall Fishman	General
	Alexander Scheeline	Program
	Terry Hunter	Arrangements
	Edward Brame	Exhibit
1987 - Detroit		
	Patricia Rouse Coleman	Governing Board Chair
	David Coleman and L. Felix Schneider	General
	John S. Beaty	Program
	Edward Brame	Exhibit
1988 - Boston		
	James Cavanaugh	Governing Board Chair
	Frank Plankey and John S. Beaty	General
	Roger Gilpin	Program
	Edward Brame	Exhibit
1989 - Chicago		
	Alexander Scheeline	Governing Board Chair
	Paul Bourassa	General
	Robert G. Michel	Program
	Edward Brame	Exhibit
1990 - Cleveland		
	Nancy Miller-Ihli	Governing Board Chair
	Charles Belle	General
	Steven Hughes	Program
	Edward Brame	Exhibit
1991 - Anaheim		
	David Coleman	Governing Board Chair
	Richard Deming and Constance Sobel	General
	James Holcombe	Program
	Edward Brame	Exhibit
1992 - Philadelphia		
	Karmie Galle	Governing Board Chair
	Matthew Klee	General
	Barry Lavine	Program
	Edward Brame	Exhibit
1993 - Detroit		
	Robert Watters	Governing Board Chair
	L. Felix Schneider and David Coleman	General
	Julian Tyson	Program
	Mildred Barber	Exhibit
1994 - St. Louis		
	Paul Bourassa	Governing Board Chair
	Terry Hunter	General
	John Koropchak	Program
	Mildred Barber	Exhibit
1995 - Cincinnati		
	Jon W. Carnahan	Governing Board Chair
	Joseph A. Caruso	General
	Richard F. Browner and R. Kenneth Marcus	Program
	Mildred Barber	Exhibit
1996 - Kansas City		
	Rachael Barbour	Governing Board Chair
	O. Karmie Galle	General
	William Fateley	Program
	Scott McGeorge	Exhibit

1997 - Providence

Mildred Barber	Governing Board Chair
Chris Brown	General
John Olesik	Program
Scott McGeorge	Exhibit

1998 - Austin

John Graham	Governing Board Chair
David Laude	General
Isiah Warner and Linda McGown	Program
Scott McGeorge	Exhibit

1999 - Vancouver

Robert G. Michel	Governing Board Chair
Michael Blades	General
Ronald Williams	Program
Scott McGeorge	Exhibit

2000 - Nashville

John Koropchak	Governing Board Chair
Arlene Garrison	General
Michael Carrabba	Program
Scott McGeorge	Exhibit

2001 - Detroit

David A. Laude	Governing Board Chair
David Coleman and L. Felix Schneider	General Co-Chairs
David J. Butcher	Program
Scott McGeorge	Exhibit

2002 - Providence

Michael Carrabba	Governing Board Chair
Robert G. Michel	General
Mark A. Hayes	Program
Scott McGeorge	Exhibit

2003 - Fort Lauderdale

Ronald Williams	Governing Board Chair
Rina Dukor	General
James Rydzak	Program
Scott McGeorge	Exhibit

2004 - Portland

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

2005 - Quebec City, Canada

Mark Hayes	Governing Board Chair
Denis Boudreau	General
Paul Farnsworth	Program
Scott McGeorge	Exhibit

2006 - Orlando

Diane Parry	Governing Board Chair
Christine Wehlburg	General
S. Douglas Gilman	Program
Mike Carrabba	Exhibit

2007 – Memphis

James Rydzak	Governing Board Chair
Paul Bourassa	General
Ian R Lewis	Program
Mike Carrabba	Exhibit

2008 - Reno

Gary Brewer	Governing Board Chair
John Hellgeth	General
Greg Klunder	Program
Mike Carrabba	Exhibit

2009 - Louisville

Becky Dittmar	Governing Board Chair
Jessica Jarman	General
Curtis Marcott	Program
Mike Carrabba	Exhibit

2010 - Raleigh

S. Douglass Gilman	Governing Board Chair
David J. Butcher	General
André J. Sommer	Program
Mike Carrabba	Exhibit

2011 - Reno

S. Douglass Gilman	Governing Board Chair
Greg Klunder	General
Pavel Matousek	Program
Mike Carrabba	Exhibit

2012 - Kansas City

Ian R. Lewis	Governing Board Chair
Brandye Smith-Goettler	SciX General
Steven Ray	SciX Program
Mike Carrabba	SciX Exhibits

2013 - Milwaukee

Ian R. Lewis	Governing Board Chair
Fred LaPlant	SciX General
Mike George	SciX Program
Mike Carrabba	SciX Exhibit

2014 – Reno

Greg Klunder	Governing Board Chair
Luisa T. M. Profeta	SciX General
José R. Almirall	SciX Program
Mike Carrabba	SciX Exhibit

2015 - Providence

Greg Klunder	Governing Board Chair
Edita Botonjic-Sehic	SciX General
Glen P. Jackson	SciX Program
Mike Carrabba	SciX Exhibit

2016 - Minneapolis

Steven Ray	Governing Board Chair
Mary Kate Donais	SciX General
Alexandra Ros	SciX Program
Mike Carrabba	SciX Exhibit

2017 - Reno

Steven Ray	Governing Board Chair
Becky Ditmar	SciX General
Matthieu Baudelet	SciX Program
Mike Carrabba	SciX Exhibit

2018 - Atlanta

Fred LaPlant	Governing Board Chair
Mark Henson	SciX General
Karen Esmonde-White	SciX Program
Mike Carrabba	SciX Exhibit

2019 – Palm Springs

Fred LaPlant	Governing Board Chair
Mark Hayes	SciX General
Garth Simpson	SciX Program
Mike Carrabba	SciX Exhibit

2020 – Virtual (in lieu of Sparks)

Chris Palmer	Governing Board Chair
Linda Kidder Yarlott	SciX General
Mary Kate Donais	SciX Program
Mike Carrabba	SciX Exhibit

2021 – Providence

Chris Palmer	Governing Board Chair
Robert Chimenti	SciX General
Jean-François Masson	SciX Program
Scott Rudder	SciX Exhibit

FACSS AWARDS

FACSS THOMAS B. HIRSCHFELD SCHOLAR AWARD

The FACSS Thomas B. Hirschfeld Scholar Award recognizes students who best exemplify the extraordinary creativity of the award's namesake, and the recipients and their work will be seen as potentially defining the future practice of analytical chemistry. There are two recipients in 2022.

Sayantan Mahapatra
Sayantan Mahapatra is currently a Ph.D. candidate in Chemistry with a focus on single-molecule chemical analysis of surface structures at the University of Illinois Chicago.

Anna Wójtowicz
Anna Wójtowicz is a 4th-year Ph.D. Candidate at the Jagiellonian University in Kraków, Poland under the mentorship of Prof. R. Wietecha-Posłuszny.

FACSS STUDENT AWARD

The prestigious FACSS Student Award is given to the student who has furthered the state-of-the-art in their chosen field(s) and in so doing, advanced the understanding of important scientific or societal questions. The recipient will have a strong research record and be identifiable as an emerging leader in analytical chemistry.

Alexis Weber
Alexis Weber is a 3rd year Ph.D. Candidate in Dr. Igor Lednev's lab in the Department of Chemistry at the University at Albany, SUNY.

FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS CALL FOR 2023 APPLICATIONS

FACSS is proud to support the development of the next generation of leaders in analytical science. Pre-doctoral students presenting at the conference are encouraged to submit applications for the FACSS Student Award and the Tomas Hirschfeld Scholar Award. Both awards recognize research excellence but highlight the different ways that this may be achieved. Recipients receive complimentary registration and financial support to attend the SciX conference.

Look for information online in January 2023 at scixconference.org. To be considered for either award, students must submit an abstract for oral presentation at SciX (submission opens later winter/early spring 2023), then submit the following as a single PDF file:

- The application form (check in early 2023 for next year's application form)
- Two letters of nomination, including one by the student's mentor
- A copy of the candidate's résumé
- A copy of the candidate's graduate transcript
- Copies of reprints and/or preprints of research accomplished

For full bios, scan here to visit scixconference.org/awards

FACSS INNOVATION AWARD

The FACSS Innovation Award is given to 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 qualifies. All attendees are eligible for the award irrespective of educational level or professional vocation. Papers submitted for SciX will be considered for these awards – authors indicate during the submission process that they wish to be considered. Finalists present at the SciX conference in an exclusive plenary session on Thursday morning, with the award winner(s) selected and announced on Friday morning to conclude SciX 2022.

2022 FACSS INNOVATION AWARD SYMPOSIUM

Thursday | 8:00 am– 10:10 am | Ballroom D&E

Talks are 20 minutes each with 10 minutes immediately following for Q&A

What Lies Beneath your Elution Peak: Imaging When and Where Analytes Adsorb to Commercial Stationary Phase Particles
Lydia Kisley

Biomimetic Transparent Nanoplasmonic Meshes by Reverse-Nanoimprinting for Bio-interfaced Spatiotemporal Multimodal Surface-enhanced Raman Spectroscopy
Aditya Garg

Opto-Lipidomics of Tissues
Mads S. Bergholt

Rapid Vibrational Circular Dichroism – Opportunities through the combination of External Cavity Quantum Cascade lasers and balanced detection
Daniel-Ralph Hermann

FACSS CHARLES MANN AWARD

The Charles Mann Award is presented to an individual who has demonstrated advancement(s) in the field of applied Raman spectroscopy, presented at the FACSS SciX conference; and/or demonstrated dedication to the advancement of the Raman spectroscopy program at the FACSS SciX conference and/or the ASTM Raman subcommittee. The Charles Mann award for Applied Raman Spectroscopy was instituted by FACSS in 2002 following the untimely death of Professor Charles (Charlie) Mann. Professor Mann was a well-known and long-standing member of the faculty of Florida State University (FSU). Professor Mann and his faculty colleague, Professor Tom Vickers, contributed significantly to the development of analytical Raman spectroscopy via publications, participation at numerous meetings including the annual FACSS meeting, and participation in the ASTM sub-committee on Raman spectroscopy E13.08. Professor Mann's research areas covered from the fundamental including data analysis (chemometrics and databases), quantitative Raman, and instrumental understanding to the applied, polymers, inorganics, etc.

Igor K. Lednev
Igor K. Lednev is a Distinguished Professor in the Department of Chemistry, University at Albany, State University of New York.

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

SAS APPLIED SPECTROSCOPY WILLIAM F. MEGGERS AWARD

2021 Meggers Award Paper Published in *Applied Spectroscopy*, 2021, Vol. 75(5) 520–530

Augmented Two-Dimensional Correlation Spectroscopy for the Joint Analysis of Correlated Changes in Spectroscopic and Disparate Sources

H. Georg Schulze, Shreyas Rangan, Martha Z. Vardaki, Diepiriye G. Iworima, Timothy J. Kieffer, Michael W. Blades, Robin F. B. Turner and James M. Piret

Georg Schulze obtained a Bsc. Eng. (Chem.) from the University of Pretoria, followed by two years of industrial experience.

Shreyas Rangan completed his B.Tech. and M.Tech. in Biotechnology from the Indian Institute of Technology Madras, followed by an M.Sc. in Genome Science and Technology from The University of British Columbia (UBC).

Martha Vardaki obtained a B.Sc. and M.Sc. in Pharmacy and Pharmaceutical analysis respectively from the University of Patras and a Ph.D. degree in physics from the University of Exeter (UK), followed by a Research Associate appointment in Imperial College London.

Diepiriye Iworima moved from Nigeria and obtained her B.Sc. (Hons) and M.Sc. in Cellular Biology from Simon Fraser University.

Timothy Kieffer completed a Ph.D. degree in Physiology from The University of British Columbia in 1994, followed by a Post-Doctoral Fellowship in Molecular Endocrinology at Massachusetts General Hospital & Harvard Medical School.

Michael Blades received a B.Sc. in Chemistry at St. Mary's University (Halifax, Nova Scotia) and a Ph.D. at the University of Alberta in 1980 working in the area of plasma spectrochemistry.

Robin Turner earned a Ph.D. degree in electrical engineering from the University of Alberta in 1990.

James Piret has a Bachelor's degree from Harvard in Applied Mathematics to Biochemistry and a Chemical Engineering doctoral degree from MIT in 1989.

For full bios, scan here to visit scixconference.org/awards

NESAS AND SAS LESTER W. STROCK AWARD

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

Igor Gornushkin
Dr. Igor Gornushkin is a senior scientist at the BAM Federal Institute for Materials Research and Testing in Berlin, Germany.

ADDITIONAL SAS AWARDS PRESENTED ON TUESDAY EVENING

SAS ATOMIC TECHNICAL SECTION STUDENT AWARDS

Recognizing outstanding student research in the area of Atomic Spectoscopy.

Ana Lores Padin
University of Oviedo
Ph.D, candidate in BionanoAnalytical Electrochemistry and Spectrochemistry

Emily Kwapis
University of Florida
Ph.D. candidate in Nuclear Engineering

Marcus von der Au
Federal Institute of Hydrology
Ph.D. candidate in analytical chemistry

Lucía Gutiérrez Romero
University of Oviedo
Ph.D. candidate in Mass Spectrometry in Biomedical Analysis

SAS EARLY CAREER INTEREST GROUP TRAVEL GRANT

Travel support for Early Career Scientists (within 5 years of earning a terminal degree) to SAS' National meeting during SciX. Awarded to Early Career scientists who demonstrate merit in the field of spectroscopy and/or those who demonstrate financial need.

Malama Chisanga
University of Montreal, Canada
Department of Chemistry

Olga Eremina
University of Southern California
Department of Biomedical Engineering

SAS BARBARA STULL GRADUATE STUDENT AWARD

Recognizing graduate students for outstanding research in spectroscopy. Presented in honor and memory of longtime SAS staff member and colleague Barbara L. Stull.

Alexis Weber, *University at Albany - SUNY*
Awarded for outstanding research efforts targeting the development of the first universal tool for the identification and analysis of body fluid traces for forensic purposes as well as an outstanding research background in forensic science.

SAS UNDERGRADUATE STUDENT AWARDS

Given to junior or senior undergraduate students for outstanding research in spectroscopy.

Ewelina Randall
City College of New York
Awarded for work in construction of hyperspectral microscopy of visible and near-infrared fluorescence and the development of near-infrared nanosensors that transduce information via spectral changes in living cells and animals.

Aaron K. Mclean
Monash University
Awarded for work in applying FTIR spectroscopy to diagnose COVID-19 in saliva and helping develop the chemometric model for the infrared based saliva screening test for COVID-19.

Aric Potter
University of Utah
Awarded for studies in reversed-phase chromatographic stationary-phase materials with covalently-bound n-alkyl chains and the influence of surface curvature on the structure of alcohol-hybrid monolayers.

SAS FELLOW

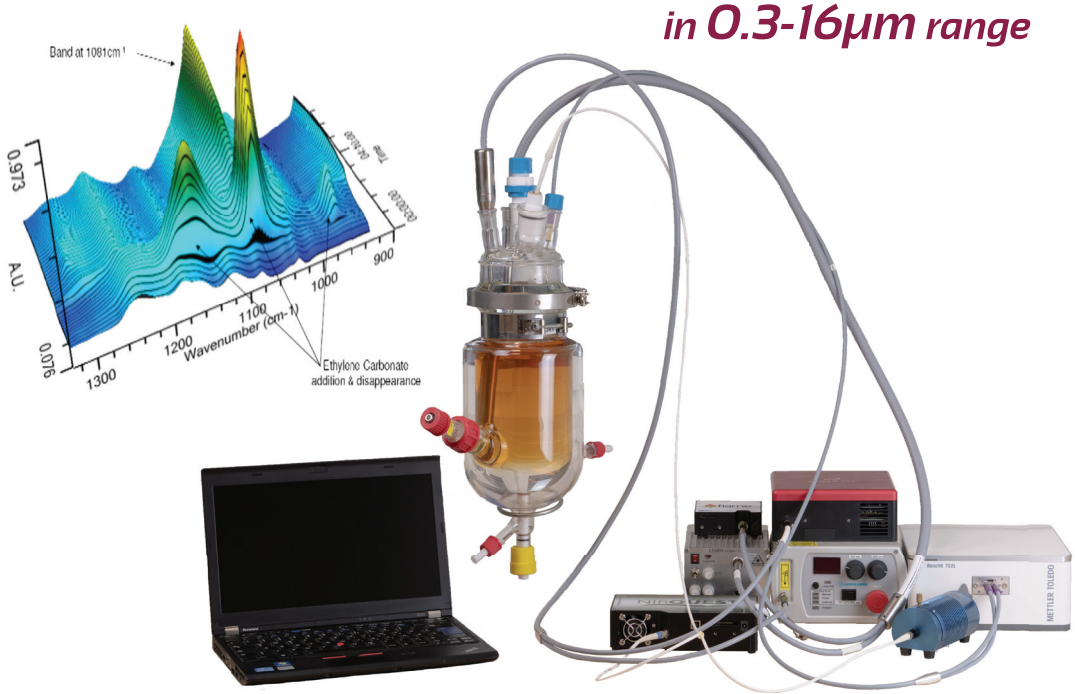
Recognizing individual members for their outstanding service to the field of spectroscopy and the Society for Applied Spectroscopy.

John H. Kalivas
Professor
Department of Chemistry
Idaho State University

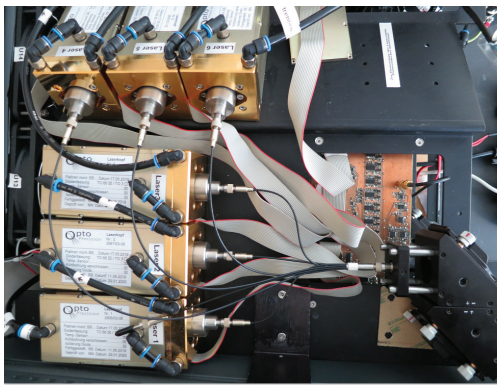
For full bios, scan here to visit scixconference.org/awards

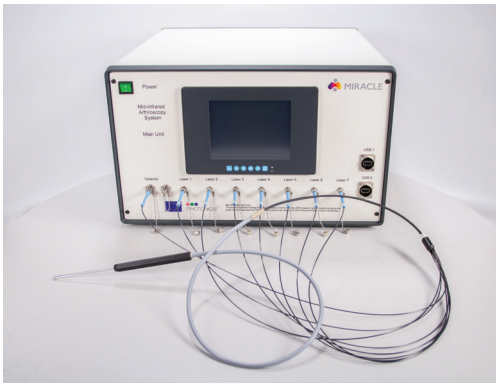
Fiber Probes
for Multi-Spectral
Process Control & Diagnostics
in 0.3-16µm range

art photonics
broad spectra fiber solutions



Multi-Wavelength Mid InfraRed QCL Fiber Sensors





Combining up to 7 QC-Lasers with Mid IR-fiber bundle in one probe – to use Lego design for spectral fiber sensors optimized to control specific process *in-line* or for medical diagnostics *in-vivo*

**Photos are due to the courtesy of EU-project MIRACLE:*

MIRACLE

SAS HONORARY MEMBERSHIP AWARD

Recognizing those individuals who have made exceptional contributions to spectroscopy.

Stanley Michael Angel
University of South Carolina
Awarded for the breadth and scope of his research and accomplishments in the fields of atomic and vibrational spectroscopies and the fact that he is among the best instrument innovators and builders of this generation.

WILLIAM J. POEHLMAN AWARD

Spectroscopy Society of Pittsburgh
The section was chosen for its efforts in attracting high attendance to meetings, collaboration with SACP and SSP, and offering virtual broadcasts of meetings.

2022 SAS SERVICE AWARDEES

President
Karl Booksh
Past President 2020,
President 2021,
Past President 2022

Treasurer
Diane Parry
2017-2022

Membership Chair
Brooke Kammrath
2019-2022

SAS DISTINGUISHED SERVICE AWARD

Howard L. Mark
Mark Electronics
Awarded for his active participation in and longtime service to the Society for Applied Spectroscopy. During his more than 40-year tenure with SAS, Dr. Mark has made exceptional contributions as a tireless volunteer and officer for the SAS New York-New Jersey Regional Section.

SAS PRESIDENT'S AWARD

Ellen v. Miseo
Awarded for recent extraordinary contributions in service the Society for Applied Spectroscopy in the area of education and training

Richard A. Crocombe
Awarded for recent extraordinary contributions in service the Society for Applied Spectroscopy related to the launch of a new society journal

COBLENTZ SOCIETY AWARDS

COBLENTZ SOCIETY CLARA CRAVER AWARD

The Clara Craver award recognizes young individuals who have made significant contributions in applied analytical vibrational spectroscopy. The Craver Award is presented annually to an outstanding young molecular spectroscopist whose efforts are in the area of applied analytical vibrational spectroscopy. 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.

Wei Min
Dr. Wei Min is currently a Professor of Chemistry at Columbia University. He is also affiliated with the Department of Biomedical Engineering, the Kavli Institute for Brain Science and NeuroTechnology Center at Columbia University.

ELLIS R. LIPPINCOTT AWARD

The Ellis R. Lippincott Award is awarded annually to recognize an individual that has made significant contributions to the field of vibrational spectroscopy. The award was jointly established in 1975 by The Optical Society (OSA), The Coblentz Society, and The Society for Applied Spectroscopy to honor the unique contributions of Professor Ellis R. Lippincott. Among other contributions, Professor Lippincott was one of the developers of the diamond anvil cell which is widely employed used in high pressure research, and because innovation was a hallmark of Lippincott's work, this quality must also be demonstrated by candidates for the award.

Martin Zanni
Martin T. Zanni is the Meloche-Bascom Professor of Chemistry at the University of Wisconsin-Madison.

COBLENTZ SOCIETY WILLIAM G. FATELY STUDENT AWARD

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

Yamuna Phal
Yamuna Phal is a Ph.D. candidate in Electrical and Computer Engineering at the University of Illinois at Urbana-Champaign (UIUC).

For full bios, scan here to visit scixconference.org/awards

COBLENTZ SOCIETY STUDENT AWARDS

For many years, the Coblentz Society has recognized outstanding young scientists pursuing studies in vibrational spectroscopy with Coblentz Student Awards. Awardees receive a copy of the Society's Desk Book of Infrared Spectra, a certificate, SciX registration, and a year's membership in the Society. The winner's faculty advisors, institution, and anticipated graduation date appear in the Society's Newsletter and website.

Sayantan Mahapatra
Sayantan Mahapatra is currently a Ph.D. candidate in Chemistry with a focus on single-molecule chemical analysis of surface structures at the University of Illinois Chicago. In 2015, he earned a bachelor's degree (B.Sc.) in Chemistry with minors in Physics and Mathematics from the University of Calcutta, India.

Lamyaa M. Almehmadi
Lamyaa M. Almehmadi is a Ph.D. student in Professor Igor K. Lednev's laboratory at the University at Albany, State University of New York (SUNY Albany).

Ethan A. Perets
Ethan A. Perets received his Ph.D. in Chemistry at Yale University, where his research focused on the development and application of vibrational spectroscopies to study hydration structures around proteins and DNA.

Coblentz SOCIETY

Headshots!

The Coblentz Society is sponsoring headshots Wednesday from noon to 3 pm. Stop by the booth in the exhibit hall to get your photos taken. Free for members; nominal charge for non-members.

ADDITIONAL AWARDS

SPECTROSCOPY MAGAZINE EMERGING LEADER IN MOLECULAR SPECTROSCOPY

Wei Lu
Wei Lu joined the faculty in the Division of Chemistry and Chemical Engineering at Caltech in 2018 after obtaining her Ph.D. in Chemistry from Columbia University, working with Prof. Wei Min.

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.

Joseph A. Loo
Joseph A. Loo is Professor of Chemistry and Biochemistry, and Biological Chemistry (David Geffen School of Medicine at UCLA) at the University of California, Los Angeles.

RSC ANALYTICAL DIVISION MID-CAREER AWARD

Karen Faulds
Karen Faulds is a Distinguished Professor in the Department of Pure and Applied Chemistry at the University of Strathclyde and an expert in the development of surface enhanced Raman scattering (SERS) and Raman techniques for novel analytical detection strategies and in particular multiplexed bioanalytical applications.

AES LIFETIME ACHIEVEMENT AWARD

Adrienne R. Minerick
Adrienne R. Minerick is currently a Professor of Chemical Engineering & Affiliated Professor of Biomedical Engineering at Michigan Technological University, where she was the founding Dean of the College of Computing and is a former Dean of the School of Technology.

AES MID-CAREER AWARD

Aditya S. Khair
Aditya Khair is a professor of chemical engineering in the Department of Chemical Engineering at Carnegie Mellon University in Pittsburgh, PA.

For full bios, scan here to visit scixconference.org/awards

SCHEDULE-AT-A-GLANCE

SUNDAY, OCTOBER 2, 2022

3:50 pm – 5:30 pm	**Oral Symposia**
	22IR11: Biological Applications of Vibrational Spectroscopy, *Meeting Room 2*
	22RAM14: Higher Order and Advanced Techniques, *Meeting Room 1*
	22SPECIAL12: Ordered Assemblies and Prepared Surfaces, *Meeting Room 3*
	22SPECIAL13: New Platforms and New Applications, *Meeting Room 4*
4:30 pm – 5:30 pm	"How to Make Connections: Student Networking at Conferences" *Meeting Room 6*
6:15 pm – 7:15 pm	Keynote: "The Future of Space Exploration: Earth-based, Deep Space-based, Robotic and Human;" Amanda Hendrix, Planetary Science Institute, *Ballroom C*
7:15 pm – 9:15 pm	Welcome Mixer and SAS Sponsored Student Poster Session, *Ballroom B*

MONDAY, OCTOBER 3, 2022

7:00 am – 8:30 am	Coblentz Annual Member Meeting and Breakfast, *Covington 1&2 (Marriott)*
8:30 am – 10:10 am	**Oral Symposia**
	22ART01: Student Research in Archaeological Chemistry, *Meeting Room 8*
	22ATOM01: LA-ICP-MS, *Meeting Room 4*
	22IR08: Advances in Vibrational Spectroscopy for PAT and Process Chemistry, *Ballroom D&E*
	22LIBS01: Fundamentals, *Meeting Room 5*
	22MASS01: Mass Spectrometry and Space, *Meeting Room 9*
	22PAT04: In Situ Spectroscopy for Industrial R&D, *Meeting Room 7*
	22PMA01: Characterization of Therapeutic Modalities: From Small Chiral Molecules to Fibrils and Nucleic Acids, *Meeting Room 10*
	22RAM01: Emerging Raman, *Ballroom C*
	22RAM02: SERS 1, *Meeting Room 1*
	22RAM16: Methods for Real Samples, *Meeting Room 3*
	22SPECIAL01: Coherent Multidimensional Spectroscopy Symposium I, *Meeting Room 2*
	22SPR01: Emerging Plasmonic Materials and Architectures, *Meeting Room 6*
10:10 am – 10:45 am	Poster Session/Break, *Ballroom B*
10:45 am – 12:00 pm	**Award Presentations and Plenary Sessions**, ***Ballroom C***
10:45 am	Award Presentations
11:00 am	RSC Analytical Division Mid-Career Award; Karen Faulds, University of Strathclyde
11:30 am	Ellis R. Lippincott Award; Martin Zanni, University of Wisconsin-Madison
12:15 pm – 1:30 pm	Coblentz Speed Mentoring, *Covington 1&2 (Marriott)*
1:30 pm – 3:10 pm	**Oral Symposia**
	22AES01: Extraterrestrial Electrokinetics, *Meeting Room 8*
	22ATOM02: Single Cell & NP ICP-MS Part I, *Meeting Room 4*
	22AWD01: RSC Analytical Division Mid-Career Award Symposium Honoring Karen Faulds, *Ballroom C*
	22CHEM02: Advances in Chemometrics, *Meeting Room 6*
	22CTP/EARLY01: Entrepreneurship in the Scientific Community, *Meeting Room 3*
	22LIBS09: Geological Applications, *Meeting Room 5*
	22PAT05: PAT Coblentz: Machine Learning, *Meeting Room 7*
	22PMA08: Bioprocess Materials and Methods, *Meeting Room 10*
	22RAM03: SERS 2, *Meeting Room 1*

	22RAM15: Raman Spectroscopy in Regenerative Medicine and 3Rs Research, *Ballroom D&E*
	22SPECIAL02: Coherent Multidimensional Spectroscopy Symposium II, *Meeting Room 2*
	22SPSJ03: Frontiers of Vacuum, Far, and Deep-Ultraviolet Spectroscopy I, *Meeting Room 9*
3:10 pm – 3:50 pm	Poster Session/Break, *Ballroom B*
3:50 pm – 5:30 pm	**Oral Symposia**
	22ATOM06: Single Cell & NP ICP-MS Part II, *Meeting Room 4*
	22AWD09: Ellis R. Lippincott Award Symposium Honoring Martin Zanni, *Ballroom C*
	22IR04: Mid-IR Lasers and Detectors as Enabling Technology for New Sensing Schemes, *Meeting Room 2*
	22IR07: Photothermal Session II, *Meeting Room 3*
	22LIBS03: Advanced Approaches II, *Meeting Room 5*
	22MASS03: Elemental and Isotopic Tracers: Technology and Applications, *Meeting Room 8*
	22PAT06: Process Analytical in Petroleum and Refinery Industries, *Meeting Room 7*
	22PMA06: Advanced Spectroscopic Techniques in PAT Part I, *Meeting Room 10*
	22RAM06: Biomedical Raman (Clirspec), *Ballroom D&E*
	22RAM10: SAS - SPECTROSCOPY IN SPACE, *Meeting Room 1*
	22SPR05: Early Career Researchers in Plasmonics, *Meeting Room 6*
	22SPSJ04: Frontiers of Vacuum, Far, and Deep-Ultraviolet Spectroscopy II, *Meeting Room 9*
5:30 pm – 6:30 pm	FACSS SciX Social Hour, *Rivercenter Lobby*

TUESDAY, OCTOBER 4, 2022

8:30 am – 10:10 am	**Oral Symposia**
	22AES02: Electrokinetic Fundamentals, *Meeting Room 8*
	22ATOM07: ICP-MS Applications, *Meeting Room 4*
	22BIM05: Nanotheranostics: Diagnosis and Treatment of Disease using Nanomaterials, *Meeting Room 3*
	22CHEM06: Pathways to Autonomous Chemometrics, *Meeting Room 6*
	22IR01: NanoIR in Material Science, *Ballroom D&E*
	22LIBS06: Space Applications, *Meeting Room 5*
	22MASS04: Rapid Screening and Assay Methods for Mass Spec and Beyond, *Meeting Room 10*
	22PAT01: SAS PAT Technical Section: PAT in Pharma, *Meeting Room 7*
	22RAM08: Raman Imaging and Microscopy, *Meeting Room 1*
	22RAM09: Spatially Offset Raman Spectroscopy, *Ballroom C*
	22SPECIAL07: Molecular Microspectroscopy and the Molecular Microspectroscopy Laboratory (MML), *Meeting Room 2*
	22SPSJ02: Near-Infrared Spectroscopy; Application to Biological and Materials Sciences, *Meeting Room 9*
10:10 am – 10:45 am	Poster Session/Break, *Event Center*
10:45 am – 12:00 pm	**Award Presentations**, ***Event Center***
10:45 am	Award Presentations
11:00 am	Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award; Lu Wei, California Institute of Technology
11:30 am	FACSS Charles Mann Award; Igor Lednev, University at Albany, State University of New York
12:00 pm – 1:30 pm	Exhibit Hall Lunch, *Event Center*

1:30 pm – 3:10 pm	**Oral Symposia**
	22AES04: Microfluidic Bioanalysis 1, *Meeting Room 8*
	22ATOM08: General Session, *Meeting Room 4*
	22AWD03: FACSS 2022 Charles Mann Award Symposium Honoring Igor Lednev, *Ballroom C*
	22BIM01: A New Stream of Intelligent Measurements and Data Science Part 1, *Meeting Room 3*
	22CHEM04: Chemometrics and Food Safety, *Meeting Room 6*
	22CTP/EARLY03: SAS Organized Session: Navigating Challenges to Achieve Success as an Early Career Spectroscopist, Part 1, *Meeting Room 7*
	22IR03: Nanoscale Spectroscopy: Advances in Instrumentation, *Ballroom D&E*
	22LIBS04: Molecular, *Meeting Room 5*
	22PMA04: SERS for Diagnostics and BioPharma Manufacturing, *Meeting Room 10*
	22RAM04: SERS 3, *Meeting Room 1*
	22SPECIAL09: Analytical Imaging I, *Meeting Room 2*
	22SPSJ01: Near-Infrared Spectroscopy; Spectral Analysis, Imaging, *Meeting Room 9*
3:10 pm – 3:50 pm	Poster Session/Break, Event Center
3:50 pm – 5:30 pm	**Oral Symposia**
	22ATOM04: Traditional and Atmospheric Glow Discharge Sources, *Meeting Room 4*
	22AWD02: Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Lu Wei, *Ballroom C*
	22CHEM01: A New Stream of Intelligent Measurements and Data Science Part 2, *Meeting Room 3*
	22CTP/EARLY04: SAS Organized Session: Navigating Challenges to Achieve Success as an Early Career Spectroscopist, Part 2, *Meeting Room 7*
	22FORENS03: Forensic Analysis in the Lab and at the Crime Scene, *Meeting Room 9*
	22LIBS05: Chemometrics, *Meeting Room 8*
	22LIBS07: Environmental and Cultural Applications, *Meeting Room 5*
	22PMA02: Pharmaceutical Forensics, *Meeting Room 10*
	22RAM13: TERS, *Ballroom D&E*
	22SPECIAL04: FACSS 2021 Charles Mann Award Symposium Honoring Roy Goodacre, *Meeting Room 1*
	22SPECIAL10: Analytical Imaging II, *Meeting Room 2*
	22SPR03: Biosensing with Plasmonics, *Meeting Room 6*
5:30 pm – 7:30 pm	Exhibitor-hosted Happy Hour, *Riverview Ballroom (Marriott)*
7:30 pm – 8:30 pm	SAS Award Presentations, *Covington 3 (Marriott)*
8:30 pm – 11:00 pm	SAS Members' Wine and Cheese Reception, *Covington 1&2 (Marriott)*

WEDNESDAY, OCTOBER 5, 2022

8:00 am – 10:30 am	Career Fair, *Terrace 3 (Marriott)*
8:30 am – 10:10 am	**Oral Symposia**
	22AES03: Microfluid Electrokinetic Devices, *Meeting Room 8*
	22BIM04: Machine and Deep Learning for Biomedical Diagnostics, *Meeting Room 3*
	22CHEM03: Chemometrics Something Borrowed, Something New, *Meeting Room 6*
	22CTP/EARLY02: Strategies for Finding Balance, *Meeting Room 5*
	22IR05: Quantum Cascade Lasers for Chemical Sensing, *Ballroom D&E*
	22IR09: Spectroscopic Methods for Materials Characterization, *Meeting Room 7*
	22MASS02: Advances in Novel Mass-Spectral Imaging, *Meeting Room 9*

	22PMA03: SERS for Drug Discovery, *Meeting Room 10*
	22RAM05: IRDG Raman, *Ballroom C*
	22RAM12: Raman Spectroscopy for Security and Forensics Purposes, *Meeting Room 1*
	22SPECIAL06: Regional Academic Research, *Meeting Room 2*
	22SPECIAL08: Spectrochimica Acta B - Award Session, *Meeting Room 4*
10:10 am – 10:45 am	Poster Session/Break, *Event Center*
10:45 am – 12:00 pm	**Award Presentations, *Event Center***
10:45 am	Award Presentations
11:00 am	Coblentz Craver Award; Wei Min, Columbia University
11:30 am	NESAS and SAS Lester W. Strock Award; Igor Gornushkin, BAM Federal Institute for Materials Research and Testing
12:00 pm – 1:30 pm	Exhibit Hall Lunch, *Event Center*
1:30 pm – 3:10 pm	**Oral Symposia**
	22AES06: Emerging Leaders Session, *Meeting Room 8*
	22AWD05: NESAS and SAS Lester W. Strock Award Symposium Honoring Igor Gornushkin, *Ballroom D&E*
	22AWD08: Coblentz Society Craver Award Symposium Honoring Wei Min, *Ballroom C*
	22BIM06: Optical Technologies for Disease Screening and Diagnostics, *Meeting Room 3*
	22FORENS04: Pharmaceutical Forensics, *Meeting Room 9*
	22LIBS08: Medical Applications, *Meeting Room 4*
	22LIBS10: Instrumentation, *Meeting Room 5*
	22PAT03: Advances in On-Line Process Analysis, *Meeting Room 7*
	22PMA07: Advances in the Analysis of Nanomaterials for Health, *Meeting Room 10*
	22RAM11: Raman Spectroscopy for Food Security, *Meeting Room 1*
	22SPECIAL05: Regional Industrial Research, *Meeting Room 2*
	22SPR02: Optical and Chiral Properties of Plasmonic Nanoparticles, *Meeting Room 6*
3:10 pm – 3:50 pm	Poster Session, *Event Center*
3:50 pm – 5:45 pm	Exhibits Closing Reception, *Event Center*

THURSDAY, OCTOBER 6, 2022 - ***Note the altered schedule for Thursday as we enjoy three plenary presenters this day!***

8:00 am – 10:10 am	FACSS Innovation Award Finalists Plenary Session (New day and time for 2022!), *Ballroom C*
10:10 am – 10:45 am	Break, *Rivercenter Lobby*
10:45 am – 12:30 pm	**Award Presentations**, ***Ballroom D&E***
10:45 am	Award Presentations
11:00 am	SAS and Applied Spectroscopy William F. Meggers Award; James Piret, The University of British Columbia
11:30 am	ANACHEM Award; Joseph Loo, University of California, Los Angeles
12:00 pm	AES Electrophoresis Mid-Career Award; Aditya Khair, Carnegie Mellon University
12:30 pm – 2:00 pm	Lunch on own
2:00 pm – 3:40 pm	**Oral Symposia**
	22ATOM03: Nuclear, *Meeting Room 3*
	22AWD06: AES Mid-Career Award Symposium Honoring Aditya Khair, *Meeting Room 7*
	22AWD07: SAS and Applied Spectroscopy William F. Meggers Award Symposium, *Ballroom D&E*
	22BIM03: Translation of Multimodal Imaging Technologies into Clinical Routine, *Meeting Room 2*
	22CHEM05: Chemometric Opportunities in the Forensic Sciences, *Meeting Room 5*

22FORENS02: Food Forensics, *Meeting Room 8*

22IR10: Coblentz, New England SAS, and New York/New Jersey SAS Celebrating Success of Nurturing Talent in Vibrational Spectroscopy, *Meeting Room 10*

22LIBS02: Advanced Approaches I, *Meeting Room 4*

22PAT02: SAS PAT Technical Section: PAT in BioPharma and Pharma, *Meeting Room 6*

22PMA09: Small Molecule Profiling, *Meeting Room 9*

22SPECIAL03: Celebrating Peter Griffiths' 80th Birthday, *Meeting Room 1*

3:40 pm – 4:00 pm Break, *Rivercenter Lobby*

4:00 pm – 5:40 pm Oral Symposia

22AES05: AES Lifetime Achievement Award Session Honoring Adrienne Minerick, *Meeting Room 7*

22ATOM05: Food, *Meeting Room 4*

22AWD04: ANACHEM Award Symposium Honoring Joseph Loo, *Ballroom D&E*

22BIM02: BioPhotonics Technologies Fighting Infections at the Point of Care, *Meeting Room 3*

22FORENS01: Nuclear Forensics, *Meeting Room 8*

22IR02: NanoIR in Life Science and Biology, *Meeting Room 2*

22PMA05: Industrial Applications of Vibrational Spectroscopy, *Meeting Room 9*

22RAM07: Transmission and Other Advanced Spectroscopic Sampling Methods in Pharmaceutical Analysis, *Meeting Room 1*

22SPECIAL11: Remembering Stanley Crouch, *Meeting Room 6*

22SPR04: Enhancing Chemical Processes with Plasmonics, *Meeting Room 5*

7:00 pm SciX Gala - All attendees welcome! Costume contest - Win free registration to SciX 2023! (New day for 2022!) *Attendees are required to come to the Gala wearing their SciX name badge.*

FRIDAY, OCTOBER 7, 2022

7:30 am – 7:45 am Continental Breakfast

7:45 am – 8:00 am Announcement of 2022 FACSS Innovation Award Winner, *Covington 3 (Marriott)*

8:00 am – 10:00 am Closing Plenary Session including Special Speakers, Announcement of 2022 FACSS Innovation Award Winner and SciX 2023 Preview

Bringing Home the Benefits of Space Exploration
Terrestrial Benefits of Space Exploration

Daniel Lockney

The Spaceflight Environment and Human Health and Performance

Charles Doarn

From Ocean Worlds to the Big Blue: How Planetary Robotics is Helping Us Explore the Deep Sea Cost-effectively

Pablo Sobron

SHORT COURSES/WORKSHOPS

Workshops are available for a separate registration fee.
Visit the registration desk to sign up. Space is limited and some courses may sell out.
All short courses/workshops will be taking place in the Marriott RiverCenter.
Please reference the App for room locations.

SUNDAY, OCTOBER 2 AND MONDAY OCTOBER 3

9:00am- 4:00pm (Both Days)
IR-Raman Interpretation
Peter Larkin, Solvay
Gloria Story, P&G
Facilitated in cooperation with Coblentz and SAS

MONDAY, OCTOBER 3

9:00am- 12:00pm (Half Day)
Fundamentals and Applications of Surface Enhanced Raman Spectroscopy (SERS)
Annie Dowgiallo, SRI International
FACSS SciX Workshop

1:00pm- 4:00pm (Half Day)
Practical Raman Spectroscopy
Sarah Shidler, Renishaw
Tim Prusnick, Renishaw
Facilitated in cooperation with Coblentz and SAS

TUESDAY, OCTOBER 4

9:00am- 12:00pm (Half Day)
Laser Fundamentals for Spectroscopy
Rob Chimenti, Rowan University

9:00am- 12:00pm (Half Day)
Problems with FT-IR Spectra and How to Avoid Them
Ellen Miseo, TeakOrigin, Inc.
Jenni Briggs, Pike Technologies
Facilitated in cooperation with Coblentz and SAS

THURSDAY, OCTOBER 6

9:00am- 4:00pm (Full Day)
Electrokinetic Microfluidics: Theory and Hands-on Problems
Neil Ivory, Washington State University
Facilitated in cooperation with AES

9:00am- 4:00pm (Full Day)
FTIR and Raman Spectroscopies Applied in Cosmetic and Beauty Industry
Samuel Gourion-Arsiquaud, TRI Princeton
Add Laurence Senek, TRI Princeton
Facilitated in cooperation with Coblentz and SAS

Please note 22BIM07 was cancelled and moved to a poster session on Tuesday prior to printing. Please reference the Tuesday Poster Session- BIM in the poster section.

22IR11: Biological Applications of Vibrational Spectroscopy *Meeting Room 2*

Chair: Mike George, *University of Nottingham*
Co-Chair: Curtis Marcott, *Light Light Solutions*

(6) **Breaking the Thiol Barrier: N-Heterocyclic Carbenes as a Robust Platform for Bioconjugation and Sensing**
Jon P. Camden[1]; [1]*University of Notre Dame*

(7) **Spectroscopic Studies Related to the Etiology of Dry Eye and Cataract**
Douglas Borchman[1]; [1]*University of Louisville*

(8) **Development and Evaluation of a Non-Contact Raman Spectroscopy Probe for In-Vivo Characterization of Otitis Media**
Sean Fitzgerald[1], Guillermo Monroy, Alexander Ho, Andrea K. Locke[1], Stephen A. Boppart[2], Anita Mahadevan-Jansen; [1]*Vanderbilt University,* [2]*University of Illinois at Urbana-Champaign*

(9) **Surface-Enhanced Raman Spectroscopy of Bacterial Metabolites to Unveil Bacterial Tolerance to Antibiotics**
Wei Wang[1], Peter J. Vikesland; [1]*Virginia Tech*

(10) **Application of Infrared Spectroscopy to Study the Stability of Biological Samples**
Anna Wójtowicz[1], Marcin Reciak, Renata Wietecha-Posłuszny; [1]*Jagiellonian University*

22RAM14: Higher Order and Advanced Techniques *Meeting Room 1*

Chair: Robert Lascola, *Savannah River National Laboratory*
Presider: Wei Zhao, *University of Arkansas at Little Rock*

(11) **Determination of Second Hyperpolarizability with Computational Raman Activities and Identification of DOVE Signatures for Selected Molecules**
Wei Zhao[1]; [1]*University of Arkansas at Little Rock*

(12) **White Light Continuum Generation in Bulk Media Triggers High-Speed Multiplex CARS in the Fingerprint Region**
Dario Polli[1], Federico Vernuccio, Arianna Bresci, Alejandro De La Cadena, Benedetta Talone, Chiara Ceconello, Francesco Manetti, Subir Das, Renzo Vanna, Giulio Cerullo; [1]*Politecnico di Milano*

(13) **Probing Coupled Folding and Binding Processes of Ribonuclease S with Temperature-Jump Multidimensional Infrared Spectroscopy**
Yumin Lee[1], Brennan Ashwood, Andrei Tokmakoff; [1]*University of Chicago*

(14) **Identifying Biomolecular Changes in Murine Cortical Tissue After Blast-Induced Traumatic Brain Injury Using Coherent Anti-Stokes Raman Scattering Microscopy**
Jacob Hardenburger[1], Pratheepa Rasiah, Anita Mahadevan-Jansen; [1]*Vanderbilt University*

(15) **Stable Isotope Raman Microspectroscopy: Applicability for Analysis of Microbial Degradation of Microplastics**
Natalia P. Ivleva[1], Julian Weng, Kara Müller, Martin Elsner; [1]*Technical University of Munich (TUM)*

22SPECIAL12: Ordered Assemblies and Prepared Surfaces *Meeting Room 3*

Chair: Robert Lascola, *Savannah River National Laboratory*
Presider: Craig Prater, *Purdue University*

(16) **Chiral-Specific Vibrational and Electronic Spectroscopy of Ordered Assemblies**
Garth J. Simpson[1]; [1]*Purdue University*

(17) **Spectroscopic and Microscopic Tracking of Multicomponent Supramolecular Nanostructures with Optoelectronic and Energy Transfer Properties**
Md Shah Alam[1], Jon Parquette, Karthikeyan Perumal, Jenae Linville; [1]*The Ohio State University*

(18) **Aerosol Jet Printed SERS Substrates for Ultrasensitive Detection of PFAS**
Rahul Rao[1], Colleen McDonnell, Faris Albarghouthi, Ryan Selhorst, Aaron Franklin; [1]*Air Force Research Laboratory*

(19) **A Non-Lithographic Universal Method to Fabricate Surface Enhanced Raman Scattering Substrates on Different Materials**
Ahmed Yousef Fouad Mahmoud[1], Alexandra Teixeira, Maria Silva, Francisca Guedes, Martin Lopez-Garcia, Sara Abalde-Cela, Lorena Diéguez; [1]*The International Iberian Nanotechnology Laboratory (INL)*

(20) **Controlled Citrate Oxidation on Gold Nanoparticle Surfaces for Improved SERS Analysis of Carboxylic and Phenolic Pollutants in Water**
Haoran Wei[1], Hanwei Wang; [1]*University of Wisconsin-Madison*

22SPECIAL13: New Platforms and New Applications *Meeting Room 4*

Chair: Robert Lascola, *Savannah River National Laboratory*
Presider: Wei Zhao, *University of Arkansas at Little Rock*

(21) **A New Hand-held FT-IR Spectrometer for Field-based Identifications of Vapor Phase Threats**
David W. Schiering[1], John Seelenbinder, Gregg Ressler; [1]*RedWave Technology*

Talks begin at 20-minute intervals.

TECHNICAL PROGRAM – SUNDAY, OCTOBER 2, 2022
Oral Symposia | 3:50 PM – 5:30 PM

(22) **Waveguide-Enhanced Raman Spectroscopy for Detection of Chemical Vapors**
Erik D. Emmons[1], Phillip G. Wilcox[1], Kevin Hung, Erik Roese, Ashish Tripathi, Jason Guicheteau, Ethan Luta, Benjamin Miller, Matthew Yates, Nathan Tyndall, Todd Stievater; [1]*US Army DEVCOM Chemical Biological Center*

(23) **Time-gated Raman Spectroscopy for Process Analyses in Downstream Purification Process of Monoclonal Antibody**
Amuthachelvi Daniel[1], Mari Tenhunen; [1]*Timegate Instruments Ltd*

(24) **Fluorescence-enhanced Photothermal Infrared Spectroscopy**
Craig Prater[1]; [1]*Photothermal Spectroscopy Corp*

(25) **Spectroelectrochemistry: More Than Just the Sum of Its Parts**
Sergey Shilov[1]; [1]*Bruker Optics*

TECHNICAL PROGRAM – SUNDAY, OCTOBER 2, 2022
Welcome and Keynote Lecture | 6:15 PM – 7:15 PM | *Ballroom C*

22SUNKEY01: Keynote Session

(26) **The Future of Space Exploration: Earth-based, Deep Space-based, Robotic and Human**
Amanda R. Hendrix[1]; [1]*Planetary Science Institute*

TECHNICAL PROGRAM – MONDAY, OCTOBER 3, 2022
Oral Symposia | 8:30 AM – 10:10 AM

22ART01: Student Research in Archaeological Chemistry *Meeting Room 8*

Chair: John Murray, *Arizona State University*

(27) **Vessels and their Residues: Exploring Nuances in the Diverse Scapes of South-Asia**
Ahana Ghosh[1]; [1]*Indian Institute of Technology*

(28) **Geochemical Data and Geospatial Methods: Characterizing Obsidian Use and Movement in Late Pleistocene Eastern Africa**
Sydney E. James[1]; [1]*Arizona State University*

(29) **pXRF as a Method to Identify Ochre Residues on Archaeological Ostrich Eggshell Fragments**
Hannah M. Keller[1], Ellery Frahm, Jessica C. Thompson[1]; [1]*Yale University*

(30) **Developing an Empirical Calibration for Elemental Characterization and Sourcing of South African Silcrete with pXRF**
John K. Murray[1], Jayde N. Hirniak[1], Andrew M. Zipkin[2]; [1]*Arizona State University,* [2]*Eurofins EAG Laboratories*

(31) **"It Starts Down Below": A Preliminary Study of Pollution Levels in Animals from the Southern Carpathian Bronze Age with ICP-MS**
Iride Tomazic[1], Amy Nicodemus, John O'Shea; [1]*University of Michigan*

22ATOM01: LA-ICP-MS *Meeting Room 4*

Chair: C. Derrick Quarles Jr., *Elemental Scientific, Inc.*

(32) **Dual fs-LIBS & fs-LA-ICPTOFMS System (Not Simultaneous) for Fast and High Dynamic Range Micro-Analysis: Pros and Cons.**
Jorge Pisonero[1], Cristina Méndez-López, Cristian Soto, Jaime Orejas, Ana Méndez, Antonia Cepedal, Nerea Bordel, Lukas Schlatt, Phil Shaw; [1]*University of Oviedo*

(33) **Recent Developments for In Situ Sr Isotope Ratios and Rb/Sr Geochronology by LA-ICP-MS/MS**
Alicia Cruz-Uribe[1], Cemil Arkula; [1]*University of Maine*

(34) **Elemental Histology: New Frontiers in LA-ICP-TOF-MS**
Keith MacRenaris[1], Andrew Crawford, David Zee, Qiaoling Jin, Thomas O'Halloran; [1]*Michigan State University*

(35) **Determination of Neurodegeneration-related Cytosolic Proteins in Individual Human Epithelial Cells by LA-ICP-MS Using Novel Matrix-Matched Standards and Metal Nanoclusters as Immunoprobes-Labels**
Ana Lores Padin[1], Beatriz Fernandez, Montserrat García, Héctor Ganzález Iglesias, Rosario Pereiro; [1]*University of Oviedo*

(36) **Elemental Distribution in Shark Teeth Using High-Speed LA-ICP-MS Imaging**
C. Derrick Quarles Jr.[1], Benjamin T. Manard[2], Christopher Hintz, Alicia Cruz-Uribe, Joseph Petrus, Cole R. Hexel[2]; *[1]Elemental Scientific, Inc., [2]Oak Ridge National Laboratory*

22IR08: Advances in Vibrational Spectroscopy for PAT and Process Chemistry *Ballroom D&E*

Chair: John Wasylyk, *Bristol Myers Squibb*
Co-Chair: Mike George, *University of Nottingham*

(37) **In Situ Monitoring of Amorphous Solid Dispersions Using Low Frequency (THz) Raman Spectroscopy**
Alison Nordon[1], Pattavet Vivattanaseth, Magdalene Chong, Elke Prasad, Gavin W. Halbert[1], John Robertson, Catriona McFarlan; *[1]University of Strathclyde*

(38) **Driving Sustainable Research by Maximizing Spectroscopy and Spectrometry Tools**
Robert Wethman[1], John M. Wasylyk[1], Ming Huang, David Fenton; *[1]Bristol Myers Squibb*

(39) **Use of Vibrational Spectroscopy in Cosmetic Science and Claims Substantiation**
Samuel Gourion-Arsiquad[1]; *[1]TRI*

(40) **Self-Optimising Flow Reactors for Multi-objective and Multistep Process Development**
Richard A. Bourne[1], Adam Clayton, John Blacker, Tom Chamberlain, Nik Kapur; *[1]University of Leeds*

(41) **Self-Optimisation of Flow Processes using A-TEEM Spectroscopy**
Ashley Love[1]; *[1]University of Nottingham*

22LIBS01: Fundamentals *Meeting Room 5*

Chair: Alessandro De Giacomo, *University of Bari*
Co-Chair: Jonathan Merten, *Arkansas State University*

(42) **Probing LIP-Atmosphere Interaction with Atomic Absorption Spectroscopy**
Jonathan A. Merten[1], Hannah Bariola, Shealyn Chestnut, Erin Nicholas, Shawnda Ethridge, Mary Foster; *[1]Arkansas State University*

(43) **Comprehensive Diagnostics of LIBS Plumes by Combining Emission and Absorption Spectroscopy**
Sivanandan Harilal[1], Elizabeth J. Kautz[1], Mark C. Phillips[2]; *[1]Pacific Northwest National Laboratory, [2]University of Arizona*

(44) **Fundamental Approaches to Broaden the Applications of Commercial Handheld LIBS**
Matthieu Baudelet[1], Kristen Livingston, Magdalena E. Jackson[2]; *[1]University of Central Florida, [2]Rensselaer Polytechnic Institute*

(45) **Femtosecond and Nanosecond Laser-assisted Surface Processing of Crystalline Silicon**
Reji Philip[1], Nancy Verma, Nithin Joy, Kiliyanamkandi Anoop; *[1]Raman Research Institute*

(46) **Vapor-phase Chemical Speciation and Condensation of Cerium Oxide Nanoparticles**
Kate Rodriguez[1], Batikan Koroglu, Joshua Hammons, Zurong Dai, Kim Knight; *[1]Lawrence Livermore National Lab*

22MASS01: Mass Spectrometry and Space *Meeting Room 9*

Chair: Theresa Evans-Nguyen, *University of South Florida*
Co-Chair: Jacob Shelley, *Rensselaer Polytechnic Institute*

(47) **Universal Liquid Sampling Ionization Mass Spectrometry**
Theresa Evans-Nguyen[1], Ashton Taylor, Cheyenne Sircher; *[1]University of South Florida*

(48) **SILICA (Surface Investigation via Lunar Imaging and Compositional Analysis): A Versatile Lunar Mission Concept**
Ricardo Arevalo[1], Ann Parsons, Soumya Ray, Ben Farcy, Mauricio Ayllon-Unzueta, Bret Bronner, Ryan Danell, Adrian Southard, Andrej Grubisic, Jacob Graham, Cynthia Gundersen, Julie Llano, Christelle Briois, Laurent Thirkell, Fabrice Colin, Alexander Makarov; *[1]University of MD*

(49) **Development of Novel Ion Inlet Designs for Laser Desorption Mass Spectrometers that Accommodate Different Surface Sampling Strategies**
Adrian Southard[1], Ricardo Arevalo, Friso Van Amerom, Ryan Danell, Desmond Kaplan, Julie Llano, Wally Rodriguez, Andrej Grubisic, Niko Minasola; *[1]University of MD*

(50) **Hypervelocity Impact Dissociation in Planetary Mass Spectrometry**
Daniel Austin[1], Brandon Turner, Eric Sevy, Matthew Asplund, Locke Hansen; *[1]Brigham Young University*

(51) **Presentation Title TBD**
Stojan Madzunkov[1]; *[1]NASA*

22PAT04: In Situ Spectroscopy for Industrial R&D *Meeting Room 7*

Chair: Mark Rickard, *DuPont*

(52) **In Situ Spectroscopy for Industrial Reaction Monitoring**
Xiaoyun (Shawn) Chen[1]; *[1]Dow*

(53) **In Situ IR Study on Polyurethane Reactions**
William Wang[1]; *[1]Lubrizol Advanced Materials*

Talks begin at 20-minute intervals.

(54) **Wide Spectral Range, Large Scanning Area, Cloud Connected and Compact FT-NIR Spectral Sensing Platform for On-site Analysis**
Yasser M. Sabry[1]; *[1]Si-Ware Systems*

(55) **Monitoring Structural and Chemical Curing Kinetics of Epoxy, Methacrylate, and Dual-Cure Resins for Additive Manufacturing Via In-Situ Raman Spectroscopy**
Robert V. Chimenti[1], Alexandra M. Lehman-Chong[1], Jianwei Tu, Joeseph F. Stanzione[1], Samuel E. Lofland[1], James T. Carriere[2]; *[1]Rowan University, [2]Coherent Inc.*

(56) **High Throughput Raman for Low-Volume Crystallization.**
Shamus Driver[1], Mark S. Kemper[2], Shaun J. Fraser[2]; *[1]Tornado Spetcral Systems, [2]Tornado Spectral Systems*

22PMA01: Characterization of Therapeutic Modalities: From Small Chiral Molecules to Fibrils and Nucleic Acids *Meeting Room 10*

Chair: Rina Dukor, *BioTools*

(57) **Presentation Title TBD**
Leo A. Joyce[1]; *[1]Arrowhead Pharmaceuticals, Inc.*

(58) **Application of Vibrational Circular Dichroism (VCD) in Drug Discovery and Development – Structure Elucidation of Chiral Molecules**
Yanan He[1]; *[1]GSK*

(59) **Presentation Title TBD" with "Lilliputian Particles: Scattering and Spectroscopy Applied to New Large Molecule Delivery Vehicles**
Kevin Dahl[1]; *[1]Particlese*

(60) **Vibrational Optical Activity to Elucidate the Conformational Behaviour of the Antibiotic Vancomycin and Derivatives**
Roy Aerts[1], Wouter Herrebout, Christian Johannessen; *[1]University of Antwerp*

(61) **Lipids Reverse Supramolecular Chirality and Reduce Toxicity of Amyloid Fibrils**
Kimberly Quinn[1], Stanislav Rizevsky, Kiryl Zhaliazka, Mikhail Matveyenka, Dmitry Kurouski; *[1]BioTools*

22RAM01: Emerging Raman *Ballroom C*

Chair: Pavel Matousek, *STFC Rutherford Appleton Laboratory*

(62) **Wearable/Flexible Surface-Enhanced Raman Spectroscopy**
Keisuke Goda[1]; *[1]The University of Tokyo*

(63) **Computational Stimulated Raman Scattering Microscopy**
Ji-Xin Cheng[1]; *[1]Boston University*

(64) **Investigating the Antimicrobial Properties of the Peptide, LL-37, in Preventing E. Coli Biofilm Forming: a Raman Microscopy-Based Approach**
Samantha L. Walker[1], William J. Tipping[1], Yun Xu, Sian Sloan-Dennison, Royston Goodacre, Howbeer Muhamadali, Duncan Graham, Donald Davidson, Karen Faulds; *[1]The University of Strathclyde*

(65) **Development of A Multifocal Spot Raman Spectrophotometer for High-Throughput Biological and Chemical Screening using 96 Microplates**
Hao-Xiang Liao[1], Kazuki Bando, Menglu Li, Katsumasa Fujita; *[1]Osaka University*

(66) **Efficient Separation and Characterization of Biomolecules by Optical Tweezers-Controlled Surface-Enhanced Raman Spectroscopy**
Jinqing Huang[1], Xin Dai, Wenhao Fu, Vince St Mesias, Wei Liu; *[1]The Hong Kong University of Science and Technology*

22RAM02: SERS 1 *Meeting Room 1*

Chair: Royston Goodacre, *The University of Liverpool*
Co-Chair: Sian Sloan-Dennison, *The University of Strathclyde*
Co-Chair: Zac Schultz, *The Ohio State University*

(67) **Automated Nanoparticle Synthesis for Improved SERS-based Sensing**
Samuel Mabbott[1]; *[1]Texas A&M University*

(68) **Development of SERS-Based Assay Platforms for Rapid and Accurate Diagnosis of SARS-CoV-2**
Jaebum Choo[1]; *[1]Chung-Ang University*

(69) **Into Another Dimension: Coupling Multidimensional Chromatography and SERS**
Christa Brosseau[1], Maddison M. Eisnor[1]; *[1]Saint Mary's University*

(70) **Differentiation of Glycans by Surface Enhanced Raman Spectroscopy**
Hannah C. Schorr[1], Zac D. Schultz[1]; *[1]The Ohio State University*

(71) **Differentiation of Structurally Similar Fentanyl Analogs with Theoretical and Experimental Analysis by Surface-Enhanced Raman Spectroscopy (SERS)**
Sevde Dogruer Erkok[1], Emily Hernandez, Bruce McCord; *[1]Florida International University*

22RAM16: Methods for Real Samples *Meeting Room 3*

Chair: Robert Lascola, *Savannah River National Laboratory*

(72) **Rapid Analysis Of Refined Fuel Properties Using A Novel Solid-State Raman Analyzer**
Brian Marquardt[1], Thomas Dearing; *[1]MarqMetrix*

(73) **New Innovative Raman Sampling Techniques Enable Quantitative Measurements on Raman Microscopes.**
Harry Owen[1]; [1]*HORC*

(74) **In-Process Laser Based Method for Detection Impurities at Trace Levels**
Edward A. Orr[1]; [1]*ABB Inc.*

(75) **Development of New Raman Gas Schemes with High Isotopic Discrimination and for the Analysis of Volatile Organic Compounds**
Torsten Frosch[1], Andreas Merian, Timea Frosch, Jürgen Popp; [1]*Technical University Darmstadt*

(76) **Capability of Portable Shifted Excitation Raman Difference Spectroscopy for Real-World Investigations**
Martin Maiwald[1], Kay Sowoidnich, André Müller, Bernd Sumpf; [1]*Ferdinand-Braun-Institut*

22SPECIAL01: Coherent Multidimensional Spectroscopy Symposium I *Meeting Room 2*

Chair: Wei Zhao, *University of Arkansas at Little Rock*

(77) **Multidimensional Floquet State Spectroscopy and Its Applications to Analytical Chemistry and Coherent Control of Reactions**
John C. Wright[1], Roger Carlson, Wei Zhao, Mark Rickard, Nathan Mathew, Lena Yurs, Erin Boyle, Peter C. Chen[2], Daniel Kohler, Kent J. Meyer[3], Jonathan Handali, Emily Kaufman, Kyle Sunden; [1]*University Wisconsin-Madison,* [2]*Spelman College,* [3]*UW Madison*

(78) **Time Resolved Nonlinear Spectroscopy of Excess Electrons in Aliphatic Ionic Liquids**
David A. Blank[1], Andrew T. Healy[1]; [1]*University of Minnesota*

(79) **High Resolution 2DIR spectroscopy**
Peter C. Chen[1], DeAunna Daniels, Thresa Wells; [1]*Spelman College*

(81) **Hyperspectral Chemical Imaging with Sum-Frequency Generation Microscopy**
Nien-Hui Ge[1], Hiroaki Maekawa, S. K. Karthick Kumar, Sudipta Mukherjee; [1]*University of California at Irvine*

22SPECIAL01: Coherent Multidimensional Spectroscopy Symposium II *Meeting Room 2*

(80) **Opportunities for Ultrafast 2D-IR Spectroscopy in Zeolite Catalysis Research**
Paul Donaldson[1], Russell Howe, Alex Hawkins, Gregory Greetham; [1]*STFC Central Laser Facility*

22SPR01: Emerging Plasmonic Materials and Architectures *Meeting Room 6*

Chair: Jean-Francois Masson, *University of Montreal*

(82) **Chemical Design of Colloidal Copper-Based Plasmonic Nanocrystals**
Xingchen Ye[1]; [1]*University of Indiana Bloomington*

(83) **Ultrabright Nanorattle Assay for Multiplexed SERS Detection of Molecular Biomarkers in Head and Neck Squamous Cell Carcinoma**
Joy Q. Li[1], Julia Canick, Hoan Ngo, Priya Dukes, Walter Lee, Tuan Vo-Dinh; [1]*Duke University School of Medicine*

(84) **Analysis of Nanostar Reshaping Kinetics for Optimal Substrate Fabrication**
Der Vang[1], Pietro Strobbia; [1]*University of Cincinnati*

(85) **A Plasmonic Puzzle: The Curious Properties of Hollow Metallic Nanoshells Prepared by the Galvanic Replacement of Silver**
Gregory Wallace[1], Ewen Smith, Tell Tuttle, Karen Faulds, Duncan Graham; [1]*The University of Strathclyde*

(86) **Plasmonic Magnesium Nanoparticles in Action**
Emilie Ringe[1], Vladimir Lomonosov, Thomas Wayman, Claire West, Elizabeth Hopper, Christina Boukouvala, Andrey Ten; [1]*University of Cambridge*

22PLEN01: Royal Society of Chemistry Analytical Division Mid-Career Award

(87) **Sensitive and Selective Bioanalysis using SERS and SESORS**
Karen Faulds[1], Duncan Graham, Matthew E. Berry[1], Anastasia Kapara, Samantha M. McCabe[1], Hayleigh Kearns; [1]*The University of Strathclyde*

22PLEN01: Ellis R. Lippincott Award

(88) **Advances in Interfacial and Voltage-gated Two-dimensional Infrared Spectroscopy**
Martin Zanni[1]; [1]*University Wisconsin-Madison*

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22AES01: Extraterrestrial Electrokinetics
Meeting Room 8

Chair: Christopher Harrison, *San Diego State University*

(89) **Single Molecule Methods to Seek Life As We Know It or Don't Know It**
Christopher E. Carr[1]; [1]*Georgia Institute of Technology*

(90) **Development and Optimization of Capillary Electrophoresis Instrumentation for Detection of Chemical Biosignatures on Future Life Detection Missions to Ocean Worlds**
Mauro Ferreira Santos[1], Konstantin Zamuruyev, Aaron Noell, Maria Mora, Peter Willis; [1]*NASA Jet Propulsion Laboratory*

(91) **Novel Deep Eutectic Solvents for the Fluorescent Labelling and Separation of Evidence of Past Life via CE-LIF**
Jessica Torres[1], Christopher R. Harrison[1], Karen S. Campos[1]; [1]*San Diego State University*

(92) **Panel & Open Discussion**

22ATOM02: Single Cell & NP ICP-MS Part I
Meeting Room 4

Chair: Alexander Gundlach-Graham, *Iowa State University*

(93) **Single Particle ICP-TOFMS: From Quantification to Interpretation**
Alexander Gundlach-Graham[1], Sarah E. Szakas[1], Stasia Harycki, Hark B. Karkee[2], Raven Buckman; [1]*Iowa State University,* [2]*Iowa State university*

(94) **Single particle/cell ICP-ToF-MS as a powerful tool in environmental and material research**
Björn Meermann[1]; [1]*Federal Institute for Materials Research and Testing (BAM)*

(95) **Towards Normalization of Quantitative Single Cell ICP-MS Experiments**
Maria Montes-Bayon[1], Roberto Alvarez-Fernandez Garcia, Juliana Severo Fagundes, Jörg bettmer, Zoltan Mester, Kelly LeBlanc; [1]*University of Oviedo*

(96) **Size Determination of Nanoparticles by ICP-ToF-MS using Isotope Dilution in Microdroplets**
Marcus von der Au[1], Sebastian Faßbender, Michail Ioannis Chronakis, Björn Meermann; [1]*Federal Institute for Materials Research and Testing (BAM)*

(97) **Metallic Environmental Particulate Matter Monitoring Using a Gas-Exchange Device Coupled to ICP-MS Run in Single Particle Mode**
Chady Stephan[1], Aaron Hineman, Ruth Merrifield; [1]*PerkinElmer Inc.*

22AWD01: Royal Society of Chemistry Analytical Division Mid-Career Award Symposium Honoring Karen Faulds *Ballroom C*

Chair: Karen Faulds, *The University of Strathclyde*

(98) **Knowledgeable Analytical Raman Enhancing Nanoparticles**
Royston Goodacre[1], Howbeer Muhamadali; [1]*The University of Liverpool*

(99) **Translating Sensors from Feasibility to Future Product**
Kristy S. McKeating[1]; [1]*Fitbit*

(100) **Turning vibrational data into music**
Colin J. Campbell[1]; [1]*University of Edinburgh*

(101) **Raman Spectroscopy and Semi-Supervised Learning for Improved Treatment of Patients Receiving HDR-Brachytherapy**
Kirsty Milligan[1], Xinchen Deng, Ramie Ali-Adeeb, Phil Shreeves, Juanita Crook, Julian Lum, Alexandre Brolo, Jeffrey Andrews, Andrew Jirasek; [1]*University of British Columbia*

(102) **SERS, SRS and Shenanigans**
Duncan Graham[1]; [1]*The University of Strathclyde*

22CHEM02: Advances in Chemometrics *Meeting Room 6*

Chair: Peter Harrington, *Ohio University*

(103) **Building Concordant Ontologies Using KNARM (Knowledge Acquisition and Representation Methodology)**
Hande Küçük McGinty[1]; [1]*Kansas State University*

(104) **Data Tensorization for Better Curve Resolution of Exponential Mixtures**
Cyril Ruckebusch[1], Adrian Gomez Sanchez, olivier devos, Anna de Juan; [1]*University of Lille*

(105) **Generative Adversarial Linear Analysis**
Garth J. Simpson[1]; [1]*Purdue University*

(106) **Using Chemometrics to Track Down the Source of Variance Between Authentic Botanical Samples**
Jim Harnly[1]; [1]*USDA ARS*

(107) **Raman Spectroscopy Of Fish Blood as a Screening Test For The Lake Pollution With Perfluoroalkyl Substances (PFAS)**
Luis Perez-Almodovar[1], Igor K. Lednev[1]; [1]*University at Albany, State University of New York*

22CTP/EARLY01: Entrepreneurship in the Scientific Community *Meeting Room 3*

Chair: Alexis Weber, *University at Albany, State University of New York*

(108) **Supporting Tech Transfer: The Funding Agency Perspective**
Gregory Dutton[1]; [1]*National Institute of Justice*

(109) **Funding a Start-up and Navigating the World of Non-Dilutive Funding.**
Jeffery Harrison[1]; [1]*Pyrochem Catalyst Company*

(110) **Time-Resolved Spectroscopy in Academia to a Successful Small Business Innovation Research Grant in Industry**
Amy Scott[1]; [1]*Beta Analytic*

(111) **Entrepreneurship for the Academic: the Good, the Baffling, and the Insanity**
Alexander Scheeline[1]; [1]*SpectroClick Inc.*

(112) **Customer Led Design and "Failing Fast" in Hardware Design**
Jonathon Speed[1]; [1]*Keit Spectrometers*

22LIBS09: Geological Applications *Meeting Room 5*

Chair: Cécile Fabre, *Universite de Lorraine / GeoRessources*

(113) **From Mineral Sources and Stalactites to Soils and Street Safety: LIBS Applications that Improve the Quality of our Lives**
Nancy J. McMillan[1]; [1]*New Mexico State University USA*

(114) **LIBS to Fight Against Climate Change: A New Approach for the In-Situ Assessment of Carbon Capture in Geological Matrices**
Josette El Haddad[1], Paul Bouchard, Christian Padioleau, Kim Renaud, Francis Vanier, Elton Soares de Lima Filho, Aïssa Harhira, Mohamad Sabsabi; [1]*National Research Council Canada*

(115) **Contribution of LIBS to Mineral Resources: from Multi-Elementary Analysis to Mineralogical Mapping**
Cécile Fabre[1]; [1]*Universite de Lorraine / GeoRessources*

(116) **Quantitative Analysis of Fluorine in Geological Samples with Handheld Laser-Induced Breakdown Spectroscopy**
Gabrielle Lambton[1]; [1]*Sciaps*

(117) **In-Situ Multispectral Investigation of the Biogeochemistry of the Geldingadalir Lava Field**
Kirby Simon[1], Pablo Sobron, Renata Barros, Giorgia Stasi, Aurélien Daussin; [1]*Impossible Sensing*

22PAT05: PAT Coblentz: Machine Learning *Meeting Room 7*

Chair: Jim Rydzak, *Specere Consulting*
Co-Chair: Mike George, *University of Nottingham*

(118) **Improving NIR Moisture Analysis through a Novel Synchronized, Automatic Calibration Data Collector**
Adam J. Hopkins[1], Elena Hagemann, Scott Segro, Frank Koch; [1]*Metrohm USA*

(119) **Sensor Agnostic Threat Anomaly Detection (ThreAD) for Explosives**
Eric R. Languirand[1], Justin Curtiss, Darren Emge; [1]*U.S. Army DEVCOM CBC*

(120) **High Throughput Raman Monitoring of Downstream Bioprocess Purifications**
Mark S. Kemper[1], Shamus Driver, Shaun J. Fraser[1]; [1]*Tornado Spectral Systems*

(121) **Tablet API Determination Via Chemometric Analysis**
William Worley[1]; [1]*JMP Statistical Discovery, LLC*

(122) **ATR-FTIR and Chemometric Techniques in Solid Biofuels Application: Targeting the Bio-coke Product**
Supitchaya Cherdkeattikul[1], Yusuke Morisawa, Tamio Ida; [1]*Kindai University*

22PMA08: Bioprocess Materials and Methods *Meeting Room 10*

Chair: John Bobiak, *Bristol Myers Squibb*

(123) **Rapid FTIR Method For Monitoring and Assessment of the Critical Quality Attribute of AAV Capsid Genome Packaging Contents**
Yelena Pyatski[1], Kimberly Quinn, Rina K. Dukor[1]; [1]*BioTools*

(124) **Characterization of Charge Tunable Nanoemulsions Stabilized by Cationic/Anionic Surfactant Mixtures**
Konnor Jones[1], Lawrence Scatena; [1]*University of Oregon*

(125) **In-Line Lipidomics of Oil-Producing Yeast Cells for a More Sustainable Palm Oil Life Cycle**
Karin Wieland[1], Mahmoud Masri, Jeremy von Poschinger, Thomas Brück, Christoph Haisch; [1]*Competence Center CHASE GmbH*

(126) **DDetermination of Protein and Peptide Conformation and Orientation at Buried Interfaces in Situ in Real Time**
Wen Guo[1], Tieyi Lu, Ralph Crisci, Satoshi Nagao, Tao Wei, Zhan Chen; [1]*University of Michigan*

(127) **Microchip Electrophoresis for Single Cells Measurements of Oxidative Stress**
Tyler Allcroft[1], Michelle L. Kovarik[1]; [1]*Trinity College*

22RAM03: SERS 2 *Meeting Room 1*

Chair: Sian Sloan-Dennison, *The University of Strathclyde*
Co-Chair: Royston Goodacre, *The University of Liverpool*
Co-Chair: Zac Schultz, *The Ohio State University*

(128) **SERS Based Monitoring of Bacterial Stress Responses**
Peter J. Vikesland[1], Wei Wang, ASIFUR Rahman, Qishen Huang; [1]*Virginia Tech*

(129) **SERS of Cells: from Status to Physiological Process**
Janina Kneipp[1], Cecilia Spedalieri, Yiqing Feng, Vesna Zivanovic, Gergo Peter Szekeres; [1]*Humboldt-Universität zu Berlin*

(130) **SERS-based Vertical Flow Assay on Plasmonic Paper for Point of Care Diagnostics**
Jeremy D. Driskell[1], Eunice Ebbah, Richard Frimpong, Wongji Jang, Jun-Hyun Kim; [1]*Illinois State University*

(131) **Gold Nanoparticle (AuNP) Based Surface-Enhanced Raman Spectroscopy (SERS) Substrates for Sensitive Detection of Environmental Contaminants**
Seju Kang[1], Peter J. Vikesland; [1]*Virginia Tech*

(132) **Biomimetic Transparent Nanoplasmonic Meshes by Reverse-Nanoimprinting for Bio-interfaced Spatiotemporal Multimodal Surface-enhanced Raman Spectroscopy**
Aditya Garg[1], Elieser Mejia, Wonil Nam, Peter J. Vikesland, Wei Zhou; [1]*Virginia Tech*

22RAM15: Raman Spectroscopy in Regenerative Medicine and 3Rs Research *Ballroom D&E*

Chair: Ioan Notingher, *University of Nottingham*

(133) **Raman Microspectroscopy and Raman Imaging in Regenerative and Personalized Medicine**
Julia Marzi[1], Katja Schenke-Layland; [1]*University of Tübingen*

(134) **Transcutaneous Raman Spectroscopy of Bones in Human Cadaver Hands**
Andrew J. Berger[1], Christine Massie, Hani Awad, Emma Knapp; [1]*University of Rochester*

(135) **Raman Spectroscopy for Monitoring Native and Engineered Cartilage Health**
Mads S. Bergholt[1], Martin Hedegaard, Michael Albro, Elzbieta Stepula, Magnus Jensen, Brian Snyder, Anders R. Walther; [1]*King's College London*

(136) **Development of Bessel-beam illumination Raman microcopy for thick samples**
Kazuki Bando[1], Shumpei Yabuuchi, Menglu Li, Toshiki Kubo, Ryosuke Oketani, Nicholas I. Smith[1], Satoshi Fujita, Katsumasa Fujita; [1]*Osaka University*

(137) **Spectral CARS Signatures Identifies Intestinal Cell Types, Including LGR5+ Intestinal Stem Cells**
Patrik K. Johansson[1], Katarina C. Klett[1], Chris Long, Sarah C. Heilshorn[1], Annika Enejder; [1]*Stanford University*

22SPECIAL02: Coherent Multidimensional Spectroscopy Symposium II *Meeting Room 2*

Chair: Wei Zhao, *University of Arkansas at Little Rock*

(138) **Local CO Behavior on Polycrystalline Pt Electrode Surface Using Compressive Sensing Sum Frequency Generation Microscopy (CS-SFGM) Combined with Electrochemistry**
Steven Baldelli[1], Hao Li; [1]*University of Houston*

(140) **Expanding Advanced Chemical Microscopy via Innovations and Commercialization**
Ji-Xin Cheng[1]; [1]*Boston University*

(141) **Ultrafast Interconversion between Excitonic Valley States in Monolayer MoS2 Due to Intrinsic Coupling**
Greg Engel[1], Lawson Lloyd, Ryan Wood, Fauzia Mujid, Siddhartha Sohoni, Karen Ji, Po-Chieh Ting, Jacob Higgins, Jiwoong Park; [1]*University of Chicago*

(142) **Stimulated Raman Excited Fluorescence: Combining the Best of Two Worlds**
Wei Min[1]; [1]*Columbia University*

22SPSJ03: Frontiers of Vacuum, Far, and Deep-Ultraviolet Spectroscopy I *Meeting Room 9*

Chair: Yusuke Morisawa, *Kindai University*

(143) **Electrochemical Far- and Deep-Ultraviolet Spectroscopy Applied for Organic Semiconductor/Ionic Liquids Interfaces**
Ichiro Tanabe[1]; [1]*Rikkyo University*

(144) **Direct Observation and Attribution of the Vertical Transitions of the**
Nami Ueno[1], Yusuke Morisawa, Yukihiro Ozaki; [1]*Kobe University*

(145) **Changes in Electronic States of Saturated Cyclic Compoud with Six-Membered Rings**
Yusuke Morisawa[1]; [1]*Kindai University*

(146) **Label-Free Autofluorescence-Detected Mid-Infrared Photothermal Microscopy**
Aleksandr Razumtcev[1], Minghe Li, Garth J. Simpson[1]; [1]*Purdue University*

(147) **Imaging Molecular Diffusion And Adsorption Through Nanoporous Silica Particles: Exploring Molecular Transport In Chromatography Separations**
Hong Bok Lee[1], Max Lei Lei Geng[1]; [1]*University of Iowa*

Talks begin at 20-minute intervals.

22ATOM06: Single Cell & NP ICP-MS Part II
Meeting Room 4

Chair: Antonio Montoro Bustos, *National Institute of Standards and Technology*
Co-Chair: C. Derrick Quarles Jr., *Elemental Scientific, Inc.*

(148) **Determination of Proteins in Single Cells by Inductively Coupled Plasma-Mass Spectrometry using Metal Nanoclusters as Labels of Specific-Recognition Reactions**
Beatriz Fernandez[1], Paula Menero-Valdés, Ana Lores Padin, C. Derrick Quarles Jr., Montserrat García, Héctor González-Iglesias, Rosario Pereiro; [1]*University of Oviedo*

(149) **Finding Small Particles in Complex Samples: Recent Advances of spICP-MS**
Carsten Engelhard[1], Darya Mozhayeva, Annika Schardt, Johannes Schmitt, Ingo H. Strenge[1]; [1]*University of Siegen*

(150) **Analysis of nanoparticles in food by single particle ICP-MS**
Katrin Loeschner[1], Janja Vidmar, Luisa Hässmann; [1]*Technical University of Denmark*

(151) **Single Cell ICP-MS (SC-ICP-MS) to Study the Uptake and Apoptotic Status of Nanoplatinum (IV) Treated Cells**
Lucía Gutiérrez-Romero[1], Elisa Blanco-González, Borja Gallego-Martínez, René Rodríguez-González, Maria Montes-Bayon; [1]*University of Oviedo*

(152) **Online Microdroplet Calibration for the Quantification of Metal and Metal Oxide Nanoparticles in Organic Matrices**
Stasia Harycki[1], Alexander Gundlach-Graham; [1]*Iowa State University*

22AWD09: Ellis R. Lippincott Award Symposium Honoring Martin Zanni *Ballroom C*

Chair: Martin Zanni, *University Wisconsin-Madison*

(153) **Dynamics of Protein Molecular Recognition via Vibrational Spectroscopy**
Megan Thielges[1]; [1]*Indiana University*

(154) **Commercialization of Ultrafast 2D Spectroscopy: How a Spectroscopy Startup Grew from the Basement into a Company**
Chris T. Middleton[1]; [1]*PhaseTech Spectroscopy, Inc.*

(155) **Structural Transitions of FUS Protein Within Liquid-Liquid Phase Separated Droplets Probed by Light Scattering and 2DIR Spectroscopy**
Arnaldo Serrano[1], Anna Zepeda, Dean Edun; [1]*University of Notre Dame*

(156) **Measuring Protein Structure and Dynamics on Nanoparticle Surfaces via 2D IR Spectroscopy**
Lauren E. Buchanan[1]; [1]*Vanderbilt University*

(157) **Applications of IR Spectroscopy from PIKE Technologies**
Kent Gundlach[1], Jenni Briggs, Andy Bean; [1]*PIKE Technologies*

22IR04: Mid-IR Lasers and Detectors as Enabling Technology for New Sensing Schemes *Meeting Room 2*

Chair: Markus Brandstetter, *Research Center for Non-Destructive Testing GmbH*

(158) **Rapid Vibrational Circular Dichroism – Opportunities through the combination of External Cavity Quantum Cascade lasers and balanced detection**
Daniel-Ralph Hermann[1], Georg Ramer, Bernhard Lendl; [1]*TU Wien*

(159) **Mid-Infrared Hyperspectral Single-Pixel Imaging Microscopy**
Alexander Ebner[1], Paul Gattinger, Ivan Zorin, Christian Rankl, Markus Brandstetter; [1]*Research Center for Non-Destructive Testing GmbH*

(160) **Introducing Temperature-controlled Desorption Separation by Nanoelectromechanical Photothermal Infrared Spectroscopy**
Niklas Luhmann[1], Robert G. West[2], Raphael Pliessnig, Josiane P. Lafleur[1], Silvan Schmid; [1]*Invisible-Light Labs,* [2]*Institute of Sensor and Actuator Systems - TU Wien*

(161) **Quantum Cascade Laser Dual-Comb Spectroscopy in Solid, Liquid, and Gas Phase Measurements**
Markus Mangold[1], Raphael Horvath, Jakob Hayden, Pitt Allmendinger; [1]*IRsweep AG*

(162) **New Approaches to High-Sensitivity QCL-IR Spectroscopy of Proteins in Water**
Young J. Lee[1], Seong-min Kim, Yow-Ren Chang; [1]*National Institute of Standards and Technology*

22IR07: Photothermal Session II *Meeting Room 3*

Chair: Rohith Reddy, *University of Houston*

(163) **O-PTIR and Raman Spectroscopic Imaging for the High Resolution Elucidation of Breast Microcalcification Heterogeneities.**
Nicholas Stone[1], Pascaline Bouzy, Keith Rogers, Robert Scott, Iain Lyburn, Eleanor Cornford, Charlene Greenwood, Jayakrupakar Nallala; [1]*University of Exeter*

(164) **Correlative Spectroscopic Analysis of Buccal Cells: O-PTIR (Far Field IR, Raman) and Superresolved Fluorescence Imaging**
Kathleen M. Gough[1], Sabine Mai, Mustafa Kansiz, Gorkem Bakir, Atacenk Baslic, Benoit Girouard, Curtis Mensforth, Darryl Dyck, Rohith Reddy, Chalapathi Gajjela; *[1]University of Manitoba*

(165) **Tissue Subtype Identification using Photothermal Mid-infrared Spectroscopic Imaging**
Chalapathi Gajjala[1], Rupali Mankar, Ragib Ishrak, Xinyu Wu, Reza Reihani, Sharmin Afrose, David Mayerich, Rohith Reddy; *[1]University of Houston*

(166) **Mid-Infrared Biomarkers of Lupus Nephritis Using Optical-Photothermal imaging**
Chalapathi Gajjala[1], Rohith Reddy; *[1]University of Houston*

(167) **High-Speed Photothermal Mid-Infrared Spectroscopic Imaging Through Optimization of Sampling Parameters**
Rupali Mankar[1], Rohith Reddy, Chalapathi Gajjala, David Mayerich, Xinyu Yu; *[1]University of Houston*

22LIBS03: Advanced Approaches II *Meeting Room 5*

Chair: Jhanis Gonzalez, *Lawrence Berkeley National Laboratory*

(168) **Femtosecond LIBS Plasmas Induced by GHz Burst Mode Ablation**
Vassilia Zorba[1], Minok Park, Xianglei Mao, Costas Grigoropoulos; *[1]Lawrence Berkeley National Laboratory*

(169) **Nuclear Safeguards with Laser-Induced Breakdown Spectroscopy**
George Chan[1]; *[1]Lawrence Berkeley National Laboratory*

(170) **Quantitative Evaluation of U-Zr Alloy Fuels Utilizing Femtosecond LIBS**
Matthew M. Jones[1], Joey Charboneau, Nick Erfurth, Laura Sudderth; *[1]INL*

zLukas Schlatt[1], Phil Shaw; *[1]Nu Instruments*

(172) **End Point Detection in Laser Machining using LIBS Emission Real Time Monitoring**
Burak E. Sancaktar[1], Eduardo A. Rojas-Nastrucci, Susan D. Allen; *[1]Embry Riddle Aeronautical University*

22MASS03: Elemental and Isotopic Tracers: Technology and Applications *Meeting Room 8*

Chair: Kaveh Jorabchi, *Georgetown University*

(173) **Structurally Specific Mass Distribution-Based Isotopic Shifts in High-Resolution Cyclic Ion Mobility Separations Coupled to Mass Spectrometry**
Gabe Nagy[1], David L. Williamson[1]; *[1]University of Utah*

(174) **The IROA Protocol for Improving Metabolomics Data Quality**
Chris Beecher[1]; *[1]IROA Technologies*

(175) **On-Line Hyphenation of Capillary Electrophoresis with Multicollector-ICP-MS (CE/MC-ICP-MS) for Species-Specific Isotope Ratio Analysis of Sulfur Species**
Björn Meermann[1], Sebastian Faßbender, Dariya Tukhmetova, Katerina Rodiouchkina, Frank Vanhaecke; *[1]Federal Institute for Materials Research and Testing (BAM)*

(176) **HPLC-Parallel Accelerator and Molecular Mass Spectrometry Analysis of 14C-Labeled Amino Acids**
David Baliu-Rodriguez[1], Ted J. Ognibene[1], Benjamin J. Stewart[1], Bruce A. Buchholz[1]; *[1]Lawrence Livermore National Laboratory*

(177) **Rapid Metabolite Quantitation by Simultaneous F and Cl Speciation**
Kaveh Jorabchi[1], Frenio Redeker, Grace Hahm; *[1]Georgetown University*

22PAT06: Process Analytical in Petroleum and Refinery Industries *Meeting Room 7*

Chair: Toni Miao, *Chevron*

(178) **Optimizing Spectroscopy Performance**
Brian G. Rohrback[1]; *[1]Infometrix, Inc.*

(179) **Qualitative and Quantitative Analysis of Total Petroleum Hydrocarbons (TPHs) in Soil by Handheld Near-Infrared (NIR) Spectroscopy**
Heinz Wilhelm Siesler[1], Toni Miao, Natasha Sihota, Frank Pfeifer, Cory McDaniel, Marina de Gea Neves; *[1]University of Duisburg-Essen*

(180) **Robust Fiber Optic Probes for Industrial Process Control**
Tatiana Sakharova[1], Viacheslav Artyushenko, Toni Miao, Alexey Bocharnikov, Alexander Novikov, Iskander Usenov, Steven Barnett; *[1]art photonics GmbH*

(181) **Process Gas Analysis by 785-nm Raman Spectroscopy**
Colin W. Couper[1]; *[1]Tornado Spectral Systems*

(182) **Near Infrared Analyzers Applied to Process Control and Optimization in the Refinery: Measurement of Light Hydrocarbon to Heavy Hydrocarbon Liquid Streams**
Allan J. Rilling[1], Edward A. Orr[2], Jose Quintero-Escorcia; *[1]ABB Inc, [2]ABB Inc.*

22PMA06: Advanced Spectroscopic Techniques in PAT Part I *Meeting Room 10*

Chair: John Wasylyk, *Bristol Myers Squibb*
Co-Chair: Mike George, *University of Nottingham*

(183) **Coherent Control of Chemical Reactions Using Floquet States**
John C. Wright[1], Kent J. Meyer[2], Lucian Hand, Martynas J. Miškinis[3], Vytautas Sinkus, Nick Adams; *[1]University Wisconsin-Madison, [2]UW Madison, [3]Light Conversion USA*

(184) **Fiber Spectroscopy for in-line Process Control in 0.3-16µm Range**
Viacheslav Artyushenko[1]; *[1]art photonics GmbH*

(185) **Upstream Process Monitoring by Time-gated Raman Spectroscopy**
Amuthachelvi Daniel[1], Mari Tenhunen; *[1]Timegate Instruments Ltd*

(186) **Quantum Cascade Laser (QCL)-based IR Liquid Analyzer for Real-Time Measurement of Protein Concentrations and Higher Order structures (HOS)**
Jeremy Rowlette[1], Santosh Hodawadekar; *[1]DRS Daylight Solutions*

(187) **A Micro-Raman Study of Structural Changes Produced in Antimony and Antimony Chalcogenide Thin Photovoltaic films as a Result of Argon Ion Sputtering During X-ray Photoelectron Spectroscopy Experiments**
Tariq Jawhari[1], Xavier Alcobé, Lorenzo Calvo-Barrio, Diego Fraga Chiva, Samuel Porcar García, Juan Bautista Carda Castelló, Isidro Martin Garcia; *[1]CCiT, Universitat de Barcelona (UB)*

22RAM06: Biomedical Raman (Clirspec) *Ballroom D&E*

Chair: Nicholas Stone, *University of Exeter*

(188) **Autofluorescence-Raman Analysis of Surgical Margins During Mohs Micrographic Surgery: Clinical Integration and Preliminary Validation Results**
Ioan Notingher[1]; *[1]University of Nottingham*

(189) **Deep Raman Spectroscopy: Multiplexed Signal Recovery for Future Theranostics**
Ben Gardner[1], Nicholas Stone, Pavel Matousek, Sara Mosca, Francesca Palombo, Megha Mehta, Marzieh Salimi; *[1]University of Exeter*

(190) **Non-Invasive Multimodal Spectroscopic Diagnosis for Early Stage Oral Cancer**
Siddra Maryam[1], Daniyal Ghauri, Rekha Gautam, Kiang Kho, Marcelo S. Nogueira[1], Sanathana k. Sekar[1], Huihui Lu, Richeal Riordain, Linda Feeley, Patrick Sheahan, Ray Burke, Stefan Andersson-Engels; *[1]Tyndall National Institute*

(191) **High-resolution Raman Imaging of >300 Cells from Human Patients Affected by Nine Different Leukemia Subtypes: Virtual Staining Using a Global Clustering Approach**
Renzo Vanna[1], Andrea Masella, Manuela Bazzarelli, Paola Ronchi, Aufried Lenferink, Cristina Tresoldi, Carlo F. Morasso[2], Caludio Masolo, Marzia Bedoni, Dario Polli, Fabio Ciceri, Giulia De Poli, Matteo Bregonzio, Cees Otto; *[1]CNR-Institute for Photonics and Nanotechnologies (IFN-CNR), [2]Istituti Clinici Scientifici Maugeri IRCCS*

(192) **Raman Endoscope for Diagnosis of Eosinophil Esophagitis**
Hidetoshi Sato[1], Riki Zakaria, Takumu Watanabe, Soichiro Ishihara, Keita Iwasaki, Bibin Andriana, Kosuke Hashimoto, Tatsuyuki Yamamoto, Naoki Oshima; *[1]Kwansei Gakuin University*

22RAM10: SAS - SPECTROSCOPY IN SPACE *Meeting Room 1*

Chair: Andrew Whitley, *HORIBA Scientific*

(193) **Recent Advances in Long-Range Remote Raman Systems for Planetary Exploration**
Shiv K. Sharma[1], Stanley M. Angel[2], Paul G. Lucey, Tayro Acosta-Maeda, Evan M. Kelly[1]; *[1]University of Hawaii at Manoa, [2]The University of South Carolina*

(194) **Exploring Jezero Crater with SuperCam on the Perseverance Rover**
Sam Clegg[1], Ann Ollila, Ryan Anderson, Olivier Forni, Agnis Cousin, Jeremie Lasue, Chip Legett, Paolo Pilleri, Elise Clave, Shiv K. Sharma[2], Olivier Beyssac, Jeff Johnson, Guillermo Lopez Reyes, Nina Louise Lanza, Baptiste Chide, Juan Manuel Madariaga, Sylvestre Maurice, Roger Wiens, The SuperCam Team; *[1]Los Alamos National Lab, [2]University of Hawaii at Manoa*

(195) **SHERLOC: Results of the First 400 Sols of Operations**
Luther Beegle[1], Rohit Bhartia, William Hug, SHERLOC Science Team; *[1]California Institute of Technology*

(196) **SHERLOC: Deep UV Raman from Earth to Mars**
Rohit Bhartia[1], Luther Beegle; *[1]Photon Systems, Inc.*

(197) **Panel & Open Discussion**

TECHNICAL PROGRAM – MONDAY, OCTOBER 3, 2022

Oral Symposia | 3:50 PM – 5:30 PM

22SPR05: Early Career Researchers in Plasmonics *Meeting Room 6*

Chair: Zac Schultz, *The Ohio State University*

(198) **Transforming Treatment of Patients with Drug Induced Liver Injury Using SERS Based Lateral Flow Testing**
Sian Sloan-Dennison[1], Ben Clark, Kathleen Scullion, James Dear, Dieter Bingemann, Paul Fineran, David Creasey, Cicely Rathmell, Karen Faulds, Duncan Graham; [1]*The University of Strathclyde*

(199) **Plasmon-Enhanced Electrochemistry in Nonaqueous Solvent**
Andrew J. Wilson[1], Padmanabh Joshi; [1]*University of Louisville*

(200) **Exploring Chemistry of Surface-Supported Nanostructures using Ultrahigh Vacuum Tip-Enhanced Raman Spectroscopy**
Sayantan Mahapatra[1], Nan Jiang; [1]*University of Illinois Chicago*

(201) **Advances in SERS Optophysiology for Neurosciences**
Stephanie M V Gallant[1], Jean-Francois Masson; [1]*University of Montreal*

(202) **Surface Enhanced Spatially Offset Raman Spectroscopy Using A 1064 nm Laser**
Andrew R. Callander[1], Karen Faulds, Duncan Graham, Neil C. Shand[2]; [1]*The University of Strathclyde,* [2]*The Defence Science and Technology Laboratory (DSTL)*

22SPSJ04: Frontiers of Vacuum, Far, and Deep-Ultraviolet Spectroscopy II *Meeting Room 9*

Chair: Igor Lednev, *University at Albany, State University of New York*

(203) **UV Raman - A Key Technology for BioPhotonics**
Jürgen Popp[1]; [1]*Leibniz Institute of Photonics Technology*

(204) **Multi-Wavelengths Ultraviolet Raman Spectroscopy for Understanding the Effect of Co-Solvents on the Structural Stability of DNA**
Barbara Rossi[1], Mariagrazia Tortora, Andrea Mele, Jacopo Vigna, Ines Mancini, Alessandro Gessini, Claudio Masciovecchio; [1]*Elettra-Sincrotrone Trieste*

(205) **Continuously Tunable Wavelength, CW Deep UV Laser for Raman Spectroscopy**
Ryan Roppel[1], Sergei V. Bykov[1], Sanford A. Asher[1]; [1]*University of Pittsburgh*

(206) **UV Resonance Raman Studies of Tryptophan in Proteins**
Judy Kim[1], Chanin Tangtartharakul; [1]*UC San Diego*

(207) **Hyphenation of Raman Microspectroscopy and Field-Flow Fractionation for Analysis of Nanoplastics**
Natalia P. Ivleva[1], Maximilian Huber, Christian Schwaferts, Florian Meier, Martin Elsner; [1]*Technical University of Munich (TUM)*

TECHNICAL PROGRAM – TUESDAY, OCTOBER 4, 2022

Oral Symposia | 8:30 AM – 10:10 AM

22AES02: Electrokinetic Fundamentals *Meeting Room 8*

Chair: Rodrigo Martinez-Duarte, *Clemson University*

(208) **High Sensitivity in Dielectrophoresis Separations**
Benjamin G. Hawkins[1]; [1]*Cal Poly, San Luis Obispo*

(209) **The synthesis of Bacterial Cellulose under AC electric fields**
Rodrigo Martinez-Duarte[1], Sindora R. Baddam[1]; [1]*Clemson University*

(210) **Particle Properties Influence on the Electrokinetic Equilibrium Condition and Nonlinear Electrophoretic Mobility**
Olivia Ernst[1], Curran Dillis, Adrian Lomeli-Martin, Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

(211) **MOF-based Janus Micromotor Locomotive Characterization**
Eric R. Languirand[1], Matthew Collins; [1]*U.S. Army DEVCOM CBC*

(212) **Methodology for characterizing the Nonlinear Electrokinetic Behavior of Microparticles**
Adrian Lomeli-Martin[1], Olivia Ernst, Richard Cobos Franco, Aditya Khair, Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

22ATOM07: ICP-MS Applications *Meeting Room 4*

Chair: Jenny Nelson, *Agilent*

(213) **Elemental Analysis of Kratom Products and E-Liquids Samples using ICP-MS**
Madhavi Mantha[1], Kevin Kubachka, Robert Wilson; [1]*US Food and Drug Administration*

Talks begin at 20-minute intervals.

(214) **Metallomics to Study Cancer Metabolism in Clear Cell Renal Cell Carcinoma**
Julio Landero[1], Dina Secic, Maria Czyzyk-Krzeska, James Reigle, Behrouz Shamsaei, Mario Medvedovic, David Plas, Tom Cunningham, Jarek Meller, Shuchi Gulati; *[1]Icahn School of Medicine at Mount Sinai*

(215) **Determination of Minerals and Trace Elements in Milk, Milk Products, Infant Formula, and Adult/Pediatric Nutritional Formula by Inductively Coupled Plasma Mass Spectrometry (ICP-MS)**
Lawrence H. Pacquette[1]; *[1]Abbott Nutrition*

(216) **Characterization of Silicon Dioxide Food Additives via Single Particle Inductively Coupled Plasma Mass Spectrometry and Other Techniques**
Monique E. Johnson[1], Sadia Khan, Antonio R. Montoro Bustos[1], Karen E. Murphy[1], Michael Winchester, Timothy Croley, Ingo H. Strenge[2], Savelas Rabb; *[1]National Institute of Standards and Technology, [2]University of Siegen*

(217) **Advanced Trace Element Analysis using Plasma Spectroscopy in Environmental Monitoring (Fine Dust, Virus, and Toxic Gas)**
Jun-Ho Yang[1], Jack Yoh; *[1]Seoul National University*

22BIM05: Nanotheranostics: Diagnosis and Treatment of Disease using Nanomaterials *Meeting Room 3*

Chair: Samuel Mabbott, *Texas A&M University*

(218) **Optimization of SORS Instrumentation for Applications in Preclinical Cancer Imaging**
Fay Nicolson[1], Bohdan Andreiuk, Bridget O'Donnell, Eunah Lee, Andrew Whitley, Scott Rudder, Kevin Haigis; *[1]Dana-Farber Cancer Institute and Harvard Medical School*

(219) **Wearable Plasmonic Paper-based Microfluidics for Sweat Analysis**
Limei Tian[1]; *[1]Texas A&M University*

(220) **Deep Raman Diagnosis: A Combined Role of SERS Nanostructure, Instrumentation and Ex Vivo Tissue Model**
Priyanka Dey[1], William Olds, Alexandra Vaideanu, Andreas Schatzlein, Idriss Blakey, Peter Fredericks, Pavel Matousek, Nicholas Stone; *[1]Teesside University*

(221) **Understanding the Intracellular Uptake of Nano-based Drug Delivery Systems in Cancer Therapeutics**
Aristea Anna Leventi[1], Kharmen Billimoria, Dorota Bartczak, Stacey Laing, Heidi Goenaga-Infante, Karen Faulds, Duncan Graham; *[1]University of Strathclyde*

(222) **Multiplexed 3D Detection of Antibody-conjugated Shell-isolated Gold Nanotags Using SERS for Breast Cancer Phenotyping**
Melissa Benison[1], Neil C. Shand[2], Duncan Graham, Karen Faulds; *[1]University of Strathclyde, [2]The Defence Science and Technology Laboratory (DSTL)*

22CHEM06: Pathways to Autonomous Chemometrics *Meeting Room 6*

Chair: John Kalivas, *Idaho State University*

(223) **Automatic Approaches for Efficient Curve Resolution of Spectral Imaging Data**
Cyril Ruckebusch[1], Laureen COIC, Raffaele Vitale; *[1]University of Lille*

(224) **Self-Optimizing Support Vector Classifiers Applied to the Analysis of Maca Metabolomic Mass Spectral Profiles**
Peter B. Harrington[1], Qudus Ayodeji Thanni; *[1]Ohio University*

(225) **Autonomous Chemometrics, Is Resistance Futile?**
John H. Kalivas[1], Jordan Peper, Nathan Woods, Rajiv Khadka, Xingyue Yang, John Koudelka; *[1]Idaho State University*

(226) **A Digital Science Platform for Process Chemometric Model Maintenance.**
David A. Joyce[1], Steve McCann, Kenneth Gonzalez, Gary Walters; *[1]Thermo Fisher Scientific*

(227) **Monitoring Worker Exposure to Respirable Crystalline Silica: Application for Data-driven Predictive Modeling for End-of-Shift Exposure Assessment**
Cody Wolfe[1], Lauren Chubb, Rachel Walker, Yekich Milan, Emanuele Cauda; *[1]CDC/NIOSH*

22IR01: NanoIR in Material Science *Ballroom D&E*

Chair: Georg Ramer, *TU Wien*

(228) **High Throughput Imaging of Composition, Thermal Conductivity and Interfacial Thermal Conductance with Nanoscale Resolution**
Andrea Centrone[1], Mingkang Wang, Georg Ramer, Georges Pavlidis, Jeffrey J. Schwartz[2], Vladimir Aksyuk; *[1]National Institute of Standards and Technology, [2]Laboratory for Physical Sciences*

(229) **Subsurface Imaging and Spectroscopy in Two-Dimensional Materials via Photothermal Induced Resonance**
Jeffrey J. Schwartz[1], Andrea Centrone; *[1]Laboratory for Physical Sciences*

(230) **A Closer Look at a Post-Consumer Recycled Polyolefin Blend: Chemical Characterization at the Nanoscale Using Tapping Mode AFM-IR**
A. Catarina V.D dos Santos[1], Davide Tranchida, Bernhard Lendl, Georg Ramer; *[1]TU Wien*

(231) **Nanoscale Infrared Study of Ryugu Samples Returned by the Hayabusa 2 Space Mission**
Jérémie Mathurin[1], Emmanuel Dartois, Alexandre Dazzi, Ariane Deniset-Besseau, Laure Bejach, Cécile Engrand, Jean Duprat, Yoko Kebukawa, Hikaru Yabuta, Hisayoshi Yurimoto, Tomoki Nakamura, Takaaki Noguchi, Ryuji Okazaki, Hiroshi Naraoka, Kanako Sakamoto, Shogo Tachibana, Seiji Watanabe, Yuichi Tsuda; *[1]Université Paris-Saclay/CNRS*

(232) **Chemical Nano-Speciation of Breast Microcalcifications in Cancerous Tissues: the Potential of AFM-IR Technique to Decipher Microcalcification Genesis**
Margaux Petay[1], Ariane Deniset-Besseau, Alexandre Dazzi, Maguy Cherfan, Dominique Bazin; *[1]University Paris-Saclay/CNRS*

22LIBS06: Space Applications *Meeting Room 5*

Chair: Pablo Sobron, *Impossible Sensing*

(233) **Exploring the Lunar Surface and Volatiles with Laser-Induced Breakdown Spectroscopy**
Jeffrey Gillis-Davis[1], Pablo Sobron, Bradley Jolliff; *[1]Washington University in St. Louis*

(234) **LIBS, Raman, and Chemometrics for Exploration of Ocean Worlds**
Laura E. Rodriguez[1], Anastasia Yanchilina, Kirby Simon, Evan Eshelman, Deborah Kelley, Pablo Sobron, Laurie Barge; *[1]NASA Jet Propulsion Laboratory, California Institute of Technology*

(235) **LIBS for Exploring the Clouds of Venus**
Kirby Simon[1], Pablo Sobron, Anastasia Yanchilina, Diana Gentry, Laura Iraci, Alfonso Davila, Andrew Mattioda, Amanda Brecht, Alan Cassell; *[1]Impossible Sensing*

(236) **Using Laboratory LIBS Acoustics Experiments to Elucidate SuperCam Microphone Data on Mars.**
Carene Larmat[1], Erin Dauson, Ann Ollila, James Ten Cate, Baptiste Chide, Adriana Reyes-Newell, Nina Louise Lanza, Roger Wiens; *[1]Los Alamos National Laboratory*

(237) **New Insights in Autonomous LIBS-based Planetary Exploration: Generalized Scale Invariant Quantitative LIBS**
Pablo Sobron[1], Daniel Van Hoesen; *[1]Impossible Sensing*

22MASS04: Rapid Screening and Assay Methods for Mass Spec and Beyond *Meeting Room 10*

Chair: Abraham Badu-Tawiah, *The Ohio State University*

(238) **Ultrasensitive Detection And Quantification Of HIV DNA And Its Polymerase Chain Reaction Products By A Novel Enzyme Linked Mass Spectrometric Assay**
Nan Cheng[1], Saaimatul Huq, Ming Miao, John G. Marshall[1]; *[1]Toronto Metropolitan University*

(239) **Rapid Screening of Suspect Drug Products Containing Designer Benzodiazepines Using DART-MS**
Skyler W. Smith[1], Travis M. Falconer[1], Sara E. Kern[2], John P. Roetting[1], Martin K. Kimani[1]; *[1]U.S. Food & Drug Administration, [2]US Food and Drug Administration*

(240) **Improvements and Characterization of Localized-Sustained Stimulation of Brain Slices On-Chip**
Colby E. Witt[1], Ashley E. Ross[1]; *[1]University of Cincinnati*

(241) **Development of Electrochemical Aptamer-Based Neuropeptide Y Sensor**
Jordan M. Seibold[1], Ryan White, Ashley E. Ross[1]; *[1]University of Cincinnati*

(242) **Feasibility Studies on the Cyto R1 Platform for Tumor-Associated Cell Sorting**
Alexandra Hyler[1], Katherine Degen, Ridi Barua, Dean Thomas, Rafael Davalos, Eva Schmelz; *[1]CytoRecovery*

22PAT01: SAS PAT Technical Section: PAT in Pharma *Meeting Room 7*

Chair: Jim Rydzak, *Specere Consulting*

(243) **The Use of a Bench Top Simulator for Economic PAT Application Development**
Stephen Hammond[1], Philip Doherty; *[1]Expo Pharma Engineering Services*

(244) **Reactions and Crystal Form Transformations Revealed Using In-Situ Raman Spectroscopy and Optical Microscopy**
Charlie Goss[1], Anthony Nocket, Andrew DiPietro, Kevin Chu, Swetha Ainampudi, Yasser Jangjou, Alexis Venere, Alicia Potuck, Anjan Pandey; *[1]GlaxoSmithKline*

(245) **Impurity, isomer, and chiral analysis in process applications using molecular rotational resonance spectroscopy**
Justin L. Neill[1], Reilly E. Sonstrom[1], Alex Mikhonin; *[1]BrightSpec, Inc.*

(246) **Improving Your Reaction Efficiency with PAT Focused Technology**
Norman A. Wright[1], Brian Wittkamp, Charlie Rabinowitz; *[1]Mettler Toledo*

(247) **Unlocking product composition using solid state Raman and Core models: From fuels to fermentation**
Brian Marquardt[1], Thomas Dearing, John Richmond; [1]*MarqMetrix*

22RAM08: Raman Imaging and Microscopy
Meeting Room 1

Chair: Katsumasa Fujita, *Osaka University*

(248) **Super Resolution DO-SRS Multiplex Metabolic Imaging for Studying Aging and Diseases**
Lingyan Shi[1], Yajuan Li, Wenxu Zhang, Anthony Fung, Hongje Jang; [1]*UC San Diego*

(249) **Plasmon-Enhanced Raman Nanoscopy for Probing Single Molecule Chemical Reactions**
Taka-aki Yano[1]; [1]*Tokushima University*

(250) **Application of Raman Spectroscopy to Investigate Ageing and Disease in Archaeological Human Bone**
Sheona I. Shankland[1], Hugh Willmott, Alexzandra Hildred, Adam M. Taylor[1], Jemma G. Kerns[1]; [1]*Lancaster University*

(251) **Opto-Lipidomics of Tissues**
Mads S. Bergholt[1]; [1]*King's College London*

(252) **Toward Photoswitchable Electronic Pre-Resonance Stimulated Raman Probes**
Dongkwan Lee[1], Chenxi Qian, Haomin Wang, Lu Wei; [1]*Caltech*

22RAM09: Spatially Offset Raman Spectroscopy
Ballroom C

Chair: Pavel Matousek, *STFC Rutherford Appleton Laboratory*

(253) **Design of SORS Systems for Biomedical and Art Conservation Applications**
Pietro Strobbia[1], Claudia Conti, Ren A. Odion[2], Tuan Vo-Dinh, Pavel Matousek, Marco Realini; [1]*University of Cincinnati,* [2]*Duke University*

(254) **Through Bottle Quantification of Adulterated Extra Virgin Olive Oil using SORS**
Royston Goodacre[1], Mehrvash Varnasseri, Yun Xu, Howbeer Muhamadali, Pavel Matousek; [1]*The University of Liverpool*

(255) **Spatially Offset Raman Spectroscopy for Non-invasive Hydration Monitoring**
Anna S. Rourke[1], Laura J. Elstub[1], Trevor Voss, Anita Mahadevan-Jansen; [1]*Vanderbilt University*

(256) **Investigation On-Depth Dependent Variation of Accuracy in API Concentration Determination of Tablet using Spatially Offset Raman Scattering Line-Mapping Measurement**
Sanghoon Cho[1], Si Won Song, Hoeil Chung, Hyung Min Kim; [1]*Hanyang University*

(257) **Raman spectroscopy for measuring systemic physiological hydration in tissue: an analysis of eccrine sweat**
Trevor Voss[1], Anita Mahadevan-Jansen; [1]*Vanderbilt University*

22SPECIAL07: Molecular Microspectroscopy and the Molecular Microspectroscopy Laboratory (MML)
Meeting Room 2

Chair: Andre Sommer, *Miami University*

(258) **The History and Beginnings of the MML**
David W. Schiering[1]; [1]*RedWave Technology*

(259) **Molecular Microspectroscopy in Art Conservation and Archeology**
Patricia L. Lang[1], Pamela A. Smith[2]; [1]*Ball State University,* [2]*Improved Pharma, LLC*

(260) **Industrial Collaborations with a Focus on Instrument Development**
Andre J. Sommer[1]; [1]*Miami University*

(261) **Kidney and Eye Disease as Studied by Molecular Microspectroscopy**
James C. Williams[1]; [1]*Indiana University School of Medicine*

(262) **Molecular Microspectroscopic Analysis of Counterfeit Drugs and Other FDA-Regulated Products**
Adam Lanzarotta[1]; [1]*US Food and Drug Administration*

22SPSJ02: Near-Infrared Spectroscopy; Application to Biological and Materials Sciences *Meeting Room 9*

Chair: Christian Huck, *University of Innsbruck*

(263) **Evaluation of Solid State of Polymers Subjected to Physical Treatments using IR/NIR Spectroscopy**
Daitaro Ishikawa[1]; [1]*Fukushima University*

(264) **New Trends in Spectral Preprocessing**
Federico Marini[1], Alessandra Biancolillo, Jean-Michel Roger; [1]*University of Rome La Sapienza*

(265) **Present and Future of Miniaturized NIR-Spectrometers Combined with Challenging Data Management Strategies**
Christian W. Huck[1], Krzysztof B. Bec[1], Justyna Grabska; [1]*University of Innsbruck*

(266) **Chemical Information vs. Instrumental Difference in Miniaturized NIR Spectroscopy**
Justyna Grabska[1], Krzysztof B. Bec[1], Christian W. Huck[1]; [1]*University of Innsbruck*

(267) **Investigation of Reaction Degree of Bio-Coke Formation using Near Infrared Spectroscopy**
Yusuke Morisawa[1], Nami Ueno, Hisanori Ozaki; [1]*Kindai University*

TECHNICAL PROGRAM – TUESDAY, OCTOBER 4, 2022

Awards and Plenary Lectures | 10:45 AM- 12:00 PM | *Event Center*

22PLEN02: Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award

(268) **Pushing the Frontiers of Stimulated Raman Imaging for Complex Subcellular Bioanalysis**
Lu Wei[1]; [1]*Caltech*

22PLEN02: FACSS Charles Mann Award for Raman Spectroscopy

(269) **Raman Spectroscopy and Machine Learning for Medical Diagnostics and Forensic Purposes**
Igor K. Lednev[1]; [1]*University at Albany, State University of New York*

TECHNICAL PROGRAM – TUESDAY, OCTOBER 4, 2022

Oral Symposia | 1:30 PM – 3:10 PM

22AES04: Microfluidic Bioanalysis 1 *Meeting Room 8*

Chair: Tayloria Adams, *University of California, Irvine*

(270) **New Approaches for using 3D Printed Devices for Cell Culture and Analysis**
R. Scott Martin[1]; [1]*Saint Louis University*

(271) **Microengineered Platforms to Culture and Measure Signaling within Organs of the Gut-Brain-Immune Axis**
Ashley E. Ross[1]; [1]*University of Cincinnati*

(272) **Dielectric Characterization of Ductal Adenocarcinoma Using Murine PyMT+/- Model**
Raphael O. Oladokun[1], Soumya Srivastava, Timothy Eubank; [1]*West Virginia University*

(273) **Construction of Microfluidic Electrochemical Cell packed with a Zirconium MOF for sensitive detection of PFOA in Source Water**
Zhenglong Li[1], Maryom Rahman, Abhishek Kumar, Robbert J Elsinghorst, Joshua M Torgeson, Julian Schmid, Charmi Chande, Radha Kishan Motkuri, Sagnik Basuray; [1]*New Jersey Institute of Technology*

(274) **Biomimetic Lipid Membranes as Effective Antifouling Interfaces for Sensing in Clinically Relevant Matrices**
Daniel Stuart[1], Caleb Pike, Quan Cheng; [1]*University of California Riverside*

22ATOM08: General Session *Meeting Room 4*

Chair: Mauro Martinez, *Icahn School of Medicine at Mount Sinai*

(275) **The Characterization of Biogenic Selenium Nanoparticles in Edible Mushrooms by ICP-MS and Complementary Techniques**
Jörg bettmer[1], Maria Montes-Bayon, Andrés Suárez Priede, Mario Corte Rodríguez, Zoltan Mester, Kelly LeBlanc; [1]*University of Oviedo*

(276) **Lithium Isotope Ratio Analysis of Geological Samples via Atomic Absorption Spectrometry**
Dalia Morcillo García-Morato[1], Alexander Winckelmann, Daniel Frick, Lars Jacobsen, Silke Richter, Sebastian Recknagel, Jochen Vogl, Ulrich Panne, Carlos Abad; [1]*Bundesanstalt für Material und -Prüfung (BAM)*

(277) **Metallic Nanoparticle Analysis in Semiconductor Grade Tetramethylammonium Hydroxide Using the PerkinElmer Current 5000 Inductively Coupled Plasma Mass Spectrometer**
Aaron Hineman[1], Ruth Merrifield, Chady Stephan; [1]*PerkinElmer Inc.*

(278) **Laser-Induced Breakdown Spectroscopy Emission Enhancement from Bacteria on a Silver Thin Film**
Emily Tracey[1], Haiqa Arain, Steven J. Rehse[1]; [1]*University of Windsor*

(279) **Parametric Optimization and Benchmarking of the Liquid Sampling Atmospheric Pressure Glow Discharge Ionization Source Coupled to an Orbitrap Mass Spectrometer for the Analysis of Plutonium**
Joseph V. Goodwin[1], Benjamin T. Manard[2], Brian Ticknor, Paula Cable-Dunlap, R. Kenneth Marcus; [1]*Clemson University,* [2]*Oak Ridge National Laboratory*

22AWD03: FACSS 2022 Charles Mann Award Symposium Honoring Igor Lednev *Ballroom C*

Chair: Igor Lednev, *University at Albany, State University of New York*

(280) **3D SERS Imaging of Nanoporous Gold-Silver Microstructures: Exploring the Formation Mechanism Based on Galvanic Replacement Reaction**
Yukihiro Ozaki[1]; [1]*Kwansei Gakuin University*

(281) **Innovative Bioanalytical Raman Spectroscopic Sensors Concepts**
Jürgen Popp[1]; [1]*Leibniz Institute of Photonics Technology*

(282) **The Challenges of Translating Research Raman in to a Dedicated Analyzer for Use by Non-Spectroscopists**
Andrew Whitley[1], Linda H. Kidder[1]; [1]*HORIBA Scientific*

Talks begin at 20-minute intervals.

(283) **Characterization of New Drug Modalities with RAMAN and ROA**
Rina K. Dukor[1]; [1]*BioTools*

(284) **Exploring the Supramolecular Chirality of Protein Fibrils Using VCD**
Laurence Nafie[1]; [1]*Syracuse University*

22BIM01: A New Stream of Intelligent Measurements and Data Science Part 1 *Meeting Room 3*
Chair: Katsumasa Fujita, *Osaka University*
Co-Chair: Ioan Notingher, *University of Nottingham*

(285) **On-the-fly Raman Microscopy with Guaranteeing Accuracy Using Reinforcement Learning II: Experiment**
Katsumasa Fujita[1]; [1]*Osaka University*

(286) **Selective Sampling Raman Spectroscopy for Biomedical Applications**
Ioan Notingher[1]; [1]*University of Nottingham*

(287) **Intelligent Image-Activated Cell Sorting 2.0**
Keisuke Goda[1]; [1]*The University of Tokyo*

(288) **Optimizing Microscopy and Spectroscopy Instrumentation for Data Throughput**
Chris Rowlands[1]; [1]*Imperial College London*

(289) **Ramanomics - A New Raman Microscopy Based Omics Technology For Quantitative Analysis Of Biomolecular Composition In Live Cells And Tissues**
Andrey Kuzmin[1], Alexander Rzhevskii, Artem Pliss, Paras Prasad; [1]*SUNY, University at Buffalo*

22CHEM04: Chemometrics and Food Safety
Meeting Room 6

Chair: Mengliang Zhang, *Middle Tennessee State University*

(290) **Raman Spectroscopy with On-board Chemometric Models and Library Spectral Matching for Plasticizer Identification**
Betsy Jean Yakes[1], Josh Moskowitz, Luke K. Ackerman[1], Kristen Reese, Timothy Begley, Katherine Carlos; [1]*U.S. Food and Drug Administration*

(291) **Chemometrics-Based Correlations Between Chemical Changes and Biological Effects in Food Safety Research**
Chi Chen[1], Qingqing Mao, Jieyao Yuan; [1]*University of Minnesota Twin Cities*

(292) **Chemometrics in Spectral Data Applied to Food Quality, Safety and Authenticity**
Mohammed Kamruzzaman[1]; [1]*University of Illinois at Urbana-Champaign*

(293) **Metabolomic Study of Wild American Ginseng and Cultivated American Ginseng Roots by UHPLC-HRMS and Chemometrics**
Roderick W. Moore[1], Mengliang Zhang, Ying Gao, Jianghao Sun, Zhihao Liu; [1]*Middle Tennessee State University*

(294) **In-Field Assessment Of Flavor Traits In Tomatoes Using Portable Scanner**
Shreya M. Nuguri[1], Celeste Matos, Peren P. Aykas[1], Luis E. E. Rodriguez-Saona[1]; [1]*The Ohio State University*

22CTP/EARLY03: SAS Organized Session: Navigating Challenges to Achieve Success as an Early Career Spectroscopist, Part 1 *Meeting Room 7*

Chair: Fay Nicolson, *Dana-Farber Cancer Institute and Harvard Medical School*
Co-Chair: Andrew Whitley, *HORIBA Scientific*

(295) **My Transatlantic Transition from Post-Doc to Professor**
Samuel Mabbott[1]; [1]*Texas A&M University*

(296) **Academic-Industrial Collaboration: Bringing New Imaging Frontiers for Pharmaceutical Processes.**
Prabuddha Mukherjee[1], Michael Olszowy; [1]*Sartorius Stedim Biotech*

(297) **Scientists at P&G**
Stefania Perticaroli[1], Ariel Lebron; [1]*The Procter and Gamble Company*

(298) **They Do Research at the FDA? How to Survive and Thrive in a Regulatory Research Environment**
Betsy Jean Yakes[1]; [1]*U.S. Food and Drug Administration*

(299) **Panel & Open Discussion**
Ariel Lebron[1], Stefania Perticaroli; [1]*The Procter and Gamble Company*

22IR03: Nanoscale Spectroscopy: Advances in Instrumentation *Ballroom D&E*

Chair: Andrea Centrone, *National Institute of Standards and Technology*
Co-Chair: Andrew Whitley, HORIBA Scientific

(300) **Emerging Trend in AFMIR: Surface-sensitive Mode on the way to Probe the Depth of a Sample**
Ariane Deniset-Besseau[1], Alexandre Dazzi, Jérémie Mathurin, Martin Wagner; [1]*University Paris-Saclay/CNRS*

(301) **Seeing Atoms: TERS in the Atomistic Near-field**
Vartkess A. Apkarian[1]; [1]*University of California, Irvine*

(302) **Single Molecule Nano-Chemical Imaging and Spectroscopy to Unravel Molecular Structure and Interactions**
Francesco Simone Ruggeri[1]; [1]*Wageningen University*

(303) **Chemically Identifying Single Adatoms with Single-bond Sensitivity During Oxidation Reactions of a Polymorphic Atomic Monolayer**
Nan Jiang[1]; [1]*University of Illinois Chicago*

(304) **Nanoscale Spectroscopic Investigations of Core-Shell Nano Particles as Potential Drug Carriers**
Volker Deckert[1], Christiane Höppener; [1]*Leibniz-IPHT*

22LIBS04: Molecular *Meeting Room 5*

Chair: Michael Gaft, *Ariel University*

(305) **Features in Molecular LIBS**
Christian G. Parigger[1]; [1]*Ariel University*

(306) **MLIBS-MLIF Methods for Quantitative and Isotopic Analysis**
Lev Nagli[1], Michael Gaft, Yosef Raichlin; [1]*Ariel University*

(307) **Molecular Formation in Nebulized Assisted LIPs: Detection of Halogens**
Nerea Bordel[1], Cristina Méndez-López, Luis Javier Fernández-Menéndez, Cristina Gonzalez-Gago, Jorge Pisonero; [1]*University of Oviedo*

(308) **REE Molecules in LIBS**
Michael Gaft[1]; [1]*Ariel University*

(309) **Pulsed Microwave-Assisted Laser-Induced Breakdown Spectroscopy and Laser Ablation Molecular Isotopic Spectrometry Using Microstrip Wavevguides**
Kelsey L. Williams[1], Steven J. Ray[2]; [1]*The State University of New York at BUffalo,* [2]*The State University of New York at Buffalo*

22PMA04: SERS for Diagnostics and BioPharma Manufacturing *Meeting Room 10*

Chair: Karin Balss, *Janssen*
Co-Chair: Courtney Morder, *The Ohio State University*

(310) **Inverse Molecular Sentinel Integrated Bimetallic Nanostar Substrate for Ultrasensitive Medical Diagnostics**
Aidan Canning[1], Hsin-neng Wang, Tuan Vo-Dinh, Joy Q. Li[2], Xinrong Chen; [1]*Duke University,* [2]*Duke University School of Medicine*

(311) **Differentiating Physical and Infectious Viral Titer using Surface Enhanced Raman Spectroscopy**
Courtney J. Morder[1], Karin M. Balss[2], Zac D. Schultz[1]; [1]*The Ohio State University,* [2]*Janssen*

(312) **Designing a COVID-19 Assay using Surface Enhanced Raman Spectroscopy (SERS)**
Taylor Payne[1], Stephen Klawa, Ronit Freeman, Zac D. Schultz[1]; [1]*The Ohio State University*

(313) **Low-Cost Sensors for the Identification and Quantification of Disease Biomarkers, Viral RNA, and Drugs Of Abuse**
Laura Fabris[1]; [1]*Rutgers, the State University of New Jersey*

(314) **Indirect Surface-Enhanced Raman Spectroscopic Detection of Biomarkers Associated with Polycystic Ovarian Syndrome**
Avery Wood[1], Bhavya Sharma; [1]*University of Tennessee*

22RAM04: SERS 3 *Meeting Room 1*

Chair: Zac Schultz, *The Ohio State University*
Co-Chair: Royston Goodacre, *The University of Liverpool*
Co-Chair: Sian Sloan-Dennison, *The University of Strathclyde*

(315) **Advancing SERS Biosensors for Diagnostic Applications**
Pietro Strobbia[1]; [1]*University of Cincinnati*

(316) **Towards semiconductor substrates in SERS: applications in biosensing**
Kristen Dellinger[1], Samuel Adesoye; [1]*North Carolina Agricultural and Technical State University*

(317) **Pushing the Limits of Chemical Detection at Depths with Spatially-Offset Raman Spectroscopy**
Bhavya Sharma[1]; [1]*University of Tennessee*

(318) **Plasmonic nanotags for the detection and treatment of glioblastomas**
Samantha M. McCabe[1], Matthew E. Berry[1], Gregory Wallace, Neil C. Shand[2], Marie Boyd, Duncan Graham, Karen Faulds; [1]*The University of Strathclyde,* [2]*The Defence Science and Technology Laboratory (DSTL)*

(319) **SERS on a chip: Multiplex detection of seroconversion and cross-reactivity of SARS-CoV-2 antibodies in non-hospitalised individuals**
Malama Chisanga[1], Jean-Francois Masson; [1]*University of Montreal*

22SPECIAL09: Analytical Imaging I *Meeting Room 2*

Chair: Max Lei Geng, *University of Iowa*

(320) **Single-molecule fluorescence imaging of electrons and ions produced in iron corrosion**
Lydia Kisley[1]; [1]*Case Western Reserve University*

(321) **Imaging Molecular Transport in Nanoporous Silica at Microsecond Time Resolution**
Max Lei Lei Geng[1], Hong Bok Lee, Ana Rodriguez, Madelyn Daley; [1]*University of Iowa*

(322) **IR Spectroscopy Beyond the Diffraction Limit at Submicron and Nanoscale Spatial Resolutions via Photothermal Techniques**
Curtis Marcott[1]; [1]*Light Light Solutions*

(323) **Raman Imaging Grasped the Molecular Changes During the Cell Differentiation of Human Induced Pluripotent Stem Cells into Erythropoietin-Producing Cells**
Mika Ishigaki[1], Hirofumi Hitomi, Yukihiro Ozaki, Akira Nishiyama; [1]*Shimane University*

(324) **Hierarchical Chemical Patterning and Imaging of Surfaces from sub-10-nm to Macroscopic Scales**
Shelley A. Claridge[1]; [1]*Purdue University*

22SPSJ01: Near-Infrared Spectroscopy; Spectral Analysis, Imaging *Meeting Room 9*

Chair: Yukihiro Ozaki, *Kwansei Gakuin University*

(325) **Development of a Monitoring Method for Peptide Synthesis with Different Amino Acid Sequences Using Near-infrared Spectroscopy**
Mika Ishigaki[1], Atsushi Ito, Risa Hara, Shun-ichi Miyazaki, Kodai Murayama, Sana Tsuji, Miho Inomata, Keisuke Yoshikiyo, Tatsuyuki Yamamoto, Yukihiro Ozaki; [1]*Shimane University*

(326) **Understanding How Near-infrared Quality Estimation Models for Agricultural Products Work with the aid of Metabolomics**
Akifumi Ikehata[1]; [1]*National Agriculture and Food Research Organization (NARO)*

(327) **New Avenues in Quantum Chemical Simulations of NIR Spectra – from Polymers to Aqueous Matrix and Interpretation of Instrumental Difference of Miniaturized Spectrometers**
Krzysztof B. Bec[1], Justyna Grabska, Christian W. Huck[1]; [1]*University of Innsbruck*

(328) **Spectrometers in Wonderland: Shrinking, Shrinking, Shrinking**
Richard Crocombe[1]; [1]*Crocombe Spectroscopic Consulting, LLC*

(329) **Use Of Handheld FT-NIR Sensors To Rapidly Quantify Cannabinoids of Hemp, in situ.**
Cameron M. Jordan[1], Siyu Yao, Luis E. E. Rodriguez-Saona[1], M. Monica Giusti, Gonzalo Miyagusuku-Cruzado, Christopher Ball; [1]*The Ohio State University*

22ATOM04: Traditional and Atmospheric Glow Discharge Sources *Meeting Room 4*

Chair: Gerardo Gamez, *Texas Tech University*

(330) **The Solution-Cathode Glow Discharge: Novel Approaches and Applications**
Steven J. Ray[1], Nicholas Hazel, Chelsey Albaladejo; [1]*The State University of New York at Buffalo*

(331) **Glow Discharge Optical Emission Spectroscopy with Array Detectors**
Arne Bengtson[1], David Bengtson; [1]*Swerim AB*

(332) **Glow Discharge Spectrometry: State of the Art and Future Directions**
Jorge Pisonero[1], Cristina Gonzalez-Gago, Nerea Bordel; [1]*University of Oviedo*

(333) **Nanoparticle Characterization via Glow Discharge Optical Emission Spectroscopy Elemental Mapping**
Gerardo Gamez[1], Kevin Finch; [1]*Texas Tech University*

(334) **Halogen Determinations using a Liquid Sampling-Atmospheric Pressure Glow Discharge Microplasma Ion Source Coupled to a Commercial Mass Spectrometer**
Cameron J. Stouffer[1], R. Kenneth Marcus; [1]*Clemson University*

22AWD02: Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Lu Wei *Ballroom C*

Chair: Lu Wei, *Caltech*

(335) **Pre-organization & Evolution of Enzyme Active Sites using the Vibrational Stark Effect**
Steven Boxer[1]; [1]*Stanford University*

(336) **Needle in a Haystack: Chasing Nanoparticles by SRS Microscopy**
Wei Min[1]; [1]*Columbia University*

(337) **Mid-infrared Photothermal Microscopy: Theory, Instrumentation, Applications**
Ji-Xin Cheng[1]; [1]*Boston University*

(338) **Raman Microscopy: A New Imaging Modality that Opens up Analytical Biology**
Katsumasa Fujita[1]; [1]*Osaka University*

(339) **Raman Image-activated Cell Sorting**
Keisuke Goda[1]; [1]*The University of Tokyo*

22CHEM01: A New Stream of Intelligent Measurements and Data Science Part 2 *Meeting Room 3*

Chair: Tamiki Komatsuzaki, *Hokkaido University*
Co-Chair: Thomas Bocklitz, *Leibniz Institute of Photonics Technology*

(340) **On-the-fly Raman microscopy with Guaranteeing Accuracy using Reinforcement Learning I: Theory**
Tamiki Komatsuzaki[1]; [1]*Hokkaido University*

(341) **Deep Learning Applied to Nonlinear Spectroscopy and Microscopy for System Control, Data Processing and Feature Extraction**
Dario Polli[1], Arianna Bresci, Federico Vernuccio, Chiara Ceconello, Francesco Manetti, Renzo Vanna, Subir Das, Giulio Cerullo, Salvatore Sorrentino; [1]*Politecnico di Milano*

(342) **Measurement Informatics and Its Application in Science**
Takashi Washio[1]; [1]*ISIR, Osaka University*

(343) **Reconstruction of Purified Optical Data from Measurements Using Deep Learning**
Rola Houhou[1], Thomas W. Bocklitz[2], Jürgen Popp, Michael Schmitt, Tobias Meyer-Zedler, Parijat Barman, Elsie Quansah, Orlando Guntinas-Lichius, Franziska Hoffmann; [1]*Friedrich-Schiller University,* [2]*Leibniz Institute of Photonics Technology*

(344) **Transforming the Food Industry with Hyperspectral Imaging**
Andrea Weeks[1]; [1]*P&P Optica*

22CTP/EARLY04: SAS Organized Session: Navigating Challenges to Achieve Success as an Early Career Spectroscopist, Part 2 *Meeting Room 7*

Chair: Benjamin Manard, *Oak Ridge National Laboratory*

(345) **Recent Applications of Laser-Induced Breakdown Spectroscopy at Oak Ridge National Laboratory**
Hunter B. Andrews[1]; [1]*Oak Ridge National Laboratory*

(346) **Use of Molecular Emission by LIBS for Fluoride Imaging in Epidemiology**
Mauro Martinez[1], Manish Arora, Christine Austine; [1]*Icahn School of Medicine at Mount Sinai*

(347) **From Planets to Plasmas: The Career Journey of a Geochemist**
Alicia Cruz-Uribe[1]; [1]*University of Maine*

(348) **Days of our Lives- Elemental Analysis at a Consumer Products Company**
Jennifer L. L. Morgan[1]; [1]*Procter & Gamble*

(349) **Panel & Open Discussion**

22FORENS03: Forensic Analysis in the Lab and at the Crime Scene *Meeting Room 9*

Chair: Igor Lednev, *University at Albany, State University of New York*
Co-Chair: Marisia Fiklet, *SupreMEtric LLC*

(350) **National Institute of Justice: Opportunities for Novel Spectroscopic and Analytical Techniques Applied to Forensic Problems**
Frances Scott[1], Gregory Dutton; [1]*National Institute of Justice*

(351) **Expert Algorithm for Substance Identification (EASI) Applied to the Mass Spectra of Structurally Similar Fentanyl Analogs**
Glen P. Jackson[1], J. Tyler Davidson, Alexandra Adeoye, Samantha Mehnert, Emily Ruiz, Jacob King; [1]*West Virginia University*

(352) **Forensic Analysis of Saliva Stains on Absorbing and Non-Absorbing Surfaces by ATR-FTIR Spectroscopy**
Entesar Alhetlani[1], Dalal Al-Sharji, Mohamed O. Amin[1], Igor K. Lednev[2]; [1]*Kuwait University,* [2]*University at Albany, State University of New York*

(353) **Detection of Postmortem Changes in Liver Samples using Infrared Spectroscopy**
Anna Wójtowicz[1], Agata Mitura, Renata Wietecha-Posłuszny; [1]*Jagiellonian University*

(354) **High Selectivity of LIBS for the analysis of OGSR**
Shelby R. Khandasammy[1], Lenka Halámková, Matthieu Baudelet, Igor K. Lednev[1]; [1]*University at Albany, State University of New York*

22LIBS05: Chemometrics *Meeting Room 8*

Chair: Josette El Haddad, *National Research Council Canada*

(355) **Interesting Features Finder (IFF): A New Tool to Better Explore Big LIBS Data Sets**
Ludovic Duponchel[1], Qicheng Wu, Vincent Motto-Ros; [1]*University of Lille*

(356) **Transfer Learning for Improved LIBS Analytical Performance**
Erik Kepes[1], Jakub Vrábel, Pavel Porizka, Jozef Kaiser; [1]*Central European Institute of Technology, Brno University of Technology*

(357) **Combination of Multiple Spectroscopy Techniques - Using Random Forest Classifiers for Correlation Analysis**
Elise Clave[1], Bruno Bousquet, Gilles Dromart, Gilles Montagnac, Olivier Beyssac, Agnis Cousin, Olivier Forni, Roger Wiens, Sylvestre Maurice, Pierre Beck; [1]*Université de Bordeaux*

(358) **Real-time Machine Learning Based LIBS Sensors for Aerosol and Particulate matter**
Prasoon K. Diwakar[1], Pramod Kulkarni, Nicholas E. Pugh[1], Margaret Thompson; [1]*South Dakota School of Mines*

(359) **Distance of Spectroscopic Data**
Jakub Vrabel[1], Erik Kepes, Pavel Porizka, Jozef Kaiser; [1]*Central European Institute of Technology, Brno University of Technology*

22LIBS07: Environmental and Cultural Applications *Meeting Room 5*

Chair: Madhavi Martin, *Oak Ridge National Laboratory*

(360) **Optimizing Hand-held LIBS Instrumentation for the Analysis of Archaeological and Historical Sites and their Environment**
Vincenzo Palleschi[1], Bruno Cocciaro, Olga De Pascale, Giorgio Senesi; [1]*CNR, Italy*

(361) **Toxicity Assessment of Cadmium on Model Plants, the Case of Industrial Hemp and White Mustard**
Jozef Kaiser[1], Ludmila Čechová, Pavlína Modlitbová, Zdenka Kozáková, František Krčma, Andrzej Miziolek, Pavel Porizka; [1]*Central European Institute of Technology, Brno University of Technology*

(362) **Recent Advances in the Use of Laser-Induced Breakdown Spectroscopy to Classify Pathogens in Clinical Specimens**
Steven J. Rehse[1], Emma J. Blanchette[1], Emily Tracey, August Baughan, Grace Johnson; [1]*University of Windsor*

(363) **Quantification of Silicon in Poplar Leaves and Wood Pellets via Laser-Induced Breakdown Spectroscopy**
Hunter B. Andrews[1], Ann Wymore, Xiaohan Yang, Wellington Muchero, Stan Martin, Elizabeth Herndon, Natalie Griffiths, Gerald Tuskan, David Weston, Madhavi Martin; [1]*Oak Ridge National Laboratory*

(364) **Statistical Sorting of Commingled Remains Using Portable LIBS**
Kristen Livingston[1], Matthieu Baudelet, Jonathan Bethard, Katie Zejdlik-Passalacqua; [1]*University of Central Florida*

22PMA02: Pharmaceutical Forensics *Meeting Room 10*

Chair: Ravi Kalyanaraman, *Bristol Myers Squibb*
Co-Chair: Scott Huffman, *Bristol Myers Squibb*

(365) **Bridge the Gap: Education and Training in Career Development**
Dale K. Purcell[1]; [1]*Chemical Microscopy, LLC*

(366) **FTIR Microscopy: big information from small samples**
Mike S. Bradley[1]; [1]*Thermo Fisher Scientific*

(367) **Pharmaceutical Forensics in Cell Therapy - Ensuring patient safety and product supply in autologous cell therapies through great science, collaboration, and patient mindset.**
Jeremy Peters[1], Alex lew, Ravi Kalyanaraman, Scott Huffman, Brittany Handzo; [1]*Bristol Myers Squibb*

(368) **The Patient Found What? Real Foreign Matter Complaints Received by Bristol Myers Squibb Forensics Laboratory**
Brittany Handzo[1], Scott Huffman, Ravi Kalyanaraman; [1]*Bristol Myers Squibb*

22RAM13: TERS *Ballroom D&E*

Chair: Andrew Whitley, *HORIBA Scientific*
Co-Chair: Andrea Centrone, *National Institute of Standards and Technology*

(369) **Sub-Diffraction Nanoscale Raman Imaging of the Interface in a 2D Semiconductor Heterostructure**
J. Pierce Fix[1], Sourav Garg, Andrey Krayev, Audrey Sulkanen, Minyuan Wang, Gang-Yu Liu, Patrick Kung, Nicholas Borys, Juan M. Marmolejo-Tejada[1], Martin A. Mosquera[1]; [1]*Montana State University*

(370) **Symmetry-Prohibited Modes in Tip-Enhanced Raman Spectroscopy**
Andreas Ruediger[1], Mohammad Bakhtbidar, Alexandre Merlen, Azza Hadj Youssef; [1]*Institut National de la Recherche Scientifique - Énergie, Matériaux et Télécommunications*

(371) **Tip-enhanced (Non)Linear Hyperspectral Nano-Imaging of Molecules and Plasmons**
Chih-Feng Wang[1], Patrick El-Khoury; [1]*Pacific Northwest National Laboratory*

(372) **Horibal Bio-TERS: from 2D Materials to Cancer Cell Nanoimaging**
Dmitri Voronine[1]; [1]*University of South Florida*

(373) **Panel & Open Discussion**

TECHNICAL PROGRAM – TUESDAY, OCTOBER 4, 2022

Oral Symposia | 3:50 PM – 5:30 PM

22SPECIAL04: FACSS 2021 Charles Mann Award Symposium Honoring Roy Goodacre *Meeting Room 1*

Chair: Royston Goodacre, *The University of Liverpool*

(374) **Mann Alive! … Or is He …….**
Duncan Graham[1]; [1]*The University of Strathclyde*

(375) **Is this Mann Awake?**
Karen Faulds[1], Hayleigh Kearns, Duncan Graham; [1]*The University of Strathclyde*

(376) **COVID-19 Diagnostic and Prognostic Analysis Using Mass Spectrometry: Weighing Viruses and Consequential Metabolic Response.**
Katherine A. Hollywood[1], Kathleen Cain, Ellen Liggett, Reynard Spiess, Caitlin Walton-Doyle, Eleanor Sinclair, Andrew Pitt, Perdita Barran; [1]*University of Manchester*

(377) **Raman Optical Activity: Raman Spectroscopy for the Twisted**
Ewan W. Blanch[1]; [1]*RMIT University*

(378) **Presentation Title TBD**
Ian Lewis[1]; [1]*Endress+Hauser*

22SPECIAL10: Analytical Imaging II *Meeting Room 2*

Chair: Max Lei Geng, *University of Iowa*

(379) **Presentation Title TBD**
Jefferson Chan;

(380) **"Locking On" to Single Molecules and the Extracellular Phase of Viral Infection**
Kevin D. Welsher[1]; [1]*Duke University*

(381) **Exploiting Infrared Light-Matter Interaction to Advance Nanoscale Characterization and Nanomanipulation of Materials**
Laurene Tetard[1]; [1]*University of Central Florida*

(382) **Integrated Simultaneous Chemical, Surface Potential, Mechanical Imaging at < 10 nm Spatial Resolution**
Xiaoji Xu[1]; [1]*Lehigh University*

(383) **Advancements in Mid-IR Imaging Techniques for the Study of Biological Liquid-Liquid Phase Separation**
Arnaldo Serrano[1], Claire Nelmark; [1]*University of Notre Dame*

22SPR03: Biosensing with Plasmonics *Meeting Room 6*

Chair: Emilie Ringe, *University of Cambridge*

(384) **Improving Selectivity for Plasmonic Biosensors**
Amanda J. Haes[1]; [1]*University of Iowa*

(385) **A Selective and Sensitive Aptamer-Based Surface Plasmon Resonance Biosensor for Serotonin Detection**
Clarice E. Froehlich[1]; [1]*University of Minnesota, Twin Cities*

(386) **Theranostic Applications of Plasmonic Nanoprobes based on Surfactant-free Caged Gold Nanostars**
Aidan Canning[1], Xinrong Chen, Ren A. Odion[1], Tuan Vo-Dinh; [1]*Duke University*

(387) **Surface Plasmon Resonance Imaging (SPRi) in Combination with Machine Learning for Microarray Analysis of Multiple Sclerosis Biomarkers in Whole Serum**
Alexander S. Malinick[1], Daniel Stuart, Alexander S. Lambert[1], Quan Cheng; [1]*University of California Riverside*

(388) **LSPR Sensing on Nanofibers and Highly Curved Objects**
Jean-Francois Masson[1], Maryam Hojjat Jodaylami, Necka Aka, Emilie Ringe; [1]*University of Montreal*

TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 5, 2022

Oral Symposia | 8:30 AM – 10:10 AM

22AES03: Microfluid Electrokinetic Devices| *Meeting Room 8*

Chair: Rucha Natu, *FDA*
Co-Chair: Josie Duncan, *Virginia Tech*

(389) **Screening Membrane Proteins in Microfluidic-Made Giant Unilamellar Vesicles**
Adam Abate[1]; [1]*UCSF*

(390) **Electrokinetic Separation of Highly Similar Microparticles**
Alaleh Vaghef Koodehi[1], Curran Dillis, Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

(391) **Combining Linear and Nonlinear Electrokinetic Effects in Microfluidic Devices**
Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

(392) **3D-Printed Electrically Triggered Droplet Microfluidics for Reduced Sample Consumption During SFX**
Diandra Doppler[1], Mukul Sonker, Ana Egatz-Gomez, Garrett Nelson, Mohammad Towshif Rabbani, Abhik Manna, Cole Errico, Jorvani Cruz Villarreal, Jose Manuel Martin Garcia, Rebecca Jernigan, Sahba Zaare, Konstantinos Karpos, Roberto Alvarez, Sabine Botha, Gihan Ketwala, Thomas Grant, Angel Pey, Alice Grieco, Miguel Angel Ruiz-Fresneda, Alexandra Tolstikova, Reza Nazari, Uwe Weierstall, Valerio Mariani, Petra Fromme, Richard Kirian, Alexandra Ros; *[1]Arizona State University*

(393) **Ionic Liquid Packed Microfluidic Device for the Selective Detection of CO2**
Sreerag Kaaliveetil[1], Yun-Yang Lee, Ruth Dikki, Zhenglong Li, Yu Husan Cheng, Charmi Chande, Burcu Gurkan, Sagnik Basuray; *[1]New Jersey Institute of Technology*

22BIM04: Machine and Deep Learning for Biomedical Diagnostics *Meeting Room 3*

Chair: Thomas Bocklitz, *Leibniz Institute of Photonics Technology*
Co-Chair: Oleg Ryabchykov, *Leibniz Institute of Photonic Technology*

(394) **Optical Microscopy for Enhancement and Automation of Antimicrobial Resistance Detection via Raman Spectroscopy**
Oleg Ryabchykov[1], Kateřina Aubrechtová Dragounová, Ute Neugebauer, Jürgen Popp, Thomas W. Bocklitz[2]; *[1]Leibniz Institute of Photonic Technology, [2]Leibniz Institute of Photonics Technology*

(395) **Deep Learning in Digital Pathology Powers Biomarker Discovery and Optical Biopsy**
Stephen T. Wong[1], Raksha Raghunathan; *[1]Houston Methodist*

(396) **Virtual Assays of Unlabeled Tissues via Fluorescence Microscopy and Deep Learning**
Hongda Wang[1]; *[1]Pictor Labs*

(397) **Integration of Raman spectroscopy and Automated Sampling for Real-Time Bioprocess Insights in Perfusion Cell Culture**
Lee LEE Asplund[1], Stacy Shollenberger, Amy Wood, Allyson Caron, Rakesh Bobbala; *[1]MilliporeSigma*

(398) **An Integrated Analysis Platform for Community-Based Drug Checking**
Lea Gozdzialski[1], Collin Kielty, Abdelhakim Qbaich, Bruce Wallace, Dennis Hore; *[1]University of Victoria*

22CHEM03: Chemometrics Something Borrowed, Something New *Meeting Room 6*

Chair: Federico Marini, *University of Rome La Sapienza*

(399) **Variable Selection Tools for Multi-Block and Multi-Way Data**
Federico Marini[1], Alessandra Biancolillo, Jean-Michel Roger; *[1]University of Rome La Sapienza*

(400) **Information Selection and Object Weighting as Potential Solutions to the Black Hole Effect in Bilinear Curve Resolution Based on Least Squares**
Raffaele Vitale[1], Mohamad Ahmad, Marina Cocchi, Cyril Ruckebusch; *[1]University of Lille*

(401) **Data Fusion in Multimodal Spectroscopic Imaging: A Real Tool to Help Interpret Data**
Ludovic Duponchel[1], Alessandro Nardecchia, Anna de Juan, Vincent Motto-Ros, Michael Gaft; *[1]University of Lille*

(402) **Applications of Classification Algorithms to Data from Portable Instrumentation**
Caelin Celani[1], Karl Booksh, Jocelyn Alcantara-Garcia, Tyler Coplen, James Jordan, William Johnston, Amelia Speed, Rachel McCormick, Olivia Jaeger, Carolyn Chen; *[1]University of Delaware*

(403) **Building Concordant Ontologies Using KNARM (KNowledge Acquisition and Representation Methodology)**
Hande Kucuk McGinty[1]; *[1]Kansas State University*

22CTP/EARLY02: Strategies for Finding Balance *Meeting Room 5*

Chair: Karen Esmonde-White, *Endress+Hauser*

(404) **Balancing Life between Science, Entrepreneurship, Doing Good and Family**
Rina K. Dukor[1]; *[1]BioTools*

(405) **Surface Pressure: A Non-Perfect Guide to the Neverending Work-Life Balance**
Luisa T. Profeta[1]; *[1]Rigaku Analytical Devices*

(406) **Managing the Early Career Transitions in Academia**
Ishan Barman[1]; *[1]Johns Hopkins University*

(407) **Mid-Career Challenges for the Sandwich Generation**
Karen A. Esmonde-White[1], Mary Lewis, Ian Lewis; *[1]Endress+Hauser*

(408) **Panel & Open Discussion**

22IR05: Quantum Cascade Lasers for Chemical Sensing
Ballroom D&E

Chair: Bernhard Lendl, *TU Wien*
Co-Chair: Pietro Patimisco, *University of Bari*

(409) **Trace Water Detection in Organic Solvents by Photothermal Spectroscopy using a Mach-Zehnder Interferometer**
Giovanna Ricchiuti[1], Alicja Dabrowska, Davide Pinto, Georg Ramer, Bernhard Lendl; [1]*TU Wien*

(410) **Solvent Absorption Compensated Quantum Cascade Laser Infrared Microscopy for Bioimaging**
Yow-Ren Chang[1], Seong-min Kim, Young J. Lee[1]; [1]*National Institute of Standards and Technology*

(411) **QCL Based Mid-IR Dispersion Spectroscopy of Liquids**
Bernhard Lendl[1], Alicja Dabrowska, Andreas Schwaighofer; [1]*TU Wien*

(412) **Diffraction-Limited Mid-Infrared Hyperspectral Ellipsometry**
Markus Brandstetter[1], Alexander Ebner, Markus Brunner, Robert Zimmerleiter, Kurt Hingerl; [1]*Research Center for Non-Destructive Testing GmbH*

(413) **Spectroscopic Applications of Quantum Cascade Laser Arrays**
Chu C. Teng[1], Christian Pfluegl; [1]*Pendar Technologies, LLC*

22IR09: Spectroscopic Methods for Materials Characterization *Meeting Room 7*

Chair: Richard Bourne, *University of Leeds*
Co-Chair: Mike George, *University of Nottingham*

(414) **Raman Spectroscopy of Individual Electrospun Fibers**
Christian Pellerin[1], Arnaud W. Laramée[1], Clarence Allen; [1]*Université de Montréal*

(415) **Imaging the 3D Orientation of Polymer Chains by 2D Polarization IR Microscopy**
Young J. Lee[1], Shuyu Xu; [1]*National Institute of Standards and Technology*

(416) **Trimodal Microscopy for Better and Faster Microplastic IdentificationIR + Raman + Fluorescence**
James R. Anderson[1], Mustafa Kansiz, Eoghan Dillon; [1]*Photothermal Spectroscopy Corp*

(417) **Automated Particle Analysis Combined with Raman spectroscopy to Study Rutile Geochemistry for Provenance Analysis**
Sarah C. Shidler[1], Tim Prusnick, Lucy Grainger, Achim Hermann; [1]*Renishaw Inc.*

(418) **Fluorescence Rejection and Improved Identification of Raw Materials and Unknowns with a 785nm Raman System**
Elena Hagemann[1], Adam J. Hopkins[1], Naimish Sardesai; [1]*Metrohm USA*

22MASS02: Advances in Novel Mass-Spectral Imaging
Meeting Room 9

Chair: Jacob Shelley, *Rensselaer Polytechnic Institute*

(419) **Fast Imaging of Polymers Via Laser-Assisted Micro-Pyrolysis Flowing Atmospheric Pressure Afterglow High-Resolution Mass Spectrometry**
Dong Zhang[1], Gerardo Gamez; [1]*Texas Tech University*

(420) Parallel Elemental and Molecular Chemical Imaging with Tandem Laser-Ablation Mass Spectrometry and Laser-Induced Breakdown Spectroscopy
Jacob T. Shelley[1], Sunil Badal, Montwaun D. Young[1], Justin Park, Julia Danischewski; [1]*Rensselaer Polytechnic Institute*

(421) **High-throughput Analysis of Leaded and Non-toxic Inorganic Gunshot Residue by spICP-TOFMS**
Sarah E. Szakas[1], Korina L. Menking-Hoggatt[2], Alexander Gundlach-Graham, Tatiana Trejos; [1]*Iowa State University,* [2]*West Virginia University*

(422) **Fingermark Beyond the Ridge Detail: Chemical Analysis of Drugs and Toxic Metals in Fingermarks using Magnetic Carbon Nanoparticles and Mass Spectrometry**
Mohamed O. Amin[1], Entesar Alhetlani, Simona Francese; [1]*Kuwait University*

(423) **Development and Characterization of Low-Cost Liquid Sample Introduction System for ICP-MS**
Tristen Taylor[1], Alexander Gundlach-Graham; [1]*Iowa State University*

22PMA03: SERS for Drug Discovery *Meeting Room 10*

Chair: Colin Campbell, *University of Edinburgh*
Co-Chair: Lamyaa Almehmadi, *University at Albany, State University of New York*

(424) **Alkyne-tag SERS imaging for drug detection in living cells**
Katsumasa Fujita[1]; [1]*Osaka University*

(425) **Surface Enhanced Raman Scattering to Assess Sub-Cellular Nanoparticle Delivery**
Brian Scarpitti[1], Zac D. Schultz[1], Sanjun Fan; [1]*The Ohio State University*

(426) **Machine Learning Enabled SERS: Applications and Potential for Medical Diagnostics and Drug Discovery**
Joy Q. Li[1], Tuan Vo-Dinh; [1]*Duke University School of Medicine*

(427) **Label-Free SERS for Drug Discovery: Hit Identification**
Lamyaa M. Almehmadi[1], Vibhav A. Valsangkar, Ken Halvorsen, Qiang Zhang, Jia Sheng, Igor K. Lednev[1]; [1]*University at Albany, State University of New York*

(428) **A new SERS approach to monitor responses to therapy in live 3D tissue models.**
Colin J. Campbell[1], William Skinner, Norbert Radacsi, Robert Gray, Michael Chung, Nicola Robinson, Gareth Hardisty; [1]*University of Edinburgh*

22RAM05: IRDG Raman *Ballroom C*

Chair: Karen Faulds, *The University of Strathclyde*

(429) **Radiation Response Monitoring in Biological Systems Using Raman Spectroscopy and Machine Learning Techniques**
Andrew Jirasek[1], Kirsty Milligan, Ramie Ali-Adeeb, Phillip Shreeves, Juanita Crook, Alexandre Brolo, Julian Lum, Jeffrey Andrews; [1]*University of British Columbia*

(430) **Effect of Laser Power and Exposure Time on Live Cell Raman Measurements.**
Alison Hobro[1], Kota Koike, Takeshi Sugiyama, Nicolas Pavillon, Takayuki Umakoshi, Prabhat Verma, Katsumasa Fujita, Nicholas I. Smith[1]; [1]*Osaka University*

(431) **Designing Assemblies of Nano-Gold for Improved Raman Sensing**
Priyanka Dey[1]; [1]*Teesside University*

(432) **Brillouin Microscopy to Probe Viscoelastic Properties of Tissues in Health and Disease**
Michelle Bailey[1], Francesca Palombo; [1]*University of Exeter*

(433) **Ratiometric SESORS Imaging and Detection: Towards Locating Nanotags at Depth in 3D**
Matthew E. Berry[1], Samantha M. McCabe[1], Sian Sloan-Dennison, Stacey Laing, Neil C. Shand[2], Duncan Graham, Karen Faulds; [1]*The University of Strathclyde,* [2]*The Defence Science and Technology Laboratory (DSTL)*

22RAM12: Raman Spectroscopy for Security and Forensics Purposes *Meeting Room 1*

Chair: Igor Lednev, *University at Albany, State University of New York*
Co-Chair: Sonivette Colón-Rodríguez, *University at Albany, State University of New York*

(434) **Understanding how Matrix Composition Influences the Detection of Drugs using Raman and SERS**
Amanda J. Haes[1]; [1]*University of Iowa*

(435) **The classification of Raman scattering patterns using wavelet transform and transfer learning**
Jorn Yu[1], Ting-Yu Huang; [1]*Sam Houston State University*

(436) **Raman Screening of Lubricants and Lubricant Residues**
Candice Bridge[1], Safiya Best, Santana Thomas, Abryana Fergus, Mark Maric; [1]*University of Central Florida & National Center for Forensic Science*

(437) **Utilizing Raman Spectroscopy to determine the Time Since Deposition of Menstrual Blood Stains**
Alexis R. Weber[1], Anna Wójtowicz, Igor K. Lednev[1]; [1]*University at Albany, State University of New York*

(438) **Latest Advances in Handheld Raman Usability and Performance**
Luisa T. Profeta[1], Brian L. Bures[1], Huwei Tan, Adam J. Maines[1], Kurt R. Bistany[1], Stefan R. Lukow[1], Michael D. Hargreaves[1]; [1]*Rigaku Analytical Devices*

22SPECIAL06: Regional Academic Research *Meeting Room 2*

Chair: Pietro Strobbia, *University of Cincinnati*

(439) **What Lies Beneath your Elution Peak: Imaging When and Where Analytes Adsorb to Commercial Stationary Phase Particles**
Lydia Kisley[1], Ricardo Monge Neria; [1]*Case Western Reserve University*

(440) **Super resolution Spectral SERS imaging**
Zac D. Schultz[1]; [1]*The Ohio State University*

(441) **Real Time, Localized Measurement of Self Assembled Monolayer Formation**
Ryan White[1], Hope Kumakli; [1]*University of Cincinnati*

(442) **Circular Dichroism study of supramolecular systems**
Angela Mammana[1]; [1]*University of Dayton*

(443) **Engineering CRISPR-Cas Biosensors for Environmental and Infectious Disease Monitoring using Nucleic Acid Nanotechnology**
Kevin Yehl[1]; [1]*Miami University*

22SPECIAL08: Spectrochimica Acta B - Award Session *Meeting Room 4*
Chair: Alessandro De Giacomo, *University of Bari*

(444) **Real-time Characterization of Particles Produced by Laser Ablation for Analysis by Inductively Coupled Plasma Mass Spectrometry**
David W. Koppenaal[1], Kaitlyn J Suski, David M Bell, Matt K Newburn, M LIz Alexander, Dan Imre, Alla Zelenyuk; [1]*Pacific Northwest National Laboratory*

TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 5, 2022
Oral Symposia | 8:30 AM – 10:10 AM

(445) **A Searchable/Filterable Database of Elemental, Doubly Charged, and Polyatomic Ions that Can Cause Spectral Overlaps in Inductively Coupled Plasma-Mass Spectrometry**
John W. Olesik[1], Madeleine C. Lomax-Vogt[1], Fang Liu; [1]*Ohio State University*

(446) **A Demonstration of Spatial Heterodyne Spectrometers for Remote LIBS, Raman Spectroscopy, and 1D Imaging**
K. Alicia Strange Fessler[1], Stanley M. Angel[2], Abigail M. Waldron[1], Arelis Colon, J. Chance Carter; [1]*Savannah River National Laboratory,* [2]*The University of South Carolina*

(447) **Calibration-Free LIBS: What's New After 20 Years?**
Vincenzo Palleschi[1]; [1]*CNR, Italy*

(448) **Glow Discharge Optical Emission Spectroscopy Ultra-High Throughput Elemental Mapping: Insights into the Underlying Mechanisms via Laser Scattering Techniques**
Gerardo Gamez[1], Kevin Finch; [1]*Texas Tech University*

TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 5, 2022
Awards and Plenary Lectures | 10:45 AM- 12:00 PM | *Event Center*

22PLEN03: Coblentz Society Clara Craver Award

(449) **Stimulated Raman Scattering Imaging: From Label-free to Metabolic to Super-multiplex and to Single-molecule Imaging**
Wei Min[1]; [1]*Columbia University*

22PLEN03: NESAS and SAS Lester W. Strock Award

(450) **Stimulated Raman Scattering Imaging: From Label-free to Metabolic to Super-multiplex and to Single-molecule Imaging**
Igor B. Gornushkin[1]; [1]*BAM Federal Institute for Materials Research and Testing*

TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 5, 2022
Oral Symposia | 1:30 PM – 3:10 PM

22AES06: Emerging Leaders Session *Meeting Room 8*

Chair: David Charlot

(451) **Towards The Use Of Commercially Available Microfluidic Chips for Zeta Potential Characterization**
Jonathan Cottet[1], Josephine O. Oshodi[1], Ariel L. Furst[1], Cullen R. Buie[1]; [1]*MIT*

(452) **ESSENCE 2.0: An Improved All-In-One POC Platform**
Yu Husan Cheng[1], Halexandra Alvarenga, Thara Balaji, Aditi Sathe, Zhenglong Li, Charmi Chande, Sagnik Basuray; [1]*New Jersey Institute of Technology*

(453) **Dielectrophoretic Pressure in Paper (DPiP): A Novel Insulator-based Dielectrophoretic Technique for Low-Cost Trapping and Separation**
Md Nazibul Islam[1], Zachary Gagnon; [1]*Texas A&M University*

(454) **Using Deep Eutectic Solvents as the Separation Media in Capillary Electrophoresis**
Christopher R. Harrison[1], Shreeya Venkatesan; [1]*San Diego State University*

(455) **Nonlinear Electrokinetics for Separating Microorganisms**
Alaleh Vaghef Koodehi[1], Olivia Ernst, Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

22AWD05: NESAS and SAS Lester W. Strock Award Symposium Honoring Igor Gornushkin *Ballroom D&E*

Chair: Igor Gornushkin, *BAM Federal Institute for Materials Research and Testing*

(456) **In-depth Characterization of ICCD Detector for LIBS Measurements**
George Chan[1]; [1]*Lawrence Berkeley National Laboratory*

(457) **Coupling Laser Ablation and Plasmic Structures for Elemental Analysis**
Alessandro De Giacomo[1], Marcella Dell'Aglio; [1]*University of Bari*

(458) **Rare-earth Elements Analysis by LIBS**
Michael Gaft[1], Lev Nagli, Yosef Raichlin; [1]*Ariel University*

(459) **A Critical Comparison of Laser-Ablation Atomic Absorption Spectroscopy Paradigms**
Jonathan A. Merten[1]; [1]*Arkansas State University*

(460) **LIBS Imaging: Recent Advances and Perspectives**
Vincent Motto-Ros[1]; [1]*Institut Lumière Matière*

22AWD08: Coblentz Society Craver Award Symposium Honoring Wei Min *Ballroom C*

Chair: Wei Min, *Columbia University*

(461) **High Performance Infrared Spectroscopic Imaging for Rapid Biomedical Assessment**
Rohit Bhargava[1], Kevin Yeh, Seth M. Kenkel[1], Yamuna Phal, Anirudh Mittal, Kianoush Falahkheirkhah; [1]*University of Illinois Urbana-Champaign*

(462) **Principles of 2D IR Imaging and Applications to Cataract and Amyloid Tissues**
Martin Zanni[1]; [1]*University Wisconsin-Madison*

(463) **Functional Stimulated Raman Imaging for Complex Subcellular A\nalysis**
Lu Wei[1]; [1]*Caltech*

(464) **Super-resolution Multiplexed Metabolic Imaging of Aging and Diseases**
Lingyan Shi[1]; [1]*UC San Diego*

(465) **Genetics Free Optoacoustic Neuromodulation**
Ji-Xin Cheng[1]; [1]*Boston University*

22BIM06: Optical Technologies for Disease Screening and Diagnostics *Meeting Room 3*

Chair: Fay Nicolson, *Dana-Farber Cancer Institute and Harvard Medical School*

(466) **Point of Care Diagnosis of Preeclampsia**
Samuel Mabbott[1]; [1]*Texas A&M University*

(467) **Breaking Multiplexity Limits of SERS Imaging to Enable Highly Specific Molecular Imaging and Spatial Profiling of Diseased Tissues**
Olga Eremina[1], Alexander Czaja, Augusta Fernando, Arjun Aron, Dmitry Eremin, Cristina Zavaleta; [1]*University of Southern California*

(468) **Development of a Compact Dual Raman and Fluorescence Spectrometer for Point-of-Care Diagnostics**
Cyril Soliman[1], Jonathan Faircloth, Samuel Mabbott, Gerard L. Coté[1], Kristen Maitland; [1]*Texas A&M University*

(469) **Multimodal Nonlinear Optical Microscopy Unveils Early Therapy-induced Senescence in Human Cancer Cells**
Dario Polli[1], Arianna Bresci, Francesco Manetti, Silvia Ghislanzoni, Federico Vernuccio, Chiara Ceconello, Benedetta Talone, Alejandro De La Cadena, Subir Das, Renzo Vanna, Italia Bongarzone, Giulio Cerullo; [1]*Politecnico di Milano*

(470) **Enhanced Tri-modal Optical-Photothermal Infrared (O-PTIR) Spectroscopy – Advances in Spatial Resolution, Sensitivity & Tri-modality (IR, Raman & Fluorescence)**
Mustafa Kansiz[1]; [1]*Photothermal Spectroscopy Corp*

22FORENS04: Pharmaceutical Forensics *Meeting Room 9*

Chair: Adam Lanzarotta, *US Food and Drug Administration*
Co-Chair: Alexis Weber, *University at Albany, State University of New York*

(471) **Parallel Column Gas Chromatography combined with Mass Spectrometry for Comprehensive Forensic Analysis of Benzodiazepines**
Matthew R. Wood[1]; [1]*Ocean County Sheriff's Office, New Jersey*

(472) **Field Deployable Analytical Toolkit for Rapid Analysis of FDA Regulated Products at International Ports of Entry**
Sara E. Kern[1], Adam Lanzarotta, JaCinta Batson, Michael Thatcher, Martin K. Kimani[2], Lisa Lorenz, Brian Boyd, Melissa Collins, Anvi Patel, Julio Arrecis, Kelsey Griffin, Fernando Gonzalez, Gregory Howe, Morgan Hudson-Davis, Mark Loh, Flavia Morales, Allison Taylor, Anthony Wetherby, Muhammed Altaf, David Laguerre, Donna LaGarde, Valerie Toomey; [1]*US Food and Drug Administration,* [2]*U.S. Food & Drug Administration*

(473) **The Advantages of Integrating Portable Spectrometers for Counterfeit Detection and Analysis Casework**
Pauline E. Leary[1], Richard Crocombe, Brooke W. Kammrath[2]; [1]*NOBLE,* [2]*University of New Haven*

(474) **Protecting Patients Using Forensics and Innovative Technologies**
Ravi Kalyanaraman[1]; [1]*Bristol Myers Squibb*

22LIBS08: Medical Applications *Meeting Room 4*

Chair: Pavel Porizka, *CEITEC Brno University of Technology*
Co-Chair: Jozef Kaiser, *Central European Institute of Technology, Brno University of Technology*

(475) **Determination of Elemental Distributions within Functionalized Polystyrene Beads**
Andreas Limbeck[1], Birgit Achleitner, Aida Fazlic, Davide Ret, Simone Knaus; [1]*TU Wien, Institute of Chemical Technologies and Analytics*

(476) **Towards Cohort Study of Cutaneous Cancers Using Laser-Induced Breakdown Spectroscopy**
Hana Kopřivová[1], Kateřina Kiss, Jakub Buday, Lucie Vrlíková, Milan Kaška, Marcela Buchtová, Jozef Kaiser, Pavel Porizka; [1]*Central European Institute of Technology, Brno University of Technology*

(477) **Looking for Laser-Induced Breakdown Spectroscopy Signatures of Diseases in Biomedical Fluids: Progress and Challenges**
Noureddine Melikechi[1], Joshua E. Landis, Khaoula Ouarak, Helmar Adler, Souheyr Meziane, Kim Berlo, Florentine Zwillich, Erin Gibbons, Farhad Pourkamali-Anaraki, Danielle Bonito, Gregory E. Chiklis, Weiming Xia; [1]*University of Massachusetts Lowell*

(478) **In Situ Multi-Elemental Imaging with LIBS for Periprosthetic Tissue Characterization**
Benoit Busser[1], Vincent Gardette, Lucie Sancey, Pat Campbell, Vincent Motto-Ros; [1]*Institute for Advanced Bisociences*

(479) **Use of Spectroscopic and Tomographic Techniques for the Detection of Microplastics in Human Tonsils**
Viktória Parobková[1], Michaela Kavkova, Daniel Holub, Gabriela Kalčíková, Pavel Porizka, Jozef Kaiser, Tomáš Zikmund, Milan Urík; [1]*Central European Institute of Technology, Brno University of Technology*

22LIBS10: Instrumentation *Meeting Room 5*

Chair: Mohamad Sabsabi, *National Research Council Canada*

(480) **Underwater-LIBS: From Laboratory to Deep Sea Towards the Applications**
Ronger Zheng[1], Yuan Lu, Jinjia Guo, Ye Tian, Wangquan Ye, Ying Li; [1]*Ocean University of China*

(481) **Tailored LIBS Systems For Industrial Applications**
Reinhard Noll[1], Joachim Makowe, Volker Mörkens, Markus Dargel; [1]*Laser Analytical Systems & Automation GmbH*

(482) **2D LIBS Elemental Mapping Analysis of Steel and Li-ion Battery Electrodes using Pico-Second Laser Irradiation**
Yoshihiro Deguchi[1]; [1]*Tokushima University*

(483) **An Overview of LIBS Instrumentation with Focus on Mining Applications**
Paul Bouchard[1], André Beauchesne, Francis Boismenu, Antoine Hamel, Christian Padioleau, Kim Renaud, Tony Vaillancourt, Josette El Haddad, Daniel Gagnon, Aissa Harhira, Elton Soares de Lima Filho, Francis Vanier, Mohamad Sabsabi; [1]*National Research Council Canada*

22PAT03: Advances in On-Line Process Analysis *Meeting Room 7*

Chair: Xiaoyun (Shawn) Chen, *Dow*

(484) **Real-Time In-Line Moisture Determination of High Rubber Graft (HRG) Acrylonitrile Butadiene Styrene (ABS) Resin in a Fluid Bed Dryer**
Yusuf Sulub[1], Dejin Li; [1]*SABIC*

(485) **Globally Monitoring 9,000+ Molecular Groups in Whole Crude Using Spectroscopy**
Bryan Bowie[1], Chad Chrostowski, Payman Pirzadeh; [1]*ExxonMobil*

(486) **Influence of Powder Stream Density on Near-Infrared Measurements upon Scale-up of a Simulated Continuous Process**
Natasha L. Velez-Silva[1], Carl A. Anderson[1], James K. Drennen, III[1]; [1]*Duquesne University*

(487) **How the chemical recovery process in the pulp and paper industry may profit from in-line Raman spectroscopy**
Karin Wieland[1], Anna Katharina Schwaiger, Barbara Weiß, Bernhard Lendl, Martin Kraft; [1]*Competence Center CHASE GmbH*

22PMA07: Advances in the Analysis of Nanomaterials for Health *Meeting Room 10*

Chair: Zahra Rattay, *University of Strathclyde*

(488) **Improving Sensitivity of Detection using Magnetic Particles Coupled with SERS**
Nikesh N. Patel[1], Duncan Graham, Karen Faulds, Stacey Laing; [1]*University of Strathclyde*

(489) **In Situ Real Time Monitoring of Emulsification and Homogenization Processes for Vaccine Adjuvants**
Nicole Ralbovsky[1], Joseph P. Smith[1]; [1]*Merck & Co*

(490) **A Breakthrough in Inline Nanoparticle Sizing and Process Control for Nanosuspension Manufacturing**
Rut Besseling[1], Carl Schuurmans, Raquel Arribas Bueno, Michiel Hermes, Remy van Tuijn, Ad Gerich; [1]*InProcess-LSP*

(491) **On/Off Fluorescent Detection of Cancer Biomarker in Cancer Cells**
Sulayman A. Oladepo[1]; [1]*King Fahd University of Petroleum and Minerals*

22RAM11: Raman Spectroscopy for Food Security *Meeting Room 1*

Chair: Royston Goodacre, *The University of Liverpool*

(493) **Understanding the Impact of Adjuvants on Pesticide Persistence and Penetration in Fresh Produce using Surface-Enhanced Raman Mapping**
Xinyi Du[1], Lili He; [1]*University of Massachusetts Amherst*

(494) **Detecting Microplastics in Plastic Teabag Leachates via Infrared and Raman Spectroscopy**
Cassio Lima[1], Royston Goodacre; [1]*The University of Liverpool*

(495) **Non-Invasive Plant Genotyping and Identification of Pathogen Resistance Using Raman Spectroscopy**
Dmitry Kurouski[1]; [1]*Texas A&M University*

(496) **Raman Spectroscopy as a Tool for Understanding Oil or Fat Quality in Food Products**
Karen A. Esmonde-White[1], Mary Lewis, Michael Donahue, Ian Lewis; [1]*Endress+Hauser*

(497) **High Throughput Microplastic Characterization Using Particle Correlated Raman Spectroscopy**
Bridget O'Donnell[1], Eunah Lee; [1]*HORIBA Scientific*

22SPECIAL05: Regional Industrial Research
Meeting Room 2

Chair: Gloria Story, *Procter & Gamble*

(498) **Developing Complex Fluids in Microgravity**
Matt Lynch[1], Thomas Kodger, William Meyer, Mark Pestak; [1]*Procter & Gamble*

(499) **Dissolution Recycling of Polyolefins Using Alkane Solvents**
John Layman[1], Dimitris Collias, Amy Waun; [1]*Procter & Gamble*

(500) **Cleaning Clothes in Space and Applications for Consumer Use**
Mark R. Sivik[1], Will Shearouse, Kristi Niehaus, Steven Patterson; [1]*Procter & Gamble*

(501) **Soft Material Characterization: Translating Clinical Magnetic Resonance Imaging Methods for Consumer Products Research**
Nicole Westrick[1]; [1]*Procter & Gamble Co.*

(502) **Dynamic Computed Tomography for Product Research and Development**
Laura Wiley[1], Alex Doukas; [1]*Kinetic Vision*

22SPR02: Optical and Chiral Properties of Plasmonic Nanoparticles *Meeting Room 6*

Chair: Xingchen Ye, *University of Indiana Bloomington*

(503) **Controlling Localized Plasmons via an Atomistic Approach**
Nan Jiang[1]; [1]*University of Illinois Chicago*

(504) **Development and Characterization of Plasmonic Terahertz Sensors for Biological Analysis**
Santino N. Valiulis[1], Alexander S. Malinick[2], Quan Cheng; [1]*University of California, Riverside,* [2]*University of California Riverside*

(505) **Field Enhancement Between the Single-Reflection ATR-FTIR and Plasmonic Surfaces**
Li-Lin Tay[1], Nelson Rowell; [1]*National Research Council Canada*

(506) **Probing Infrared Plasmons with Electron Energy Loss Spectroscopy**
Jon P. Camden[1]; [1]*University of Notre Dame*

(507) **Ligand Rotational Isomer Effects on Optoelectronic Properties of Gold Clusters**
Christopher J. Ackerson[1], Gowri Udayangani Kuda-Singappulige, Christopher Hosier, Ian Anderson, Christine Aikens; [1]*Colorado State University*

(508) **Biomimetic Transparent Nanoplasmonic Meshes by Reverse-Nanoimprinting for Bio-interfaced Spatiotemporal Multimodal Surface-enhanced Raman Spectroscopy**
Aditya Garg[1], Elieser Mejia, Wonil Nam, Peter J. Vikesland, Wei Zhou; [1]*Virginia Tech*

(509) **Rapid Vibrational Circular Dichroism – Opportunities through the combination of External Cavity Quantum Cascade lasers and balanced detection**
Daniel-Ralph Hermann[1], Georg Ramer, Bernhard Lendl; [1]*TU Wien*

(510) **What Lies Beneath your Elution Peak: Imaging When and Where Analytes Adsorb to Commercial Stationary Phase Particles**
Lydia Kisley[1], Ricardo Monge Neria; [1]*Case Western Reserve University*

(511) **Opto-Lipidomics of Tissues**
Mads S. Bergholt[1]; [1]*King's College London*

22PLEN04: SAS and Applied Spectroscopy William F. Meggers Award

(512) **Process Analytical Utility of Raman Microspectroscopy for Cell Therapy Manufacturing Validation**
James Piret[1], Robin Turner, Georg Schulze, Shreyas Rangan, Martha Vardaki, Diepiriye Iworima, Timothy Kieffer, Michael Blades; [1]*The University of British Columbia*

22PLEN04: ANACHEM Award

(513) **Mass Spectrometry Au Naturel: A Tool for Structural Biology**
Joseph A. Loo[1]; [1]*University of California, Los Angeles*

22PLEN04: AES Electrophoresis Mid-Career Award

(514) **Nonlinear Electrophoresis of Colloidal Particles**
Aditya Khair[1]; [1]*Carnegie Mellon University*

22ATOM03: Nuclear *Meeting Room 3*

Chair: Benjamin Manard, *Oak Ridge National Laboratory*

(515) **Direct Analysis of Swipe Surfaces for Uranium by a Novel Microextraction-ICP-MS Approach**
Benjamin T. Manard[1], Brian Ticknor, Veronica Bradley, Cole R. Hexel[1], Shalina Metzger, Tyler Spano; [1]*Oak Ridge National Laboratory*

(516) **Predicting Gas Phase Ion Reactivity in Collision Cell ICP-MS/MS Analyses Through Theoretical and Experimental Analyses.**
Khadouja Harouaka[1], Kali Melby, Amanda French, Caleb Allen, Eric Bylaska, Richard Cox, Gregory Eiden, Maria Laura di Vacri, chelsie beck, brienne seiner, brian archambault, Eric Hoppe, Isaac Arnquist; [1]*Pacific Northwest National Laboratory*

(517) **LIBS and Its Role in Nuclear Energy Applications**
Supathorn Phongikaroon[1]; [1]*Virginia Commonwealth University*

(518) **Laser Ablation Spectroscopy for Radioactive Plume Detection**
Kyle C. Hartig[1], Kyle Latty, Emily Kwapis; [1]*University of Florida*

(519) **Spectroscopic Signatures and Oxidation Characteristics of Laser-produced Cerium Plasmas**
Emily Kwapis[1], Kyle C. Hartig[1]; [1]*University of Florida*

22AWD06: AES Mid-Career Award Symposium Honoring Aditya Khair *Meeting Room 7*

Chair: Henry Chu, *University of Florida*
Co-Chair: Christopher Easley, *Auburn University*

(520) **Electrohydrodynamic interactions of drops**
Petia Vlahovska[1]; [1]*Northwestern University*

(521) **Nonlinear Electrokinetic Flows in Insulator-based Dielectrophoretic Microdevices**
Xiangchun Xuan[1]; [1]*Clemson University*

(522) **Harnessing Nonlinear Electrophoresis Effects**
Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

(523) **Presentation Title TBD**
Todd Squires;

(524) **Diffusiophoresis-controlled Separation of a Colloid-electrolyte Suspension under Gravity and Solvent Evaporation**
Henry C. W. Chu[1], Jinjie Xu, Zhikui Wang; [1]*University of Florida*

22AWD07: SAS and Applied Spectroscopy William F. Meggers Award Symposium *Ballroom D&E*

Chair: Michael Blades, *The University of British Columbia*
Co-Chair: James Piret, *The University of British Columbia*

(525) **Extracting Pertinent Information from Congested and Overlapped Vibrational Spectra using Filtering Techniques Like 2D-COS and Node Attenuation**
Isao Noda[1]; [1]*University of Delaware*

(526) **The Role of Raman Spectroscopy in Bioprocess Automation**
Karen A. Esmonde-White[1], Maryann Cuellar, Justin Moretto, Ian Lewis; [1]*Endress+Hauser*

(527) **Non-Destructive Infrared Spectroscopic Assessment of Developing Tissue**
Nancy Pleshko[1], William Querido; [1]*Temple University*

(528) **Countering COVID-19 through Better Diagnostics: On Label-free Spectroscopic Methods for Virus Detection**
Ishan Barman[1]; [1]*Johns Hopkins University*

(529) **Complexity in Raman Spectroscopy: The Curse of the n's with Samples from Biopharmaceutical Manufacturing**
Alan G. Ryder[1]; [1]*National University of Ireland Galway*

22BIM03: Translation of Multimodal Imaging Technologies into Clinical Routine *Meeting Room 2*

Chair: Michael Schmitt, *Friedrich-Schiller University*
Co-Chair: Jürgen Popp, *Leibniz Institute of Photonics Technology*

(530) **Clinical Translation of Label-Free Multimodal Multiphoton Imaging for Point-of-Procedure Digital Pathology**
Stephen A. Boppart[1]; [1]*University of Illinois at Urbana-Champaign*

(531) **Raman Spectroscopy Devices for Intraoperative and in Situ Tumor Detection: Multicenter Retrospective Studies in Brain and Breast Cancer**
Frédéric Leblond[1]; [1]*Polytechnique Montréal*

(532) **Monitoring of Photodynamic Therapeutic Process of Cancer Cells with Pump-Probe Imaging Techniques**
Zhiwei Huang[1]; [1]*National University of Singapore*

(533) **Detecting Real-Time In Vivo Esophageal Biochemical Changes in Pediatric Eosinophilic Esophagitis Using Raman Spectroscopy**
Ezekiel Haugen[1], Andrea K. Locke[1], Girish Hiremath, Hernán Correa, Regina N. Tyree[1], Justin S. Baba[1], Anita Mahadevan-Jansen; [1]*Vanderbilt University*

(534) **Detection of Osteoporotic Related Bone Changes in Human Fingers Using ex vivo Raman Spectroscopy**
Christine Massie[1], Andrew J. Berger[1]; [1]*University of Rochester*

22CHEM05: Chemometric Opportunities in the Forensic Sciences *Meeting Room 5*

Chair: Igor Lednev, *University at Albany, State University of New York*

(535) **Fast Blue BB and 4-Aminophenol Colorimetric/Fluorometric Tests for the Differentiation of Hemp-Type and Marijuana-Type Cannabis and for the Determination of THC in Oral Fluid**
Jose R. Almirall[1], Alexander G. Acosta[1], Ryan Capote, Nicole Valdes, Maira Kerpel dos Santos, Roberta Gorziza; [1]*Florida International University*

(536) **FTIR Spectroscopy in Forensic Applications Advanced by Machine Learning Approaches: Making Data-Driven Decisions**
Lenka Halámková[1]; [1]*Texas Tech University*

(537) **Chemometrics for Extraction Useful Information from Raman Data: A Data Analysis Protocol**
Thomas W. Bocklitz[1]; [1]*Leibniz Institute of Photonics Technology*

(538) **Rapid Detection and Classifications of Pathogens using Raman Spectroscopy and Artificial Intelligence.**
Siva Umapathy[1], Sanchita Sil, Dipak Kumbhar, Dhanya Reghu, Divya Shrungar; [1]*Indian Institute of Science*

(539) **DART-High Resolution Mass Spectrometry (DART-HRMS) for Identification of the Resource That Necrophagous Insects Fed on**
Samira Beyramysoltan[1], Amy M Osborne, Jennifer Y. Rosati, Rabi A. A. Musah[1]; [1]*University at Albany-SUNY*

22FORENS02: Food Forensics *Meeting Room 8*

Chair: Luis E. Rodriguez-Saona, *The Ohio State University*

(540) **Development of a Handheld Sensor Technology for Real-time Measurement of Food Quality Traits**
Christopher Ball[1], Luis E. E. Rodriguez-Saona[1]; [1]*The Ohio State University*

(541) **NMR Techniques in Edible Oil Analysis and Authentication**
Emmanuel Hatzakis[1]; [1]*Ohio State University*

(542) **Detection of Some Common Food Adulterations in Türkiye Using Vibrational Spectroscopy**
Huseyin Ayvaz[1]; [1]*Canakkale Onsekiz Mart University*

(543) **Developing Surface Enhanced Raman Scattering-based biosensors for In Situ Detection of Agriculturally Relevant Targets**
Lyndsay Kissell[1], Pietro Strobbia; [1]*University of Cincinnati*

(544) **Real-Time Screening of Major Cannabinoids Content in Hemp by a Novel Handheld FT-NIR Spectroscopic Approach**
Siyu Yao[1], Christopher Ball, Gonzalo Miyagusuku-Cruzado, M. Monica Giusti, Luis E. E. Rodriguez-Saona[1]; [1]*The Ohio State University*

22IR10: Coblentz, New England SAS, and New York/New Jersey SAS Celebrating Success of Nurturing Talent in Vibrational Spectroscopy *Meeting Room 10*

Chair: John Wasylyk, *Bristol Myers Squibb*
Co-Chair: Larry McDermott, *Vertex Pharmaceuticals*

(545) **The Impact of Hot-Carriers on Surface Enhanced Raman Spectroscopy**
Chelsea Zoltowski (Goetzman)[1], Zac D. Schultz[1]; [1]*The Ohio State University*

(546) **Sensitive Nitric Oxide detection using Interferometric Cavity-Assisted Photothermal Spectroscopy**
Davide Pinto[1], J.P. Waclawek, Stefan Lindner, Harald Moser, Giovanna Ricchiuti, Bernhard Lendl; [1]*TU Wien*

(547) **Quantification of Drugs in Brain and Liver Mimetic Tissue Models using Raman Spectroscopy**
Nathan Woodhouse[1]; [1]*University of Nottingham*

Talks begin at 20-minute intervals.

(548) **Mid-Infrared Biomarkers of Lupus Nephritis Using Optical-Photothermal imaging**
Chalapathi Gajjela[1], Rohith Reddy, Chandra Mohan, Anto Crosslee, Camille Artur; [1]*University of Houston*

(549) **How to Survive as an Early Career Researcher**
Mike George[1]; [1]*University of Nottingham*

22LIBS02: Advanced Approaches I *Meeting Room 4*

Chair: Vassilia Zorba, *Lawrence Berkeley National Laboratory*

(550) **Nanoparticle Enhanced Laser Induced Breakdown Spectroscopy for Biological Applications**
Alessandro De Giacomo[1], Marcella Dell'Aglio, Rosalba Gaudiuso; [1]*University of Bari*

(551) **Back Deposition of Titanium Oxides under Laser Ablation of Titanium: Simulation and Experiment**
Igor B. Gornushkin[1], Vadim Veiko, Julia Karlagina, Andrey Samokhvalov, Dmitry Polyakov; [1]*BAM Federal Institute for Materials Research and Testing*

(552) **Multi Sensor Laser Ablation Analysis of Complex Samples**
Jhanis J. Gonzalez[1], Charles Sisson, Chunyi Liu, Vassilia Zorba, Dayana Oropeza, Jose Chirinos, Richard Russo; [1]*Lawrence Berkeley National Laboratory*

(553) **Using LIBS to Characterize High Entropy Alloys for Extreme Environments**
Prasoon K. Diwakar[1], Bharat Jasthi, Nicholas E. Pugh[1]; [1]*South Dakota School of Mines*

(554) **Laser-induced Breakdown Spectroscopy for Analysis of Molten Salts**
Daniel Diaz[1], David Hahn; [1]*University of Arizona*

22PAT02: SAS PAT Technical Section: PAT in BioPharma and Pharma *Meeting Room 6*

Chair: Dan Hill, *Biogen*
Co-Chair: Hossein Hamedi, *Biogen*

(555) **Enhanced Process Understanding of Lentiviral Manufacturing by Real-Time Raman Spectroscopy**
Erin Masucci[1], Karin M. Balss[1], Brynne Jensen, Carl Rafferty, Ryan Morrison, Emily Curtis; [1]*Janssen*

(556) **Raman Backed Model Predictive Control: Strengthening Raman's Utilization in Small-Scale Bioprocess Development**
Matthew Demers[1]; [1]*Amgen Inc*

(557) **Multi-Attribute Raman Spectroscopy (MARS) for Monitoring Product Quality Attributes in Formulated Monoclonal Antibody Therapeutics**
Bingchuan Wei[1]; [1]*Genetech*

(558) **Rapid Amino Acid Quantitation by an Integrated CE-MS Analyzer**
Kenion H. Blakeman[1], Hannah Wilker, Colin Gavin, Ji Young Anderson, Scott Miller; [1]*908 Devices*

(559) **In Situ Raman Spectroscopy for Real Time Detection of Cysteine**
Justin Lomont[1], Joseph P. Smith[2]; [1]*Merck,* [2]*Merck & Co*

22PMA09: Small Molecule Profiling *Meeting Room 9*

Chair: Katherine Hollywood, *University of Manchester*
Co-Chair: Royston Goodacre, *The University of Liverpool*

(560) **Good, Fast and Cheap in Metabolomics and Synthetic Biology, Choose One?**
Karl E V Burgess[1], Joan Cortada Garcia, Georgie Barrett, Tessa Moses, Jennifer Haggarty; [1]*University of Edinburgh*

(561) **NMR-based Isotope Editing, Chemoselection and Isotopomer Distribution Analysis in Stable Isotope Resolved Metabolomics**
Andrew N. N. Lane[1], Penghui Lin, Teresa Fan; [1]*University of Kentucky*

(562) **Stable Isotope Tracing of Nutrients From Consumption to Energy Production in Humans: A Step Towards Understanding Metabolism and Developing Therapeutic Interventions in the Fanconi Anemia Population**
Lindsey Romick-Rosendale[1], Sara Vicente-Munoz, Thomas Galletta, Suzanne Summer, Stella Davies; [1]*Cincinnati Children's Hospital Medical Center*

(563) **Direct Nanoelectrospray Ultra-high Resolution Mass Spectrometry in Stable-Isotope Labeled Metabolomics**
Richard M. Higashi[1], Teresa Fan, Andrew N. N. Lane[1]; [1]*University of Kentucky*

(564) **High Throughput Analysis and Ultra-Small Volume Detection of Biological Samples Using Droplet Imbibition Mass Spectrometry**
Taghi Sahraeian[1], Abraham Badu-Tawiah; [1]*The Ohio State University*

22SPECIAL03: Celebrating Peter Griffiths' 80th Birthday *Meeting Room 1*

Chair: Ian Lewis, *Endress+Hauser*

(565) **Microfluidic Modulation Spectroscopy: A New Approach for Probing Protein Secondary Structure**
Don Kuehl[1], Eugene Ma; [1]*Cerno Bioscience*

(566) **Laboratory Mentoring to become a President**
Christine Pharr[1]; [1]*Mount Mary University*

(567) **Data Preprocessing Method for the Analysis of Spectral Components in the Spectra of Mixtures.**
Richard Jackson[1], Qian Wang, John Lien; [1]*Galaxy Scientific, Inc.*

(568) **A Brief History of Optical Metrology**
Chris Manning[1], Andrew Helbers, Mathew Philippou, Yoav Kargon, Alexander Bianco, Tyler Morgus; [1]*Thorlabs, Inc.*

(569) **Mid-Infrared Sensors - From Emerging Tool to Enabling Technology**
Boris Mizaikoff[1]; [1]*Ulm University and Hahn-Schickard*

TECHNICAL PROGRAM – THURSDAY, OCTOBER 6, 2022
Oral Symposia | 4:00 PM – 5:00 PM

22AES05: AES Lifetime Achievement Award Session Honoring Adrienne Minerick *Meeting Room 7*

Chair: Christopher Easley, *Auburn University*

(570) **Ion Gradients in Dielectrophoretic Microdevices: Spatiotemporal Development and Impacts on Cells**
Adrienne R. Minerick[1], Azade Tahmasebi, Sanaz Habibi, Jeana Collins, Ran An; [1]*Michigan Technological University*

(571) **Multiplexed Traumatic Brain Injury (TBI) Assays using Particle Capture and Sorting**
Mark A. Burns[1], Frederick Korley, Alyse Krausz, Sanaz Habibi; [1]*University of Michigan*

(572) **Experiments in Mass Transfer: Inductive Heating and Micro Ring-Disk Electrodes**
David O. Wipf[1], Timothy J. Wipf[1]; [1]*Mississippi State University*

(573) **Presentation Title TBD**
Tayloria Adams[1]; [1]*University of California, Irvine*

22ATOM05: Food *Meeting Room 4*

Chair: Todor I. Todorov, *US Food and Drug Administration*

(574) **Occurrence and Quantification of Toxic Elements in Ready to Eat Baby Foods**
Patrick J. Gray[1]; [1]*US Food and Drug Administration*

(575) **Analysis of Toxic and Other Trace Elements in Baby Foods by ICP-MS**
Chady Stephan[1], Liyan Xing, Aaron Hineman; [1]*PerkinElmer Inc.*

(576) **Lowering Detection Limits for Arsenic Speciation in Baby Food**
Kevin Kubachka[1], Sean D. Conklin[1], Dominique Stutts, Kimberly Beers; [1]*US Food and Drug Administration*

(577) **Detection of Endogenic Copper Nanoparticles in Streptomyces Coelicolor and its Effect on Secondary Metabolism**
Paula García Cancela[1], Nathaly González Quiñónez, Mario Corte Rodríguez, Ángel Manteca fernández, Jörg bettmer, Maria Montes-Bayon; [1]*University of Oviedo*

(578) **Characterization of Elemental and Ligated Cobalt in Vitamin B12 using the Liquid Sampling-Atmospheric Pressure Glow Discharge Microplasma**
Cameron J. Stouffer[1], Sarah K. Wysor[1], Joseph V. Goodwin[1], R. Kenneth Marcus; [1]*Clemson University*

22AWD04: ANACHEM Award Symposium Honoring Joseph Loo *Ballroom D&E*

Chair: Joseph Loo, *University of California, Los Angeles*
Co-Chair: Rachel Ogorzalek Loo, *University of California, Los Angeles*

(579) **Multidimensional Mass Spectrometry of Advanced Materials**
Chrys Wesdemiotis[1]; [1]*University of Akron*

(580) **Coupling Accelerated Droplet Chemistry with LC-MS for Saccharide Analysis**
Abraham Badu-Tawiah[1], Enoch Amoah, Derik Heiss; [1]*The Ohio State University*

(581) **Lysine Acylation is Linked with Metabolism in Syntrophic Communities**
Rachel Ogorzalek Loo[1], Janine Fu, Robert Gunsalus, Michael McInerney, Joseph A. Loo[1]; [1]*University of California, Los Angeles*

(582) **Next-Generation Protein Stability Measurements in the Absence of Bulk Solvent**
Brandon Ruotolo[1]; [1]*University of Michigan*

(583) **From Protein Biochemist to Protein Mass Spectrometrist**
Kenneth D. Greis[1]; [1]*University of Cincinnati*

22BIM02: BioPhotonics Technologies Fighting Infections at the Point of Care *Meeting Room 3*

Chair: Ute Neugebauer, *Leibniz Institute of Photonic Technology*
Co-Chair: Jürgen Popp, *Leibniz Institute of Photonics Technology*

(584) **Automated Raman Spectroscopic Pathogen and AMR Detection from Research Lab to Diagnostic Solutions**
Markus Lankers[1]; [1]*mibic GmbH & Co. KG*

(585) **SERS Combined with Chemometric Analysis for Detection and Identification of Bacteria.**
Agnieszka Kamińska[1], Sylwia Berus, Krzysztof Niciński, Evelin Witkowska, Monika Adamczyk-Popławska, Beata Młynarczyk-Bonikowska,, Tomasz Szymborski; [1]*Polish Academy of Sciences*

Talks begin at 20-minute intervals.

(586) **Label-free, Raman-Based Analysis of Leukocytes for Rapid Characterization of Immune Response to Infection**
Ute Neugebauer[1], Natalie Arend, Anuradha Ramoji, Daniel Thomas-Rüddel, Oleg Ryabchykov, Aikaterina Pistiki, Michael Kiehntopf, Frank Bloos, Thomas W. Bocklitz[2], Iwan Schie, Michael Bauer, Juergen Popp; *[1]Leibniz Institute of Photonic Technology, [2]Leibniz Institute of Photonics Technology*

(587) **Antimicrobial Resistance Sensing Using a Solid Phase RPA-Resonant Raman Spectroscopy Combination: Application on the Big Five Carbapenemase Genes**
Waleed Hassanain[1], Christopher Johnson, Neil Keegan, Karen Faulds, Duncan Graham; *[1]The University of Strathclyde*

(588) **Asymptomatic Malaria Detection using Microfluidic Paper Device Capable of On-Chip Mass Spectrometry**
Abraham Badu-Tawiah[1], Suji Lee, Ayesha Seth, Girish Muralikrishnan; *[1]The Ohio State University*

22FORENS01: Nuclear Forensics *Meeting Room 8*

Chair: Robert Lascola, *Savannah River National Laboratory*

(589) **Microscopy and Spectroscopy of Actinide Dioxide Aging as a Function of Temperature and Relative Humidity**
Amy E. Hixon[1], Meena Said, Samuel Perry, Savannah Benjamin; *[1]University of Notre Dame*

(590) **Laser Fluorescence Spectroscopy and Multivariate Chemometrics for the Quantification of Uranium(VI), Samarium, Nitric Acid, and Temperature**
Luke Sadergaski[1], Hunter B. Andrews[1]; *[1]Oak Ridge National Laboratory*

(591) **Simultaneous Determinations of Uranium and Plutonium Utilizing Ultra-high Mass Resolution: The Liquid Sampling Atmospheric Pressure Glow Discharge/Orbitrap Coupling**
Joseph V. Goodwin[1], Benjamin T. Manard[2], Brian Ticknor, Paula Cable-Dunlap, R. Kenneth Marcus; *[1]Clemson University, [2]Oak Ridge National Laboratory*

(592) **Reaction Dynamics Of The Hydrolysis Molybdenum Hexafluoride By Cryogenic Layering On A Diamond Substrate**
Abigail M. Waldron[1], K. Alicia Strange Fessler, Patrick O'Rourke, Louis McNamara, Michael Thomas; *[1]Savannah River National Laboratory*

(593) **Simultaneous DSC–FTIR Reflectance Spectroscopy of the Insensitive High Explosive Triaminotrinitrobenzene (TATB) undergoing Thermal Degradation**
Greg L. Klunder[1], Malik Oliver, Batikan Koroglu, Keith Coffee, Adele Panasci-Nott, Joseph Van horn, Evan Kahl, Taylor Miller, Alan Burnham, John Reynolds; *[1]LLNL*

22IR02: NanoIR in Life Science and Biology
Meeting Room 2

Chair: Francesco Simone Ruggeri, *Wageningen University*

(594) **Nanoscale Structural Analysis of a Lipid-Driven Aggregation of Insulin**
Dmitry Kurouski[1]; *[1]Texas A&M University*

(595) **Peak Force Infrared Microscopy for Label-free Chemical Imaging of Biological Structures**
Xiaoji Xu[1]; *[1]Lehigh University*

(596) **Nanoscale Bio-Spectroscopy using Multivariate Data Analysis**
Georg Ramer[1], Bernhard Lendl, A. Catarina V.D dos Santos; *[1]TU Wien*

(597) **Application of Nano-FTIR Technology in Amyloid-β (Aβ) Research: A Revolutionary Tool in Disease Diagnosis**
Tobias Gokus[1], Suman Paul, Artem Danilov; *[1]Attocube Systems AG*

22PMA05: Industrial Applications of Vibrational Spectroscopy *Meeting Room 9*

Chair: Patrick Wray, *Bristol Myers Squibb*
Co-Chair: James Kimber, *Pfizer*

(598) **The Importance of Spectral Pre-processing for On-line Process Analysis Using Vibrational Spectroscopy**
Alison Nordon[1]; *[1]University of Strathclyde*

(599) **Infrared Spectroscopic, Imaging and Nano-Spectroscopic Analysis of Cells for Drug Development**
Andrew Chan[1]; *[1]King's College London*

(600) **Applications of Spectroscopic Imaging and PAT to 3D Printed Formulations**
Zoë Whalley[1], Patrick Wray, Tom Mills, Richard Greenwood; *[1]The University of Birmingham*

(601) **Process Analytical Technology: Applications to Batch and Flow Processes for Active Pharmaceutical Ingredient Development**
Courtney Talicska[1], Howard Ward, Eamon O'Connell; *[1]Pfizer*

(602) **Fluorescence Recovery after Photobleaching Based Diffusion Mapping within Heterogeneous Sample**
Ziyi Cao[1], Dustin M. Harmon[1], Ruochen Yang, Minghe Li, Aleksandr Razumtcev, Garth J. Simpson[1], Lynne S. Taylor[1]; *[1]Purdue University*

22RAM07: Transmission and Other Advanced Spectroscopic Sampling Methods in Pharmaceutical Analysis *Meeting Room 1*

Chair: Julia Griffen, *Agilent Technologies*

(603) **Transmission Low-Frequency Raman Spectroscopy**
Motoki Inoue[1]; *[1]Meiji Pharmaceutical University*

(604) **Frequency-Domain Terahertz Spectroscopy for Solid Samples in Normal Humidity Conditions with a Method for Suppressing Absorption Peaks by Water Vapor**
Kei Shimura[1], Touya Ono, Tetsuo Sasaki, Mizuki Mohara, Kenji Aiko, Tomoaki Sakamoto; *[1]Hitachi High-Tech Corporation*

(605) **Transmission Raman as Modern Backbone of Development for Oral Solid Dosage Forms**
Valentina Manici[1], Stefan Busche; *[1]Merck Group KGaA*

(606) **The Challenge for Real Time Release of Extended-Release Formulations by Raman Spectrometry**
Gregory K. Webster[1], Bharat Mankani, Sergey Mozharov, Brian Marquardt; *[1]AbbVie*

22SPECIAL11: Remembering Stanley Crouch *Meeting Room 6*

Chair: Dana Spence, *Michigan State University*
Co-Chair: F. Holler, *University of Kentucky*

(607) **A Half-Century of Working, Conducting Research, Teaching, Learning, Writing, and Laughing with Stanley Ross Crouch**
F. James Holler[1]; *[1]University of Kentucky*

(608) **Woodworking Science: Demystifying the Homemade Ebonizing Solution**
Robert Q. Thompson[1]; *[1]Oberlin College*

(609) **Novel, Autonomous, Microliter-scale, Integrated Sampling and Wet-Chemical-Analysis Platform for At-site Environmental, Industrial-Process, and Agricultural Monitoring**
Charles J. Patton[1], Curt Goodknight, Frank Goodknight; *[1]Segmented Solutions, LLC*

(610) **Anomalous Properties of Ionic Liquids. Using Fundamental Information to Advance Novel Applications**
Gary J. Blanchard[1]; *[1]Michigan State University*

(611) **Applying the Concept of the Complete, Multi-step Analysis to Complex Health-related Problems: Lessons Learned in the Crouch Group**
Dana Spence[1]; *[1]Michigan State University*

22SPR04: Enhancing Chemical Processes with Plasmonics *Meeting Room 5*

Chair: Amanda Haes, *University of Iowa*

(612) **Assessing Plasmon Associated Electron Transfer**
Zac D. Schultz[1]; *[1]The Ohio State University*

(613) **Localized Surface Plasmon Resonance in Hydrogels**
Francis P. Zamborini[1], Harikrishnan Nambiar; *[1]Louisville*

(614) **Spectroscopic Signatures of Plasmonic Hot Carrier Effects in the Steady State**
Matt Sheldon[1], Matthew Sheldon; *[1]Texas A&M University*

(615) **Development of Highly Sensitive and Reproducible SERS Substrates**
Jodie Fergusson[1], Stacey Laing, Sian Sloan-Dennison, Neil C. Shand[2], Duncan Graham, Karen Faulds; *[1]The University of Strathclyde, [2]The Defence Science and Technology Laboratory (DSTL)*

22SCIFRI: SciFri Closing Plenary Session

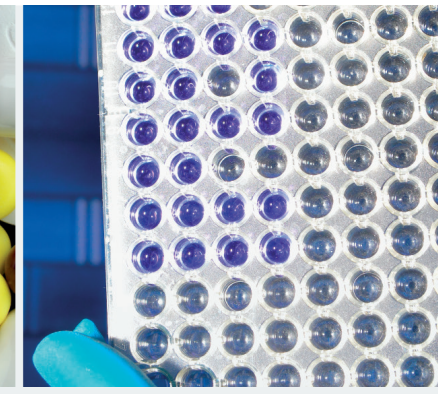
Chair: Robert Lascola, *Savannah River National Laboratory*

(616) **Terrestrial Benefits of Space Exploration**
Daniel Lockney[1]; *[1]NASA*

(617) **The Spaceflight Environment and Human Health and Performance**
Charles Doarn[1], *[1]University of Cincinnati*

(618) **From Ocean Worlds to the Big Blue: How Planetary Robotics is Helping Us Explore the Deep Sea Cost-Effectively**
Pablo Sobroni[1], *[1]Impossible Sensing*





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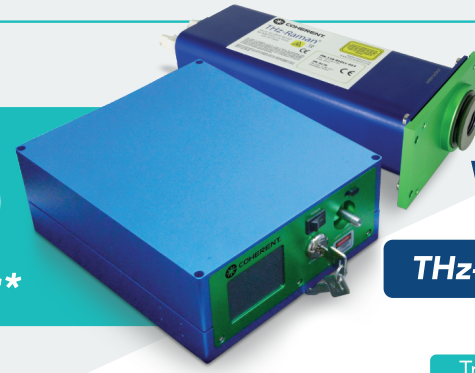

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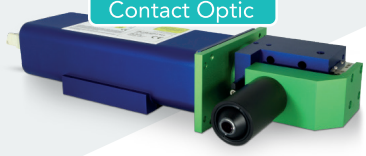

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Monday Poster Session - ART/ARCH

(Mon-P01) **Silcrete Geological Source Discrimination with Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry for Minimally Destructive Archaeological Stone Tool Provenience Studies**
Andrew M. Zipkin[1], Jayde N. Hirniak[2], John K. Murray[2]; *[1]Eurofins EAG Laboratories, [2]Arizona Stat e University*

(Mon-P02) **Application of Portable LIBS and XRF to Analysis of Archaeological Artifacts**
Magdalena E. Jackson[1], Kristen Livingston, Mary Kate Donais, Matthieu Baudelet, Jacob T. Shelley[1], Douglas Perrelli; *[1]Rensselaer Polytechnic Institute*

(Mon-P03) **The use of time of flight ICP-MS and very fast washout laserablation systems to accurately image major and minor isotopes aswell as elemental ratios in geological samples**
Lukas Schlatt[1], Phil Shaw; *[1]Nu Instruments*

(Mon-P04) **Confocal Raman Microscopy for the Detection of Calcium Phosphates in Fluorescent Soil Matrices**
Kay Sowoidnich[1], Peteh Mehdi Nkebiwe, Martin Maiwald, Bernd Sumpf, Tobias Edward Hartmann, Daniel Wanke, Torsten Müller; *[1]Ferdinand-Braun-Institut*

(Mon-P05) **In situ SEM-EDS-Raman investigation of ancient microfossils and their mineral matrix**
Justin D. Morrow[1], Andrea Corpolongo, Camden Goland, Desiree Baker, Andrew D. Czaja[2]; *[1]Thermo Fisher Scientific, [2]University of Cincinnati*

Monday Poster Session - FORENS

(Mon-P06) **Multivariate factor analysis to study the variations of ignitable liquid GC/MS profiles during the weathering process**
Briza Marie R. Dedicatoria[1], Shruthi Perna, Ngee Sing Chong, Mengliang Zhang; *[1]Middle Tennessee State University*

(Mon-P07) **Formation of spermine phosphate hexahydrate crystals in semen probed by Raman microspectroscopy**
Sonivette Colón-Rodríguez[1], Igor K. Lednev[1]; *[1]University at Albany, State University of New York*

(Mon-P08) **A Universal Test for the Forensic Identification of All Main Body Fluids Including Urine**
Bhavik Vyas[1], Lenka halamkova, Igor K. Lednev[1]; *[1]University at Albany, State University of New York*

(Mon-P09) **Identification and Discrimination of Fibers by Raman Spectroscopy**
Sergey Mamedov[1]; *[1]HORIBA Scientific*

(Mon-P10) **Stand-off Raman Spectroscopy: A Novel Method for the Detection and Identification of Body Fluid Traces**
Lamyaa M. Almehmadi[1], Igor K. Lednev[1]; *[1]University at Albany, State University of New York*

(Mon-P11) **Universal Method for Body Fluid Identification for Forensic Purposes: The Commercialization Effort**
Alexis R. Weber[1], Igor K. Lednev[1]; *[1]University at Albany, State University of New York*

(Mon-P12) **Surface-Enhanced Raman Spectroscopy Enables Highly Accurate Identification of Different Brands, Types and Colors of Hair Dyes**
Samantha Higgins[1], Dmitry Kurouski; *[1]Texas A&M University*

(Mon-P48) **Probing Menstrual Bloodstain Aging with Fluorescence Spectroscopy**
Anna Wójtowicz[1], Alexis R. Weber[2], Renata Wietecha-Posłuszny, Igor K. Lednev[2]; *[1]Jagiellonian University, [2]University at Albany, State University of New York*

Monday Poster Session - IR

(Mon-P13) **A Deep Convolutional Neural Network for bond/functional group identification from gaseous Infrared Spectra**
Fernando Fischer[1]; *[1]Universidad Católica Boliviana San Pablo*

(Mon-P14) **Quantum Cascade Laser-based Rapid Vibrational Circular Dichroism Spectroscopy**
Yamuna Phal[1], Rohit Bhargava, Ruo-Jing Ho; *[1]University of Illinois Urbana-Champaign*

(Mon-P15) **A Deep Learning Encoder-Decoder model for SMILES sequence generation from gaseous Infrared Spectra**
Fernando Fischer[1]; *[1]Universidad Católica Boliviana San Pablo*

(Mon-P16) **Rapid Screening of Clover Honey Adulteration with Infrared Spectroscopy and Chemometrics**
William Limm[1], Sanjeewa R. Karunathilaka[1], Magdi Mossoba; *[1]FDA*

Monday Poster Session - IR

(Mon-P17) **Measurement of Workplace Aerosols by simultaneous IR and Raman using Optical Photothermal Infrared Spectroscopy**
Vasileia Vogiazi[1], Nicholas E. Pugh[2], Orthodoxia Zervaki, Pramod Kulkarni; *[1]NIOSH / CDC, [2]South Dakota School of Mines*

(Mon-P18) **The Effect of Particle Size on Measurement Uncertainty of Analyte Quantification in Infrared Spectroscopy**
Kabir Rishi[1], Bon-Ki Ku, Chen Wang, Vasileia Vogiazi, Orthodoxia Zervaki, Pramod Kulkarni; *[1]NIOSH / CDC*

(Mon-P19) **Examining The Impact Of Gold Nanoparticles On Amylin Aggregation Via Two-dimensional Infrared Spectroscopy**
Kayla Hess[1], Sophia Vogelsang, Nathan Spear, Janet Macdonald, Lauren E. Buchanan[1]; *[1]Vanderbilt University*

(Mon-P20) **Long short-term memory and Transformer in Classification and Correction of ATR distorted spectrum**
Rui Cheng[1], Johannes Kiefer; *[1]Universität Bremen*

(Mon-P21) **Rapid Detection of COVID-19 Using Ultra-Compact MEMS Based Spectrometer and Supervised Machine Learning**
Yasser M. Sabry[1], Ahmed M. Abdelkhalik[2], Mazen Erfan, Ahmed M. Othman[2], Mohamed Kilany, Bassem Mortada, Mostafa Mohamed, Mohamed Gaber, Shereen Saeed, Ghada ismail, Bassam Saadany, Diaa Khalil; *[1]Si-Ware Systems, [2]Ain Shams University*

(Mon-P22) **Using TG-IR Hyphenation for Advanced Material Insight**
Samantha L. Nania[1]; *[1]PerkinElmer*

(Mon-P23) **Identification and Quantification of High-Consequence Chemical and Biological Toxin Surrogates with Infrared Spectroscopy**
Izabella A. Antczak[1], Elly Breves, Mandoye Ndoye, Richard Fauconier, Jacob T. Shelley[1]; *[1]Rensselaer Polytechnic Institute*

(Mon-P24) **Metabolic Fingerprinting For Diagnosis of Fibromyalgia and Other Rheumatology Disorders**
Haona Bao[1], Luis E. E. Rodriguez-Saona[1]; *[1]The Ohio State University*

(Mon-P26) **Visible-Near-Infrared Spectroscopy and Machine Learning Methods for the Identification of Amaranthus Species**
Soo-In Sohn[1], Subramani Pandian, Young-Ju Oh, Hyeon-Jung Kang, Eun-Kyoung Shin, Senthil Kumar Thamilarasan, Tae-Hun Ryu, Youn-Sung Cho, Tae-Sung Park; *[1]National Institute of Agricultural Sciences*

Monday Poster Session - MASS

(Mon-P27) **Accurate identification, examination and differentiation ofmultielement nanoparticles using time of flight ICP-MS and sub-millisecondspectral acquisition times**
Lukas Schlatt[1], Phil Shaw; *[1]Nu Instruments*

(Mon-P28) **Optimization of Surface Assisted Laser Desorption Ionization by Studying Material Properties of Polymer Nanofibers with a Photothermal Heterodyne Imaging Setup**
Yechan Moon[1], Zac D. Schultz[2], Susan V. Olesik[2]; *[1]The Ohio State Univerisity, [2]The Ohio State University*

(Mon-P29) **Diagnosis of Agglomeration of Crystallinity of Active Pharmaceutical Ingredients in Quartin Pills by Electrospray Laser Desorption Ionization Mass Spectrometry Ionization**
Margaret A. Sperry[1]; *[1]Marian University*

(Mon-P30) **Diagnosis of Agglomeration and Crystallinity of Active Pharmaceutical Ingredients in Pharmaceutical Preparations of Clotrimazole by Electrospray Laser Desorption Ionization Mass Spectrometry Imaging**
Kelsey K. Ramp[1], Patrick A. McVey[1]; *[1]Marian University*

(Mon-P31) **The Development of High Throughput Metabolomics To Aid The Synthetic Biology Design-Build-Test-Learn Cycle**
Georgie Barrett[1], Susan Rosser, Karl E V Burgess[1]; *[1]University of Edinburgh*

(Mon-P32) **Quantitation of Boron in Carbon Rich Matrices via Alkoxylation Gas Chromatography Mass Spectrometry as an Alternative to Plasma Spectrochemical Analysis**
Matthew Masters[1], Ron Tecklenburg, Eb Debrah; *[1]The Dow Chemical Company*

(Mon-P33) **Characterization and Quantification of Natural and Anthropogenic Titanium Nanoparticles using single-particle Inductively Coupled Plasma Time-of-Flight Mass Spectrometry**
Hark B. Karkee[1], Sarah E. Szakas[2], Alexander Gundlach-Graham; *[1]Iowa State university, [2]Iowa State University*

(Mon-P34) **Laser Ablation Mass Spectrometry for Interrogating Nuclear Materials**
Peter S. Boone[1], William Mason, Peter Hosemann, David Weisz, Brett H. Isselhardt[1]; *[1]Lawrence Livermore National Laboratory*

Monday Poster Session - MASS

(Mon-P35) **Semi-supervised Machine Learning to Classify Cerium Nanoparticles Measured with spICP-TOFMS**
Raven Buckman[1], Sarah E. Szakas[1], Alexander Gundlach-Graham; [1]*Iowa State University*

(Mon-P36) **Automated GC-MS analysis by KnowItAll MS Expert**
Karl Nedwed[1], Ty Abshear, Michelle D'Souza, O. David Sparkman, James Little; [1]*Wiley Science Solutions*

Monday Poster Session - PAT

(Mon-P37) **Non-Invasive In-Line Raman Spectroscopy Enables Readiness for Flexible Bioprocess Monitoring**
Christian Ott[1], Karin Wieland, Kristina Gruber, Christoph Haisch, Thomas Brück; [1]*Schott AG*

(Mon-P38) **Automated Sampling in Upstream Process Development for Accelerated Access to Critical Process Parameters and Critical Quality Attributes**
Lee LEE Asplund[1], Srijana Chapagain, Rakesh Bobbala, Khin Myint, Stacy Shollenberger, Allyson Caron; [1]*MilliporeSigma*

(Mon-P39) **On Digital Bioprocessing for manufacturing intelligence: Application of Process Analytical Technology (PAT) and Process Data Analytics (PDA) for upstream process development and intensification**
Ricardo Suarez Heredia[1], Marina Hincapie, Kevin Brower, Henry Lin, Nihal Tugcu; [1]*Sanofi*

(Mon-P40) **Carbon Dioxide Species In Tetramethylammonium Hydroxide Systems Using Macroscopic Raman Spectroscopy**
Michelle N. Sestak[1], Timothy M. Holt[1]; [1]*HORIBA Instruments Incorporated*

Monday Poster Session - PMA

(Mon-P41) **TD-NMR of Albumin Sources**
Gregory K. Webster[1], Steven Doherty; [1]*AbbVie*

(Mon-P42) **Recent Trends in Active Pharmaceutical Ingredient Profiles of Counterfeit Alprazolam Tablets**
Melanie N. Parsons[1], Enrique Yanes, Kelsey Griffin, Mary Jones, Valerie Toomey, Skyler W. Smith[1], Flavia Morales-Garcia; [1]*U.S. Food & Drug Administration*

(Mon-P43) **Continuous Mixing Technology: Characterization of a Vertical Mixer Using Residence Time Distribution**
James Kimber[1], Kai Lee, Giuseppe Cogoni, Jenna Brandon, David Wilsdon, Hugh Verrier, Sally Grieb, Ashwinkumar Jain, Pankaj Doshi, Daniel Blackwood; [1]*Pfizer*

(Mon-P45) **Comparison of Raman and Near-Infrared Chemical Imaging for Analysis of 3D Printed Formulations**
Zoë Whalley[1], Patrick Wray, Tom Mills, Richard Greenwood; [1]*The University of Birmingham*

Monday Poster Session - SPECIAL

(Mon-P46) **Characterizing Aromaticity of Triplet Corannulene and Coronene**
Dmitrii Govorov[1], Niroodha R. Pitawela[1], Anna Gudmundsdottir; [1]*University of Cincinnati*

(Mon-P47) **Photofracking of 1-Azido-2-Nitrobenzene Crystals**
Brandi James[1], Kristine Maxwell, Anna Gudmundsdottir; [1]*University of Cincinnati*

Tuesday Poster Session - ATOM

(Tu-P01) **Synthesis and Purification of 4-(1H-pyrrol-2-yl)pyridine and its Application in Sulfite Sensing**
Mallory E. Thomas[1], Lynn Scmitt, Alistair Lees; [1]*Binghamton University*

(Tu-P02) **Analysis of Micronutrients in Fruit Juice by Inductively Coupled Plasma Optical Emission Spectroscopy**
Andrea M. Palpini[1]; [1]*PerkinElmer Inc.*

(Tu-P03) **TotalQuant Technique - more than Semi-Quantitative Analysis**
Ewa M. Pruszkowski[1], Chady Stephan; [1]*PerkinElmer Inc.*

(Tu-P04) **Fast, High-Resolution Full Elemental Laser Ablation Imaging using Time-Of-flight ICP-MS for Endogenous Metal Analysis and Label Identification in Biological Samples**
Lukas Schlatt[1], Phil Shaw; [1]*Nu Instruments*

(Tu-P05) **Development and Validation of a Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) Method for the Analysis of Multivitamins**
Claudia Martinez Lopez[1], Todor I. I. Todorov[1]; [1]*US Food and Drug Administration*

(Tu-P06) **Iodine content in seaweed sold in the United States**
Todor I. I. Todorov[1], Mesay M. Wolle[1], Sean D. Conklin[1]; [1]*US Food and Drug Administration*

(Tu-P07) **Wavelength Dependent Photochemistry of Styrene Azide at Cryogenic Temperatures**
Dinindu P. Mendis[1], Anna Gudmundsdottir, Katrin Vilinsky, Baker Alomari; [1]*University of Cincinnati*

(Tu-P08) **Photodynamic Behavior of 1-(2-Azidophenyl)-3,5-Dimethylpyrazole**
Janaka P. Kavikarage[1]; [1]*University of Cincinnati*

Tuesday Poster Session - BIM

(Tu-P09) **Mechanistic Studies Of Flavanone Synthesis Using Flow Photochemistry**
Niroodha R. Pitawela[1], Anushree Das, Anna Gudmundsdottir; [1]*University of Cincinnati*

(Tu-P10) **Automated Feeding System for Normoglycemic Blood Storage**
Logan D. Soule[1], Lauren Skrajewski, Dana Spence; [1]*Michigan State University*

(Tu-P11) **Development of a Catalytic Sensing Mechanism to Enhance the Sensitivity of Homogenous Surface-Enhanced Raman Sensors for Viral Genetic Targets**
Steven M. Quarin[1], Amanda Macke, Ruxandra Dima, Pietro Strobbia; [1]*University of Cincinnati*

(Tu-P12) **Difference of Electronic Transition of Saccharides and its Monosaccharide ; Aime to the Unlabeled Analysis of Saccharide by Attenuated Total Reflection Far-UV (ATR-FUV) Spectroscopy**
Ryosuke Sasaki[1], Yusuke Morisawa; [1]*Kindai University*

(Tu-P13) **Numerical Investigation on Microfluidic Devices to Maintain Purity and Concentration of Separated Fractions of Bioparticles**
A K M Fazlul Karim Rasel[1], Sean L. Seyler[1], Mark A. Hayes[1]; [1]*Arizona State University*

(Tu-P14) **Linearly Polarized and Integrating Sphere-Assisted Resonance Synchronous Spectroscopies as Bioscience Tools: An Example Application with Protein and Silver Nanoparticle Interactions**
Kyle R. Carter[1], Max C. Wamsley[1], Joseph Emerson, Dongmao Zhang; [1]*Mississippi State University*

(Tu-P15) **Screening and Subsampling: A Successive Analysis of Nile Red Stained Microplastics Using Nanoparticle Tracking Analysis, Fluorescence (Hyperspectral) Imaging and Particle Correlated Raman Spectroscopy**
Eunah Lee[1], Julie Chen Nguyen, Bridget O'Donnell, Li Yan; [1]*HORIBA Scientific*

(Tu-P16) **Inertial Microfluidics for the Separation and Enrichment of Microscale Particles**
Elizabeth Ruscitti[1], Stephen C. Jacobson[1]; [1]*Indiana University*

(Tu-P17) **Vis-NIR Spectral Characterization of Joint Tissues for Arthroscopy**
Amanda Spurri[1], William Querido, Mohammed Shahriar Arefin, Chetan Patil, Nancy Pleshko; [1]*Temple University*

(Tu-P18) **Differentiation of Neurotoxic Arsenic Species in Biological Fluids Using Surface-Enhanced Raman Spectroscopy (SERS)**
Paula A. Evans-Pimiento[1], Bhavya Sharma; [1]*University of Tennessee*

(Tu-P19) **Enrichment of Green Fluorescent Proteins by Gradient Insulator-Based Dielectrophoresis**
Jerry Sheu[1], Mark A. Hayes[1]; [1]*Arizona State University*

(Tu-P20) **A Combined Near-Infrared and Mid-Infrared Spectroscopic Approach for the Detection and Quantification of Glycine in Human Serum**
Thulya Chakkumpulakkal Puthan Veettil[1], Bayden Wood; [1]*Monash University*

Tuesday Poster Session - BIM

(Tu-P21) **High-Throughput Droplet Microfluidic System For Antimicrobial Susceptibility Testing Of Antibiotics Against Common Drug-Resistant Bacterial Strains**
Yesman Akuoko[1], Adam T. Woolley[1]; [1]*Brigham Young University*

(Tu-P22) **A Reversed-Phase High Performance Liquid Chromatographic Method for the Determination of Ceftriaxone in Human Plasma**
Peter Tang[1]; [1]*Cincinnati Children's Hospital Medical Center*

(Tu-P24) **Can Radiolabeling Techniques Reveal Interferon-β's Mechanism of Action in Patients with Multiple Sclerosis?**
Morgan Geiger[1], Monica Jacobs, Kurt Zinn, Rany Aburashed, Dana Spence; [1]*Michigan State University*

(Tu-P43) **Investigating Bacteriophage-Host Interaction Using Raman Spectroscopy Combined with Stable Isotope Labeling**
ASIFUR Rahman[1], Wei Wang, Peter J. Vikesland; [1]*Virginia Tech*

(Tu-P44) **Analysis of Infection Steps of Virus with Culturing Cells by Raman Spectroscopy to Detect Viruses**
Keita Iwasaki[1], Kazuto Takami, Momoko Imai, Kosuke Hashimoto, Hidetoshi Sato; [1]*Kwansei Gakuin University*

(Tu-P45) **Simple Near-infrared Analysis of an Organic Phase Extracted from Bile Juice to Identify Gall Bladder Cancer**
Yunjung Kim[1], Eunjin Jang, Hoeil Chung; [1]*Hanyang University*

(Tu-P46) **Microfluidic Devices for Tracking Z-ring Dynamics in Response to Deletion of Negative Regulators in Bacillus subtilis**
Laura C. Lastra[1], Yuanchen Yu, Daniel Kearns, Stephen C. Jacobson[1]; [1]*Indiana University*

Tuesday Poster Session - CHEM

(Tu-P24) **Back to the Drawing Board: A Unifying First-Principle Model for Correlating Sample UV–Vis Absorption and Fluorescence Emission**
Max C. Wamsley[1], Samadhi N. Nawalage[1], Juan Hu, Willard Collier, Dongmao Zhang; [1]*Mississippi State University*

(Tu-P25) **Integrating-Sphere-Assisted Resonance Synchronous Spectroscopy for Quantification of Materials Double-Beam UV-vis Absorption**
Pathum D. Wathudura[1], Max C. Wamsley[1], Juan Hu, Dongmao Zhang; [1]*Mississippi State University*

(Tu-P26) **Photodynamic Behavior in Solid-State Vinyl Azides That Vary Due to the Flexibility of Substituents Upon Gas Release**
Fiona J. Wasson[1], Nayera Abdelaziz, Anna Gudmundsdottir; [1]*University of Cincinnati*

(Tu-P27) **Direct Analysis of Plutonium(IV) in Acidic Process Solutions Using UV-Vis Spectrophotometry and Partial Least-Squares Regression**
Guillaume Bailly[1], Didier Maloubier, Guillaume Legay; [1]*Commissariat à l'énergie atomique et aux énergies alternatives (CEA)*

(Tu-P28) **Adapting Models from a Source Calibration Set to a Target Deployment Domain with Repeat Spectra or a Constant Analyte Sample Target Set**
Jordan Peper[1], John H. Kalivas[1]; [1]*Idaho State University*

(Tu-P29) **Exploring Prenol as a Bioblendstocks Additive for Gasoline-type blendstocks**
Lorenzo Vega-Montoto[1]; [1]*Idaho National Laboratory*

Tuesday Poster Session - LIBS

(Tu-P30) **A Novel Platform For High-Speed, High-Resolution Laser Induced Breakdown Spectroscopy Imaging**
Shayne M. Harrel[1], Jean-Michel Laurent, Antoine Varagnat, Adrian Tercier, Vincent Motto-Ros; [1]*Andor Technology*

(Tu-P31) **Remote Isotopic Analysis of Lithium in Solids by Femtosecond Filament-Laser Induced Breakdown Self-Reversal Isotopic Spectrometry**
Kévin F. Touchet[1], Jose Chirinos, Zach Alvidrez, Changmin Kim, Xianglei Mao, Vassilia Zorba; [1]*Lawrence Berkeley National Laboratory*

(Tu-P32) **Isotopic Analysis of Glassy Uranium Samples by UV-LIBS**
Kévin F. Touchet[1], Jhanis J. Gonzalez[1], Richard Russo, Vassilia Zorba; [1]*Lawrence Berkeley National Laboratory*

(Tu-P33) **Mass and Morphology of Yttrium Plasma as Function of Ablation Energy**
Shealyn Chestnut[1], Mary Foster, Jonathan A. Merten[1]; [1]*Arkansas State University*

(Tu-P34) **Compact, Combined Laser-Induced Breakdown Spectroscopy (LIBS) and Raman System for the Detection and Investigation of Food Contamination. System Description and Preliminary Findings**
Sungho Shin[1], Iyll-Joon Doh, Euiwon Bae, Bartek Rajwa, J. Paul Robinson; [1]*Purdue University*

Tuesday Poster Session - LIBS

(Tu-P35) **Laser-Induced Breakdown Spectroscopy as a Readout Method for Detection of Biomolecules Labeled with Photon-Upconversion Nanoparticles**
Karolina Vytiskova[1], Radka Oborilova, Karel Novotny, Zdenek Farka, Pavel Porizka, Jozef Kaiser; [1]*Central European Institute of Technology, Brno University of Technology*

(Tu-P36) **Using LIBS to Characterize MPEAs in Extreme Conditions**
Nicholas E. Pugh[1]; [1]*South Dakota School of Mines*

(Tu-P37) **Iron Measurement in Wastewater Outfall by Laser-Induced Breakdown Spectroscopy**
CR BHATT[1], Daniel A. Hartzler[1], Dustin L. McIntyre[1]; [1]*NETL*

(Tu-P38) **Increasing Signal-Noise Ratio in Laser-Induced Breakdown Spectroscopy using a 3D-Printed Ar(g)-Flushed Partial-Vacuum Chamber (ArVaC)**
Sofia Paraoulaki de Miranda[1], Max Vallone, Victoria Paraoulaki de Miranda[1], Francisco J. Gomez Rivas-Vazquez[1], Claudia Ochatt, Robert C. DuBard[1]; [1]*Ransom Everglades School*

(Tu-P40) **Developments in the Rapid Diagnosis of Bacterial Pathogens Using Laser-Induced Breakdown Spectroscopy**
Emma J. Blanchette[1], Emily Tracey, Haiqa Arain, Alayna Tieu, Chloe Clement, Hadia Malik, Caroline Alionte, August Baughan, Grace Johnson, Isabella Arthur, Steven J. Rehse[1]; [1]*University of Windsor*

(Tu-P41) **A Customizable Modular Axes Positioning System (MAPS) For Laser-Induced Breakdown Spectroscopy**
Victoria Paraoulaki de Miranda[1], Max Vallone, Sofia Paraoulaki de Miranda[1], Francisco J. Gomez Rivas-Vazquez[1], Claudia Ochatt, Robert C. DuBard[1]; [1]*Ransom Everglades School*

(Tu-P42) **A 3rd Tuned PLS Model for Coal Property Analysis Using fs-LIBS System: A Comparative Study to Industrial Coal Analyzer**
Sahar Sheta[1]; [1]*Tsinghua University*

TECHNICAL PROGRAM – WEDNESDAY POSTERS

Poster Sessions | 10:10 AM – 10:45 AM & 3:10 PM – 3:50 PM | *Event Center*

Wednesday Poster Session - AES

(Wed-P01) **Electrokinetic lithography to engineer the collagen fiber microarchitecture**
Adrian Lomeli-Martin[1], Adeel Ahmed, Mehran Mansouri, Vinay V. Abhyankar, Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

(Wed-P02) **Towards an Understanding of AC-Electrokinetic Effects in the Separation of Nanoplastics**
Shulin Bu[1], Alexandra Ros; [1]*Arizona State University*

(Wed-P03) **Using Deep Eutectic Solvents as Reaction and Separation Media for Capillary Electrophoresis**
Karen S. Campos[1], Jessica Torres, Shreeya Venkatesan, Christopher R. Harrison[1]; [1]*San Diego State University*

(Wed-P04) **Solvent Mediated Forces in Protein Dielectrophoresis**
Michael Sauer[1], Mark A. Hayes[1], Matthias Heyden; [1]*Arizona State University*

(Wed-P05) **Isolation, Enrichment, and Recovery of Microparticles using Dielectrophoresis**
Jared P. Smithers[1], Mark A. Hayes[1]; [1]*Arizona State University*

(Wed-P06) **High-Frequency Dielectrophoresis Reveals Distinct Bioelectric Signature of Cancer Cells with Varying Ploidy and Nuclear Size**
Josie L. Duncan[1], Mathew Bloomfield, Vahid Farmehini, Nathan Swami, Daniela Cimini, Rafael Davalos; [1]*Virginia Tech*

(Wed-P07) **Biovariability Of Single Bacteria Isolate Measured With Label-free Insulator-Based Dielectrophoresis**
Hoai T. Nguyen[1], Mark A. Hayes[1]; [1]*Arizona State University*

(Wed-P08) **Nonlinear Electrokinetics of Non-spherical Particles**
Olivia Ernst[1], Alaleh Vaghef Koodehi, Blanca H. Lapizco-Encinas[1]; [1]*Rochester Institute of Technology*

(Wed-P09) **Trapping and Finite Element Analysis of Fluorescently-Tagged Gold Nanoparticles via Gradient Insulator Dielectrophoresis**
Alex Ramirez[1], A K M Fazlul Karim Rasel, Sean L. Seyler[1], Mark A. Hayes[1]; [1]*Arizona State University*

(Wed-P10) **Dielectric Characterization of Babesia Bovis using the Dielectrophoretic Crossover Frequency**
Raphael O. Oladokun[1], Soumya Srivastava; [1]*West Virginia University*

(Wed-P11) **Vis-NIR Spectroscopy and Machine Learning Methods for Discrimination of Transgenic Canola (Brassica napus L.) and their Hybrids with B. rapa**
Soo-In Sohn[1], Subramani Pandian, Young-Ju Oh, Hyeon-Jung Kang, Eun-Kyoung Shin, Senthil Kumar Thamilarasan, Tae-Hun Ryu, Woo-Suk Cho, Youn-Sung Cho, Tae-Sung Park; *[1]National Institute of Agricultural Sciences*

(Wed-P12) **In situ Raman spectroscopy Monitors the Corrosion of Mild Steel in a Salt Fog Chamber**
Dieter Bingemann[1], Arie Bleij, Maria Ponomareva, Markus Nadlinger, Gabriela Schimo-Aichhorn, Gerald Luckeneder, Gerald Haslehner, Pierluigi Bilotto; *[1]Wasatch Photonics*

(Wed-P13) **Super-resolution Surface Enhanced Raman Imaging of Protein Receptors in Cells**
Abigail E. Smith[1], Zac D. Schultz[1]; *[1]The Ohio State University*

(Wed-P14) **Analysis of Raman Spectra of Human Primary Keratinocytes and Melanocytes Under Y-Ray Irradiation Exposure**
Sila Jin[1], Yeonju Park, Hyo-Ji Lee, Yu-Jin Jung, Young Mee Jung; *[1]Kangwon National University*

(Wed-P15) **Raman Study on The Toxicity of Amyloid-β to Live Neurons**
Miyu Moriyama[1], Shogo Sato, Kosuke Hashimoto, Hidetoshi Sato; *[1]Kwansei Gakuin University*

(Wed-P16) **Raman Study on Early Reaction in Live Cells Infected with Virus**
Momoko Imai[1], Kazuto Takami, Keita Iwasaki, Kosuke Hashimoto, Hidetoshi Sato; *[1]Kwansei Gakuin University*

(Wed-P17) **Radiation Biodosimetry Using Mouse Hair by Raman Spectroscopy**
Spencer A. Witte[1], Courtney J. Morder[1], Zac D. Schultz[1], Naduparambil K. Jacob[1]; *[1]The Ohio State University*

(Wed-P18) **Effect of TIR at the air/medium interface on SORS scattering profiles**
Kate Whittaker[1]; *[1]Agilent Technologies*

(Wed-P19) **Classification of Glioblastoma Cancer Stem Cells Using Magnetically Sorted Surfaced Enhanced Raman Spectroscopy and Extracellular Matrix Peptide Mimics**
David W. Rist[1], Zac D. Schultz[1], Aleksander Skardal, Monica Venere, Tom Depalma, Miranda Montgomery; *[1]The Ohio State University*

(Wed-P20) **What Lies Beneath the Surface? – Raman Spectroscopy for Detection of Life in Space**
Nicholas Robins[1], Bhavya Sharma, Grace Sarabia; *[1]University of Tennessee, Knoxville*

(Wed-P21) **A Wide-Field Imaging Approach for Simultaneous Super-Resolution Surface-Enhanced Raman Scattering Imaging and Spectroscopy**
Deben Shoup[1], Zac D. Schultz[1]; *[1]The Ohio State University*

(Wed-P22) **Raman Spectroscopic Determination of Cellular Composition in Novel 3D Neuronal Cell Cultures**
Natalie Dunn[1], Meaghan Harley, Emily Travis, Wilson A. aruba[1], Avery Wood, Larry Millet, Madhu Dhar; *[1]University of Tennessee, Knoxville*

(Wed-P24) **Detection and Monitoring of Neuroinflammation With Surface Enhanced Raman Spectroscopy.**
Wilson A. Garuba[1]; *[1]University of Tennessee, Knoxville*

(Wed-P25) **Development of Surface-Enhanced Raman Spectroscopic Assay for Analysis of Traumatic Brain Injury Biomarkers**
Kevin Ledford[1], Avery Wood, Bhavya Sharma; *[1]University of Tennessee, Knoxville*

(Wed-P26) **Raman Spectroscopy and chemometrics: A Potential Method for Fingermark Discrimination from Gentle Touch of Drugs Tablets.**
Mohamed O. Amin[1], Entesar Alhetlani, Igor K. Lednev[2]; *[1]Kuwait University, [2]University at Albany, State University of New York*

(Wed-P27) **Effect of Hormone Replacement Therapy on Sex Determination Through Raman Spectroscopy**
Emily Miller[1], Brooke W. Kammrath[1], Igor K. Lednev[2], Alexis R. Weber[2]; *[1]University of New Haven, [2]University at Albany, State University of New York*

(Wed-P28) **Chemical Effects in Protein Analysis: A Systematic Investigation of Amino Acid Spontaneous Raman and SERS Responses**
Richard A. Dummitt[1], Zac D. Schultz[1]; *[1]The Ohio State University*

(Wed-P29) **Liquid Chromatography - Sheath Flow Surface Enhanced Raman Spectroscopy for Identification of Resveratrol in Red Wine**
Kristen Wang[1], Zac D. Schultz[1]; *[1]The Ohio State University*

(Wed-P30) **"Point of use" And Non-destructive Qualitative Screening of Long-lasting Insecticidal Mosquito Nets With Handheld Raman Spectroscopy For Malarial Prevention**
Ed Bethea[1], Matt Eady, David Jenkins; *[1]FHI360*

(Wed-P31) **Dual-mode SERS-based Lateral Flow Assay Strips for Simultaneous Diagnosis of SARS-CoV-2 and Influenza A Infection**
Mengdan Lu[1], Jaebum Choo; *[1]Chung-Ang University*

(Wed-P32) **SERS-ELISA Using Silica-Encapsulated Au Core-Satellite Nanotags for Sensitive SARS-CoV-2 Detection**
Qian Yu[1], Jaebum Choo; *[1]Chung-Ang University*

(Wed-P33) **Raman Spectroscopy: An Effective Analysis Tool for Lithium-ion Battery Manufacturing and Quality Control Processes**
Bruno Beccard[1], Shaileshkumar Karavadra, Sudhir Dahal; *[1]Thermo Fisher Scientific*

Wednesday Poster Session - SPECIAL

(Wed-P34) **Dimethyl Carbonate as a Mobile Phase Modifier for Normal Phase and Hydrophilic Interaction Liquid Chromatography**
Philip Boes[1], Sophie Elleman, Neil Danielson; [1]*Miami University*

(Wed-P35) **Applications of Digital Microscopy for the Analytical Chemistry Teaching Laboratory**
Hannah Newell[1], Krista Wilson, Alexander Igwebuike, Andre J. Sommer[1], Neil Danielson; [1]*Miami University*

Wednesday Poster Session - SPR

(Wed-P36) **Comparing Localized Surface Plasmon Resonance on Single Gold Sphere Nanoparticle and Nanorod Using Two-Trace Two-Dimensional Correlation Spectroscopy**
Sila Jin[1], Yeonju Park, Young Mee Jung; [1]*Kangwon National University*

(Wed-P37) **Construction of Solid-State Plasmonic Rulers Comprising Sharp Tip Gold Nanostructures tethered with Photoswitchable Molecular Machines**
Sarah R. Langlais[1], Sumon Hati, Rajesh Sardar; [1]*Indiana University - Purdue University Indianapolis*

(Wed-P38) **Investigation of Electronic Interactions Influencing the Plasmonic Property of Conjugated Ligand-Passivated Gold Nanostructures**
Sumon Hati[1], Xuehui Yang, Jing Zhang, Rajesh Sardar; [1]*Indiana University - Purdue University Indianapolis*

(Wed-P39) **Exploring Optimal Gold Nanoparticles for Single Particle Surface-Enhanced Raman Scattering Sensing**
Sanjun Fan[1], Brian Scarpitti, Zac D. Schultz[1]; [1]*The Ohio State University*

(Wed-P40) **Effects of Nanoparticle Multiplicative Scattering on Optical Spectroscopic Measurements**
Samadhi N. Nawalage[1], Pathum D. Wathudura[1], Dongmao Zhang; [1]*Mississippi State University*

AUTHOR INDEX

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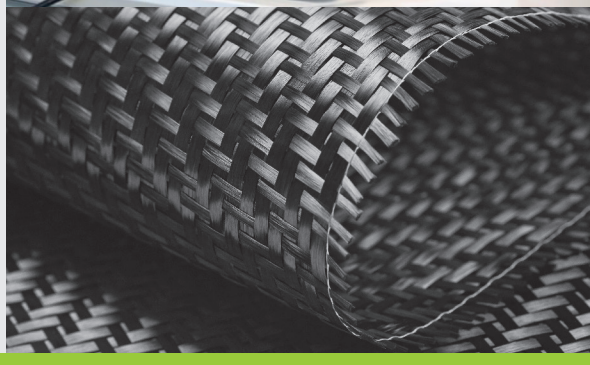

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