

FACSS PRESENTS

# SCIX 2023



OCTOBER 8-13, 2023

Nugget Casino Resort | Sparks, Nevada

**NATIONAL MEETING**

AES Electrophoresis Society

The Coblentz Society

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

Society for Applied Spectroscopy (SAS)



***SOCIETY FOR APPLIED  
SPECTROSCOPY  
AWARDS CEREMONY***

***AND  
WINE AND CHEESE  
RECEPTION***

***Tuesday, October 10, 2023  
Nugget Casino Resort***

***Awards Ceremony  
7:30 p.m. Sierra 5 Room***

***Wine and Cheese Reception  
8:30 p.m. Sierra 1 Room***

***Ticket must be presented for admission  
as this is a members only event.***

***Pick up your ticket at Booth #110 at***

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Check the mobile app and registration desk for any recent changes, or if you need assistance.

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## SciX Conference and FACSS International Office

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# WELCOME TO SciX 2023

On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS), it is our pleasure to welcome you to SciX 2023, our 50th meeting! Reaching this major milestone is quite an achievement, so this year's meeting will be a celebration of both the past and the future of SciX and analytical chemistry. We started out as a small meeting, with our first "FACSS" conference being in Atlantic City in 1974. At the time, some thought organizing a meeting with "papers presented in the fields of Analytical Chemistry and allied fields" with the purpose to "to disseminate technical information dealing with the applied, pure, or natural sciences" may be a bit of a gamble. It is perhaps fitting, therefore, that for our 50th meeting, like our first meeting, we are in another gambling location, Sparks, Nevada. It turns out that holding such a meeting was never going to be a gamble, thanks to the wonderful FACSS community and member societies, now 14 strong, always bringing a strong spirit of innovation and camaraderie, to share great science and have fun doing it. I can say that FACSS/SciX has, since my very first meeting in Detroit 1993, always been my favorite conference. The meeting has consistently delivered what it needed to be successful, great science, great collaborations, and great friendships. SciX is truly the conference of collaboration and networking – the Great Scientific Exchange. We will be using our long history to contrast with and highlight the future of analytical chemistry, with many sessions organized by early career spectroscopists in exciting new and/or booming areas of analytical science. The organizing and management team have toiled diligently to provide extremely high-quality sessions to highlight the latest exciting science and to provide excellent social events to allow you to network through your work and have fun doing it.

Our Program Chair, Karen Faulds, has done an amazing job to assemble a scientific program that balances the past and the future. It is with great delight that we see Peter Griffith giving Sunday's opening Keynote Lecture - *Fifty years of FACSS and SciX Conferences: The Remarkable Correspondence with Advances in Vibrational Spectroscopy*. Along with James de Haseth, Peter was a guiding light for me during my PhD due to their seminal book "Fourier Transform Infrared Spectrometry". Peter is truly a legend in vibrational spectroscopy, and he is recognized as such as the recipient of this year's Ellis R. Lippincott Award. Congratulations Peter! Our programming this year in state-of-the-science highlights advances in instrumentation and applications including numerous sessions in the fields of life science. Biopharma and biomedicine rightly take a front stage position - this is an area that is obviously critical for health and our standard of life. Catalyzed by COVID we have seen huge advances in the last four years, our role to provide analytical solutions for the development, production and quality of human diagnostics and treatments has never been more important. In parallel with this the application of artificial intelligence and machine learning to accelerate and focus solutions for biomedical spectroscopy and imaging, and manufacturing process solutions is currently in a renaissance period. We are pleased to see so many sessions and talks in this area this year. Two of our plenary lectures this year, from Juergen Popp and Ishan Barman will highlight this juxtaposition of biological analytical science and AI to provide treatment solutions. For me this period is certainly one of the most exciting few years to date in the last 50 years of analytical science. Our oral sessions begin on Sunday afternoon, providing non-stop scientific knowledge until Friday morning with more than 120 oral sessions, plus posters Sunday through Thursday. The fourteen FACSS member societies will again this year delight us with plenary talks from their new awardees, all of a very high quality like the two highlighted above. Organized by Awards Chair Jacob Shelley, this section will have many high points which you can find elsewhere in the program. Please celebrate and enjoy the scientific insights provide by all our awardees through their plenary lectures beginning at 10:45am each day.

A huge thank you to our section and session chairs! It cannot be understated how much work these volunteers put into SciX; it is not an exaggeration to say that this is somewhere in the region of 50 to 100 hours work each for them a year. This is in general a thankless task. So, when you see our section and session chairs please thank them, applaud them because without them SciX would not be possible and you would not be here learning, networking and having fun. Thank you!

As part of our celebration of FACSS/SciX we will have an exhibition and story board detailing our 50 meetings history. This will be located at the back of the exhibits area from Monday night to Wednesday. There will be many pictures and images showing our scientific and fun history. Go along and you might see Mike Carrabba, our FACSS Governing Board Chair, as a young man, when he was less grumpy or dressed as an elephant! You might also catch pictures of your friends! Thanks to Randy Heyler and James Carriere for stepping up to the plate to put this historical and fun montage together. Thanks also to Tina Gong, our Marketing Chair, for supporting this and all our marketing activity so you all can be informed about what is going on pre, during and post SciX – this is a challenging job to maintain good communications. The scientific program would not be complete without our short courses which provide continuous education through our member societies, industrial sponsors, and talented experienced scientific contributors. Short Courses Chair, Ellen Miseo has really stepped up to the plate this year - thanks Ellen! Our courses target technical skills and applications, through to softer career skills. It is not too late to register onsite! Related to this in this rapidly changing world we provide our attendees not only the opportunity to expand their skills but also provide new career opportunities through our Career Fair, organized by Robert Chimenti, on Wednesday morning. Please grab some coffee and snacks, you never know it might change your life!



Many of our career fair participants are also part of our yet again sold-out exhibition. The SciX Exhibition is an essential part of and is at the heart of SciX. The exhibition provides significant funding and highlights the essential tools of our analytical scientific trade. These exhibiting companies also sponsor our sessions and without them we would not have a conference. Be sure to visit the Exhibit Hall! Our Exhibits Chair Scott Rudder has yet again organized a fantastic exhibits experience. The Exhibition Opening Reception is back, in the Nugget Ballroom, and we will have fun activities arranged during this event. Also grab the chance to catch some sun and refreshments on the balcony during the Tuesday night Exhibitors Happy Hour. Get one of the collectable 50th anniversary SciX pins from our exhibitors on Tuesday before the event. Some of them may also have drink tickets that they can share when you engage in interesting conversations. Networking at SciX is what makes our conference so special and we encourage you to attend these events. Wednesday afternoon is our Exhibit Only closing event: with no technical sessions – to give you an opportunity to see any of our exhibitors before the exhibition concludes. The floor should be packed for an exhibits send-off.

The culmination of our social program – the SciX Gala – is again on Thursday evening. After a full week of celebrating our history and our future we will take a step back to our very beginning in 1974 with a 70's disco themed SciX Gala. There will be glitz, glamor and certainly Thursday Night Disco Fever. So put on your dancing shoes, 70's disco costumes, practice your Night Never and Grease moves and boogey on down to the Nugget Ballroom. There will be prizes, photo opportunities, and a 360-video booth for you to show off your moves. The night is yours to create new memories!

Sincerely,



**SciX 2023 General Chair**  
Andrew Whitley  
*HORIBA Scientific*

## SciX 2023 Committee



**SciX 2023 Program Chair**  
Karen Faulds  
*University of Strathclyde*



**SciX 2023 Exhibits Chair**  
Scott Rudder  
*OptoSigma Corporation*



**SciX 2023 Short Courses Chair**  
Ellen Miseo  
*Miseo Consulting*



**SciX 2023 Awards Chair**  
Jacob Shelley  
*Rensselaer Polytechnic Institute*



**FACSS & SciX Marketing Chair**  
Tina Gong  
*Revvity*

# 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 Coblenz 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

## 2023 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 2023 Section Chairs

### 2023 PROGRAM CHAIR

Karen Faulds  
*University of Strathclyde Glasgow*

### 2023 AWARDS CHAIR and 2024 PROGRAM CHAIR

Jacob Shelly  
*Rensselaer Polytechnic Institute*

### AES ELECTROPHORESIS

Tayloria Adams  
*University of California*

Erin Henslee  
*Wake Forest University*

### ART & ARCHAEOLOGY

Mary Kate Donais  
*Saint Anselm College*  
 Aj White  
*University of California, Berkeley*

### ATOMIC SPECTROSCOPY

Derrick Quarles Jr.  
*Elemental Scientific*  
 Benjamin Manard  
*Oak Ridge National Laboratory*  
 Alexander Gundlach-Graham  
*Iowa State University*

### 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*  
 Caelin Celani  
*University of Delaware*

### CONTEMPORARY ISSUES & EARLY CAREER RESEARCHERS

Karen Esmonde-White  
*Endress+Hauser*  
 Alexis Weber  
*University at Albany, SUNY*

### FORENSICS AND SECURITY

Betsy Jean Yakes  
*U.S. Food and Drug Administration*  
 Alexis Weber  
*University at Albany, SUNY*

### MASS SPECTROMETRY

Kaveh Jorabchi  
*Georgetown University*  
 Gabe Nagy  
*University Of Utah*  
 Chris Chouinard  
*Clemson University*

### MOLECULAR SPECTROSCOPY (IR)

Curt Marcott  
*Light Light Solutions*  
 Michael George  
*University of Nottingham*  
 Bernhard Lendl  
*TU Wien*  
 Georg Ramer  
*TU Wien*

### NASLIBS

Matthieu Baudelet  
*University of Central Florida*  
 Hunter Andrews  
*Oak Ridge National Laboratory*

### PHARMACEUTICAL ANALYSIS

John Wasyluk  
*Bristol-Myers Squibb*  
 Katherine Hollywood  
*The University of Manchester*

### PROCESS ANALYTICAL TECHNOLOGY

Shawn Chen  
*Dow Chemical*  
 Jim Rydzak  
*Specere Consulting*  
 Marissa Dobulis  
*Dow Chemical*  
 Zoe Whalley  
*University of Birmingham*

### RAMAN SPECTROSCOPY

Ian Lewis  
*Endress+Hauser*  
 Duncan Graham  
*University of Strathclyde*  
 Pavel Matousek  
*Rutherford Appleton Laboratory*  
 Sian Sloan-Dennison  
*University of Strathclyde*  
 Bhavya Sharma  
*University Of Tennessee*

### SPECIAL SESSIONS

Karen Faulds  
*University of Strathclyde Glasgow*

### 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

## CONFERENCE REGISTRATION / INFORMATION DESK

is located on the 2nd Floor of the Nugget Casino Resort.

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 Windows 10/MS Office 2016 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, Sierra 1**

7:15 pm – 9:15 pm SAS Student Poster Session

Poster set up 5:30 pm – 6:00 pm, remove at 9:00 pm

### **Monday, Nugget Foyer**

10:10 am – 10:45 am; 3:10 pm – 3:50 pm

### **Tuesday & Wednesday, Nugget Ballroom**

10:10 am – 10:45 am; 3:10 pm – 3:50 pm

### **Thursday, Nugget Foyer**

10:10 am – 10:45 am; 3:10 pm – 3:50 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 and may be removed after the afternoon poster session- 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

**Monday – 5:30- 7:30 pm | Exhibits Opening Reception**

**Tuesday – 10:00 am – 5:00 pm**

Coffee break/poster viewing	10:10 am – 10:45 am
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
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 – 5:00 pm

**BREAKFAST** is on-own every day of the conference. There will be breakfast for purchase Monday through Thursday near the registration area. A complimentary continental breakfast will be served Friday morning outside the plenary session room.

**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.

**SHORT COURSES** offer introductory and fundamental topics. Onsite registration is available at the registration desk – space permitting. See page 36 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, *Sierra 1*

### **Exhibits Opening Reception**

Monday, 5:30 pm, *Nugget Ballroom*

### **Exhibitor-Hosted Happy Hour**

Tuesday, 5:30 pm, *Chalet Terrace Room*

### **SciX Career Fair**

Wednesday, 8:00 am, *Sierra 1*

### **Exhibit Closing Reception**

Wednesday, 3:50 pm, *Nugget Ballroom*

### **SciX 2022 Gala**

Thursday, 7:00 pm, *Nugget Ballroom*

**COMPANION REGISTRATION** includes the Sunday Evening Welcome Mixer, Monday Exhibits Opening Reception, 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. See the registration desk for app details.

## SOCIETY AND COMMITTEE MEETINGS

### FACSS/SciX

#### Sunday, October 8

- 1:00 pm – 3:00 pm SciX 2024 Raleigh: Budget/General Planning/Program | *Redwood 6*
- 3:00 pm – 4:15 pm FACSS Long Range Planning Meeting (Federation) | *Redwood 6*
- 4:15 pm – 5:30 pm SciX Long Range Planning Meeting (Conference) | *Redwood 6*

#### Monday, October 9

- 12:15 pm – 1:30 pm SciX 2024 General Planning | *Redwood 6*

#### Tuesday, October 10

- 12:30 pm – 1:30 pm FACSS Budget Committee and Finance Committee | *Redwood 6*

#### Wednesday, October 11

- 7:00 am – 8:30 am Executive Committee Meeting (for the Executive Committee only) | *Redwood 6*

#### Thursday, October 12

- 12:30 pm – 2:00 pm Governing Board Meeting | *Redwood 6*

### COBLENTZ SOCIETY

#### Sunday, October 8

- 7:15 pm – 9:15 pm Coblentz Society Student Award Presentations at SAS Student Poster Session | *Sierra 1*

#### Monday, October 9

- 7:00 am – 8:30 am Coblentz Annual Member Meeting and Breakfast | *Sierra 4*
- 12:00 pm – 1:30 pm Coblentz Speed Mentoring Session | *Sierra 4*

*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 to those who pre-register.*

#### Wednesday, October 11

- 12:00 pm – 3:00 pm Headshots in Exhibit Hall | *Nugget Ballroom*
- 7:00 pm – 10:00 pm Members Only Coblentz Reception: *Stop by the Coblentz booth for details!*

### SOCIETY FOR APPLIED SPECTROSCOPY

#### Sunday, October 8

- 7:15 pm – 9:15 pm SAS Student Poster Session | *Sierra 1*

#### Monday, October 9

- 12:00 pm – 1:30 pm Meet the New SAS Office (bring your own lunch) | *Sierra 4*
- 8:00 pm SAS Student & Early Career Even | *Game On, Nugget Casino Resort*

#### Tuesday, October 10

- 7:30 pm – 8:30 pm SAS Award Presentations | *Sierra 5*
- 8:30 pm – 11:00 pm SAS Members' Wine and Cheese Reception | *Sierra 1*



# 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.
- For themed events where costumes are allowed or encouraged, attendees must be mindful of what level of taste is acceptable for a professional conference, and must take care not to wear anything that could be considered insulting to other cultures or social groups.

## **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](mailto: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](https://crisistextline.org): Text HOME to 741741

# PROGRAM SPONSORS

## PLATINUM

### **Agilent Technologies**

*Atomic, Forensics, Pharmaceutical Analysis, Mass Spectrometry*

### **Bristol-Myers Squibb**

*Pharmaceutical Analysis*

### **The Coblenz Society**

*Coblentz Award Sessions*

## GOLD

### **Bruker Optics/Nano**

*Molecular/IR*

### **Metrohm USA**

*Process Analytical, Art and  
Archaeology, Raman*

### **Elsevier**

*Special*

### **Endress + Hauser**

*Contemporary Issues/Early Career*

### **Photothermal Spectroscopy Corp**

*Molecular/IR*

### **Thermo Fisher Scientific**

*Mass Spectrometry*

### **Yyz Pharmatech Inc**

*Pharmaceutical Analysis*

## SILVER

Eigenvector Research, Inc. — *Atomic*

Elemental Scientific, Inc. — *Atomic*

ESL — *Atomic*

Glass Expansion, Inc — *Atomic*

Hamamatsu Corporation — *Forensics*

Harrington Center for  
Intelligent Instrumentation — *Chemometrics*

Ionflight — *Atomic*

Leco Corporation — *Atomic*

Mike and Mary Carrabba — *FACSS Student Awards*

Meinhard — *Atomic*

Mobilion Systems — *Mass Spectrometry*

Necsel Ip, Inc. — *Lanyards*

Nu Instruments — *Atomic*

PerkinElmer — *Atomic*

Royal Society of Chemistry — *Raman*

Sociedad de Espectroscopia Aplicada — *Atomic*

Society For Applied Spectroscopy — *Chemometrics*

tec5usa Inc. — *Process Analytical Technology*

Teledyne — *Atomic*

Tofwerk Ag — *Atomic*

Sciaps Inc. — *Art and Archaeology, Chemometrics*

Spectruma Analytik GmbH — *Atomic*

Wasatch Photonics — *Conference Bags*

Waters — *Mass Spectrometry*

## BRONZE

Excelitas Canada Inc.

— *Atomic*

Ownby Analytical, LLC

— *Art and Archaeology*

Society for Archaeological  
Sciences — *Art and Archaeology*

Thorlabs, Inc.

— *Literature Insert*

Spu System Inc.

— *Literature Insert*

## **PREMIER MEDIA PARTNER**

**Spectroscopy Magazine**

## **MEDIA PARTNERS**

**American Pharmaceutical Review**

**The Analytical Scientist**

**AuthentiCHEM**

**Applied Spectroscopy**

**BioPharma Asia**

**BioPhotonics, A Photonics Media Publication**

**ICP Winter Conference**

**Separations**



# SCIX EXHIBITS FLOORPLAN AND BOOTH KEY

As of September 18, 2023

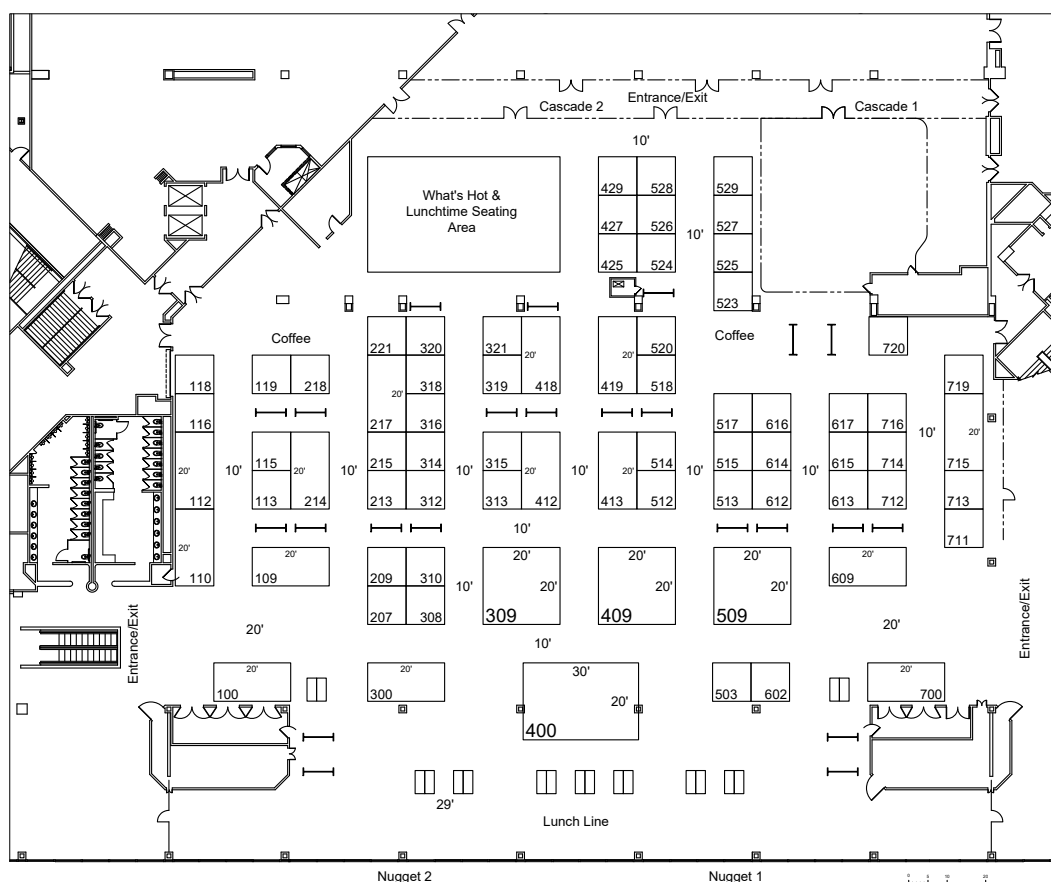


ABB Measurement and Analytics .....	517
ACS Division of Analytical Chemistry .....	319
Agilent Technologies .....	418
Alluxa .....	218
Andor Technology .....	529
Applied Spectra Inc.....	100
Armadillo SIA .....	316
Art Photonics GmbH.....	427
attocube systems Inc.....	221
Avantes .....	520
Barnett Technical Services .....	419
BaySpec, Inc.....	216
Biophotonics Diagnostics GmbH ....	429
Block Engineering .....	518
Bruker .....	425
Chroma Technology.....	615
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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

<b>1997 - Providence</b>			<b>2010 - Raleigh</b>	
Mildred Barber	Governing Board Chair		S. Douglass Gilman	Governing Board Chair
Chris Brown	General		David J. Butcher	General
John Olesik	Program		André J. Sommer	Program
Scott McGeorge	Exhibit		Mike Carrabba	Exhibit
<b>1998 - Austin</b>			<b>2011 - Reno</b>	
John Graham	Governing Board Chair		S. Douglass Gilman	Governing Board Chair
David Laude	General		Greg Klunder	General
Isiah Warner and Linda McGown	Program		Pavel Matousek	Program
Scott McGeorge	Exhibit		Mike Carrabba	Exhibit
<b>1999 - Vancouver</b>			<b>2012 - Kansas City</b>	
Robert G. Michel	Governing Board Chair		Ian R. Lewis	Governing Board Chair
Michael Blades	General		Brandye Smith-Goettler	SciX General
Ronald Williams	Program		Steven Ray	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibits
<b>2000 - Nashville</b>			<b>2013 - Milwaukee</b>	
John Koropchak	Governing Board Chair		Ian R. Lewis	Governing Board Chair
Arlene Garrison	General		Fred LaPlant	SciX General
Michael Carrabba	Program		Mike George	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibit
<b>2001 - Detroit</b>			<b>2014 - Reno</b>	
David A. Laude	Governing Board Chair		Greg Klunder	Governing Board Chair
David Coleman and L. Felix Schneider	General Co-Chairs		Luisa T. M. Profeta	SciX General
David J. Butcher	Program		José R. Almirall	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibit
<b>2002 - Providence</b>			<b>2015 - Providence</b>	
Michael Carrabba	Governing Board Chair		Greg Klunder	Governing Board Chair
Robert G. Michel	General		Edita Botonjic-Sehic	SciX General
Mark A. Hayes	Program		Glen P. Jackson	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibit
<b>2003 - Fort Lauderdale</b>			<b>2016 - Minneapolis</b>	
Ronald Williams	Governing Board Chair		Steven Ray	Governing Board Chair
Rina Dukor	General		Mary Kate Donais	SciX General
James Rydzak	Program		Alexandra Ros	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibit
<b>2004 - Portland</b>			<b>2017 - Reno</b>	
Michael Blades	Governing Board Chair		Steven Ray	Governing Board Chair
David Trimble	General		Becky Ditmar	SciX General
George Agnes	Program		Matthieu Baudalet	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibit
<b>2005 - Quebec City, Canada</b>			<b>2018 - Atlanta</b>	
Mark Hayes	Governing Board Chair		Fred LaPlant	Governing Board Chair
Denis Boudreau	General		Mark Henson	SciX General
Paul Farnsworth	Program		Karen Esmonde-White	SciX Program
Scott McGeorge	Exhibit		Mike Carrabba	SciX Exhibit
<b>2006 - Orlando</b>			<b>2019 - Palm Springs</b>	
Diane Parry	Governing Board Chair		Fred LaPlant	Governing Board Chair
Christine Wehlburg	General		Mark Hayes	SciX General
S. Douglas Gilman	Program		Garth Simpson	SciX Program
Mike Carrabba	Exhibit		Mike Carrabba	SciX Exhibit
<b>2007 - Memphis</b>			<b>2020 - Virtual (in lieu of Sparks)</b>	
James Rydzak	Governing Board Chair		Chris Palmer	Governing Board Chair
Paul Bourassa	General		Linda Kidder Yarlott	SciX General
Ian R Lewis	Program		Mary Kate Donais	SciX Program
Mike Carrabba	Exhibit		Mike Carrabba	SciX Exhibit
<b>2008 - Reno</b>			<b>2021 - Providence</b>	
Gary Brewer	Governing Board Chair		Chris Palmer	Governing Board Chair
John Hellgeth	General		Robert Chimenti	SciX General
Greg Klunder	Program		Jean-François Masson	SciX Program
Mike Carrabba	Exhibit		Scott Rudder	SciX Exhibit
<b>2009 - Louisville</b>			<b>2021 - Northern Kentucky</b>	
Becky Dittmar	Governing Board Chair		Mike Carrabba	Governing Board Chair
Jessica Jarman	General		Matthieu Baudalet	SciX General
Curtis Marcott	Program		Robert Lascola	SciX Program
Mike Carrabba	Exhibit		Scott Rudder	SciX Exhibit

# FACSS AWARDS

## FACSS THOMAS B. HIRSCHFELD SCHOLAR AWARD

*This 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.*



### **Dongkwan Lee**

Dongkwan earned a B.S. in Chemical Engineering and a minor in Electrical and Computer Engineering from the University of Illinois at Urbana-Champaign. During his undergraduate years, he worked with Prof. Rohit Bhargava to build a mid-infrared absorption microscope. Deeply intrigued by spectroscopic imaging, he pursued his Ph.D. at California Institute of Technology under Prof. Lu Wei's guidance, building a stimulated Raman scattering microscope and a fluorescence-infrared (IR) hybrid microscope.

His current research interest is mainly focused on expanding the vibrational imaging toolbox that enables investigation of complex biological systems. Understanding many biological systems requires high sensitivity, specificity, and spatial resolution imaging capabilities that are often out of reach in existing vibrational imaging technologies. In his recent work, he developed a new bond-selective imaging technique that enhances the sensitivity of direct mid-IR absorption microscopy. Mid-IR absorption provides rich chemical information, but its cross-sections are limited to  $\mu\text{M}$ -mM range. By coupling fluorescence and IR absorption and using fluorescence as a readout, bioimaging with single-molecule sensitivity and vibrational contrast was achieved. He seeks to continue his work in developing powerful vibrational imaging technologies that can be widely used in biological studies.



### **Adam Rish**

Adam Rish is a current Ph.D. candidate in Pharmaceutics at Duquesne University (Pittsburgh, PA) under the direction of Dr. Carl A. Anderson. In his Ph.D. work, Adam is focused on addressing limitations in calibration-free modeling approaches for spectroscopic process analytical technology (PAT) toward improving industrial and regulatory acceptance of these approaches. He received his bachelor's degree in Biochemistry at Grove City College (Grove City, PA) prior to beginning his doctoral studies in 2018.

The goal of his Ph.D. research has been enhancing the applicability of calibration-free modeling approaches to PAT deployment in pharmaceutical manufacturing. The majority of the work has focused on iterative optimization technology (IOT) algorithms and their current restrictions: limited model diagnostics and lack of prediction robustness. The strategies developed by Adam have been shared in multiple accepted and upcoming peer-reviewed publications. These research results have been presented and well received at several national conferences.

During his Ph.D. research, Adam has had the opportunity to collaborate and work for major pharmaceutical companies including Pfizer and Bristol-Meyer Squibb. These collaborations have resulted in several scientific publications in high impact, peer-reviewed journals. During his free time, Adam enjoys cooking, hiking, and gardening.



## FACSS STUDENT AWARD

*This prestigious 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.*



### **Aleksandr Razumtcev**

Aleksandr is a Ph.D. candidate in Professor Garth Simpson's group at Purdue University, where he conducts research at the intersection of vibrational spectroscopy and nonlinear optics. Prior to his graduate studies, he obtained a bachelor's degree in Chemistry from Saint-Petersburg State University, Russia. During his undergraduate studies, he focused on characterizing multilayered thermoelectric semiconductor nanofilms fabricated by pulsed laser deposition. After joining Purdue University, Aleksandr has been working on developing a novel method

for mid-infrared photothermal microscopy. This method relies on detecting temperature-induced changes in fluorescence intensity. By leveraging the high sensitivity of fluorescence quantum yield to local temperature variations, this new approach enhances the signal-to-noise ratio in sub-diffraction fingerprint region imaging by two orders of magnitude compared to conventional optical photothermal microscopy.

Aleksandr's work in F-PTIR microscopy was recognized with the ALS Doctoral Fellowship awarded by Lawrence Berkeley National Laboratory (LBNL). This fellowship currently supports his research at LBNL, focusing on further advancements in F-PTIR. His ongoing research interests involve utilizing F-PTIR for sub-micron chemical-specific imaging of fluorescently-labeled brain tissue sections to study neurodegenerative diseases and exploring broadband imaging using synchrotron radiation as an infrared light source. In total, Aleksandr has authored nine research publications and received several awards, including an outstanding poster award at the "Vibrational Spectroscopy" Gordon Research Conference.

## FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS CALL FOR 2024 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 2024 at [scixconference.org](https://scixconference.org).** To be considered for either award, students must submit an abstract for oral presentation at SciX (submission opens later winter/early spring 2024), then submit the following as a single PDF file:

- The application form (check in early 2024 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

## FACSS INNOVATION AWARD

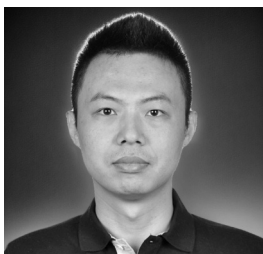
*The FACSS Innovation Award is given to the most innovative and outstanding new research advancements debuted orally at the SciX Conference. All program areas are included. Only research findings presented for the first time in the public domain qualify for entry. Work based on submitted papers not yet 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. Finalists present at the SciX conference in an exclusive plenary session on Thursday, with the award winner(s) selected and announced on Friday morning to conclude SciX.*

### 2023 FACSS INNOVATION AWARD SYMPOSIUM

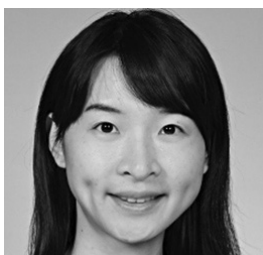
Thursday | 3:30 – 5:40 | Sierra 5



New Opportunities for Mass Spectrometry in Nanocrystal Surface Chemistry  
**Mengliang Zhang**



Unveiling Superior Spectroscopic Precision: A Shoebox-Sized, Low-Cost Spatial Heterodyne Spectrometer with 1-pm Resolution  
**Yi You**

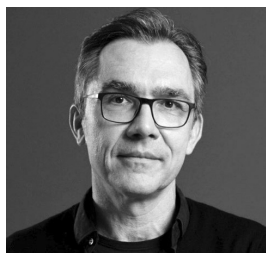


Real-time Controlling a Single DNA in Hotspot for Programmable Surface-enhanced Raman Spectroscopy Scanning in Solution  
**Jinqing Huang**



Acoustic Ion Manipulation: A Novel Approach to Enhance Ion-based Spectroscopies  
**Jacob Shelley**

*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.*



### **Juergen Popp**

Juergen Popp studied chemistry at the universities of Erlangen and Würzburg, Germany. After his PhD in Physical Chemistry, he joined Yale University for postdoctoral work. He subsequently returned to Würzburg University where he finished his habilitation in 2002. Since 2002 Juergen Popp holds a chair for Physical Chemistry at the Friedrich-Schiller University Jena, Germany. Since 2006 he is also the scientific director of the Leibniz Institute of Photonic Technology, Jena.

Juergen Popp is a world leading expert in Biophotonic / optical health technology research covering the complete range from photonic basic research towards translation into clinically applicable methods. The core of the biophotonic research activities lies in the realization of multicontrast microspectroscopic imaging approaches and instruments as well as in the implementation of fiber-, chip- and nanoparticle-based methods together with chip-based molecular point-of-care or point-of-use concepts to address biomedical, environmental and life-science problems. In particular, his expertise in the development and application of innovative linear and non-linear Raman spectroscopy approaches according to the needs of pathology, oncology, and infection/sepsis should be emphasized. A further research focus of Prof. Popp is the Raman spectroscopic investigation of material science issues. All his research is supported by the development and application of sophisticated data analysis procedures based on machine learning methods or other data analysis methods like 2D-correlation analysis.

Juergen Popp has published more than 960 journal papers and has been named as an inventor on 20 patents. His work has been cited more than 31.000 times and he has an h-index of 77. Juergen Popp is a leading partner in various national and international research projects in cooperation with academic, clinical and industrial partners (e.g. initiator and CEO of the research campus “InfectoGnostics” a public-private partnership researching new paths in infection diagnosis and infection research or initiator and core-partner of the “Leibniz Center for Photonics in Infection Research (LPI)” - the LPI is one of three projects that the German government has put on the national roadmap for research infrastructures). In doing so, he and his group raised more than 100 million Euro third party funding. He gave more than 200 invited talks on national and international conferences (among them more than 60 keynote/plenary lectures). Juergen Popp has been organizer and chairman of several large national and international conferences (e.g. ICOB 2012, ICORS 2014, ECONOS 2016 and many more) and of several interdisciplinary and translatory workshops and symposia. In this context, Juergen Popp shows great national, international and political commitment for interdisciplinary and translation (e.g. as member of the program committee „Optical Technology“ of the German Federal Ministry of Education and Research (BMBF) or as Member Board of Stakeholders European Technology Platform “Photonics21”). He has been frequently asked as a contact person for media and politics.

In 2012, he received an honorary doctoral degree from Babeş-Bolyai University in Cluj-Napoca, Romania. Professor Jürgen Popp is the recipient of the 2013 Robert Kellner Lecture Award and the prestigious 2016 Pittsburgh Spectroscopy Award. In 2016 he was elected to the American Institute for Medical and Biological Engineering (AIMBE) College of Fellows. 2018 Juergen Popp was awarded the renowned Ioannes Marcus Marci Medal of the Czechoslovak Spectroscopy Society, he won the third prize of the Berthold Leibinger Innovationspreis and received the Kaiser-Friedrich-Forschungspreis. In 2019 he was awarded the Ralf-Dahrendorf-Preis für den Europäischen Forschungsraum and in 2020 he became an OSA senior fellow. In 2021 he became a Fellow (FRSC) of the Royal Society of Chemistry. In 2022 he was awarded the Kuivila Lectureship Award of the University of Albany, USA and was named among the Photonics100 2023.

# SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

## DUAL AWARDEE:

### SAS APPLIED SPECTROSCOPY WILLIAM F. MEGGERS AWARD

Awarded to the most outstanding paper appearing in *Applied Spectroscopy*,  
2022, Volume 76, Issue 8, August 2022, Pages 926-936

### AND SAS/NASLIBS BEST PAPER AWARD

This award is for the Best Paper Published in *Applied Spectroscopy* on Laser Induced Breakdown Spectroscopy,  
2022, Volume 76, Issue 8, August 2022, Pages 926-936

## Femtosecond Single-Pulse and Orthogonal Double-Pulse Laser-Induced Breakdown Spectroscopy (LIBS): Femtogram Mass Detection and Chemical Imaging with Micrometer Spatial Resolution

Nikolaos Giannakaris, Anna Haider, Christoph M. Ahamer, Stefan Grünberger, Stefan Trautner and Johannes D. Pedarnig



### Presented by Johannes D. Pedarnig

Johannes Pedarnig received a Ph.D. in Physics from the Ludwig-Maximilians-Universität (LMU) in Munich / Germany under the supervision of Prof. Ted W. Hänsch (Ted Hänsch received the Nobel Prize in Physics in 2005). Johannes then joined the Johannes Kepler University JKU Linz as postdoctoral researcher to investigate laser-matter interaction processes in the research group of Prof. Dieter Bäuerle. Johannes is associate Professor at JKU Linz in the Institute of Applied Physics and his research group is applying optical spectroscopy for the element analysis of complex materials. Techniques include laser-

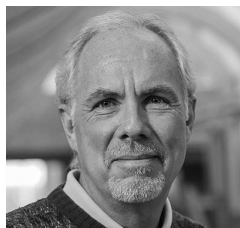
induced breakdown spectroscopy (LIBS) and different kinds of optical absorption and emission spectroscopies. A further research topic of his group is the pulsed-laser deposition of functional oxide thin films. Johannes is author and co-author of more than 130 research papers and he has organized the 8th Euro-Mediterranean Symposium on Laser-Induced Breakdown Spectroscopy. He is cooperating with different industries to apply LIBS in industrial processes.



**Nikolaos Giannakaris** is a Ph.D. student in Engineering at the Applied Physics Institute at Johannes Kepler University (JKU) in Linz/Austria under the supervision of Assoc. Prof. Dr. Johannes D. Pedarnig.



**Anna Haider** studied Technical Physics at the Johannes Kepler University JKU Linz, Austria. She was working on femtosecond-LIBS for her Master thesis and received a M.Sc. degree from JKU Linz.



**Stefan Grünberger** was born in Austria and began his career as a scientist at the Johannes Kepler University (JKU) in Linz, close to his hometown. Throughout his studies, he remained devoted to the Institute of Applied Physics and the esteemed group leader Prof. Dr. Johannes D. Pedarnig.

## NOT PICTURED

**Christoph M. Ahamer** studied Technical Physics at the Johannes Kepler University JKU Linz, Austria, and investigated industrial oxide materials by calibration-free laser-induced breakdown spectroscopy (CF-LIBS). He received a PhD degree in technical sciences from JKU Linz working on femtosecond-LIBS with high spatial resolution. Christoph has published his results in several papers in international journals

**Stefan Trautner** was also an author on this award-winning paper.



## NESAS AND SAS LESTER W. STROCK AWARD

*This award is given by the New England Section of the Society of Applied Spectroscopy in recognition of a selected publication of substantive research in/or application of analytical atomic spectrochemistry in the fields of earth science, life sciences, or stellar and cosmic sciences.*



### **Maria Montes-Bayón**

Maria Montes-Bayón holds a bachelor in Chemistry (1993, University of Oviedo, Spain), a master in Analytical Chemistry (1994, University of Plymouth, UK/ University of Oviedo) and a PhD (1999, University of Oviedo; awarded) degree. From April 2000 till July 2002, she joined the research group of Prof. Joseph A. Caruso at the Department of Chemistry at the University of Cincinnati (Ohio, USA) as Postdoctoral Fulbright Fellow. After this period, she got a Ramón y Cajal Senior Researcher contract at the University of Oviedo for five years. Later, in 2008, she became Associate Professor and in 2017, Full Professor of Analytical

Chemistry at the University of Oviedo (Spain). Her main research interests are: a) Development of quantitative strategies for determination of molecular biomarkers of clinical relevance at the single cell level using ICP-MS; b) Evaluation of encapsulated metallodrugs for their potential use in chemotherapy using mass spectrometry and c) Analytical tools to study biogenic nanoparticles and metal nano-debris from metallic implants.

## ADDITIONAL SAS AWARDS PRESENTED ON TUESDAY EVENING

### SAS ATOMIC TECHNICAL SECTION STUDENT AWARDS

*Recognizing outstanding student research in the area of Atomic Spectroscopy.*



### **Catharina Erbacher**

Ph.D. candidate in Analytical Chemistry under the supervision of Prof. Dr. Uwe Karst at the University of Münster, Germany



### **Cristina Mednez Lopez**

4th year Ph.D. student working on Laser-Induced Breakdown Spectroscopy (LIBS) at the Spectroscopy, Lasers and Plasmas Research Group (GELP) led by Profs. Nerea Bordel and Jorge Pisonero at the University of Oviedo.



### **Madeleine Lomax-Vogt**

PhD candidate in analytical chemistry at The Ohio State University Department of Chemistry and Biochemistry



### **Dariya Tukhmetova**

PhD at the Federal Institute for Materials Research and Testing under the guidance of Dr. Björn Meermann in Berlin, Germany.

Read full biographies at  
[scixconference.org/awards](https://scixconference.org/awards)

## SAS EARLY CAREER INTEREST GROUP TRAVEL GRANT

*Travel support for Early Career Scientists (within 10 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.*



**Hunter Andrews** is an early career researcher in the Isotope Applications Research Group within the Radioisotopes Science and Technology Division at Oak Ridge National Laboratory (ORNL).



**Stephanie Zaleski** joined the Department of Chemistry & Biochemistry as an Assistant Professor at CSU East Bay in 2020. She obtained her B.A. in Biochemistry from Barnard College in 2011 and her Ph.D. in Chemistry from Northwestern University in 2016 working in the lab of Richard P. Van Duyne.

Read full biographies at  
[scixconference.org/awards](https://scixconference.org/awards)

## SAS BARBARA STULL GRADUATE STUDENT AWARDS

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



### **Lamyaa M. Almeahmadi**

Lamyaa M. Almeahmadi is a Ph.D. candidate in Professor Igor K. Lednev at the University at Albany, State University of New York. She received her B.S. in Chemistry with an emphasis on Chemical Biology and an M.S. degree in Chemistry from the University at Albany, completing her master's thesis in only one year. Lamyaa's Ph.D. research focuses on using enhanced Raman spectroscopy techniques for drug discovery, mRNA vaccine stability assessment, and forensic purposes. Lamyaa has received several awards, including the 2023 Rising Star in Analytical Chemistry award from the ACS ANYL Division and the prestigious Coblentz student award. She was elected president of a local Society for Applied Spectroscopy chapter for two consecutive years and has chaired and co-chaired a symposium and conference sessions. This Fall, Lamyaa will be joining the Department of Materials Science and Engineering at the Massachusetts Institute of Technology (MIT) as a post-doctoral fellow and will work under the mentorship of Prof. Juejun Hu in the Photonic Materials Group. Her upcoming research will revolve around utilizing on-chip photonic sensors.



### **Thulya Chakkumpulakkal Puthanveettil**

Thulya is pursuing a joint PhD degree in analytical chemistry from Monash University, Australia, and the University of Bath, United Kingdom, under the guidance of Prof. Bayden R. Wood (Monash University), Dr. Paul De Bank (University of Bath), Dr. Keith Bamberg (Australian Synchrotron), and Prof. Karen J. Edler (Lund University, Sweden). In her PhD, Thulya has been working on a highly multidiscipline project combining microfluidics, spectroscopy and machine learning modelling to develop new diagnostic tests for blood and water borne pathogens particularly focusing on malaria parasites, leishmania parasites and bacteria.

During her PhD career, her work has been acknowledged on several occasions. She has published ten articles in internationally reputed journals, five of which are first author articles. She has been able to secure a highly prestigious Postgraduate Research Award from the Australian Institute of Nuclear Science and Engineering (AINSE) to conduct impactful research on malaria diagnosis at the Australian Nuclear Science and Technology

Organisation (ANSTO) facilities. This top-up award provides additional funding to support experiments at ANSTO facilities such as Australian synchrotron. In addition to this, she has been awarded an AINSE Technical Skills Scholarship for developing advanced machine learning skills to support her research on malaria diagnosis. She has been awarded the following accolades: The Association of British Spectroscopists Trust (ABS Trust) Student Bursary Award for 2023, a Research Development Grant from the Royal Society of Chemistry, study away travel grant from Monash University, Doctoral Recognition Award for 2023 from the University of Bath, and the Coblentz society student award 2023.

## SAS UNDERGRADUATE STUDENT AWARD

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



**Julia Clista Galeckiv**

Recognizing work in the utilization of Raman spectroscopy to characterize antibody-ligand association at supported phospholipid bilayers, and for developing approaches for functionalizing silica surfaces, measuring the protein association on lipid monolayers and bilayers, gathering isotherm data, and resolving features in vibrational spectra.

## SAS FELLOWS

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



**Sebastian Schlücker**

Sebastian Schlücker (born 1973) is a professor of physical chemistry at the University Duisburg-Essen (UDE) in Essen, Germany. He studied chemistry at the University of Würzburg where he also obtained his PhD in the field of linear and nonlinear Raman spectroscopy. After postdoctoral work at the laboratory of chemical physics, NIDDK, NIH in Bethesda on Raman imaging in biomedical research and his habilitation he became associate professor of experimental physics at the University of Osnabrück in 2008 before joining UDE in 2012.

His research interests are the development and applications of innovative laser spectroscopic techniques with a focus on selectivity and sensitivity as well as the physics and chemistry of molecularly functionalized plasmonic nanoparticles for applications in biomedicine (diagnostics and therapy) and chemical energy conversion (catalysis, plasmonic chemistry).

Sebastian received numerous awards for his scientific work. Examples of awards from the German Chemical Society (GDCh) include the Carl-Duisberg Memorial Award, the Bunsen-Kirchhoff Award and an ADUC Award. Last year, he received the ICORS 2022 Award for the most innovative technological development.

He serves as deputy director of the Center for Nanointegration Duisburg-Essen (CENIDE) and as a member of the International Steering Committees of the International Conference on Raman Spectroscopy (ICORS) & International Conference on Enhanced Spectroscopies (ICES). In 2018 he was elected as a Fellow of the Royal Society of Chemistry (FRSC). He is the founder of NanoWerke for high-quality SERS particles and initiated experimentamus! for inquiry-based learning with STEM experiments in primary schools.

**SAS FELLOWS**  
(Continued on next page)

## SAS FELLOWS (Continued)



### Gloria Story

Gloria Story received her A.S. in Science Technology from the University of Cincinnati - Blue Ash (1981) and worked towards a B.S. in Chemistry from UC and the University of Utah. She is currently retired from the Procter & Gamble Company, where she was a Senior Scientist with the Corporate R&D Organization. She has over 40 years of experience in vibrational spectroscopy applications.

With over 25 years of membership in the Society for Applied Spectroscopy, Gloria is currently serving as President-elect. She served as Governing Board Delegate, Section Affairs Coordinator, Secretary, Membership Coordinator, Tour Speaker Coordinator, and workshop instructor at PittCon and SciX. She's been an active member of the Coblenz Society for over 30 years, currently serving as a mentee in the Speed Mentoring program. An ACS member since 1994, she is currently serving as coordinator for her local section's membership, Education Grants, undergraduate travel awards, and museum NCW programming.

Gloria Story has co-authored 28 research publications and presented over 25 oral presentations. She has received numerous awards including the SAS Distinguished Service Award (2015), the ACS Cincinnati Section's Research Associate of the Year, Outstanding Service, and Outreach Volunteer of the Year Awards, the Procter & Gamble Company's Global Analytical Community of Practice Recognition and Pete Rodriguez Analytical Excellence Awards, and the America Service to Youth Award from the Dan Beard Council of the Boy Scouts of America.



### Bayden R. Wood

Prof. Bayden R. Wood completed his PhD in Chemistry in 1999. He has since pursued his research interest applying vibrational spectroscopy to biological/biomedical problems. In 2008, he was awarded an Australian Research Council QEII Research Fellowship and a Humboldt Fellowship, followed by an ARC Future Fellowship in 2012. Since 2015, he has headed the Monash Biospectroscopy Group pioneering the application of vibrational spectroscopy and chemometrics to investigate a range of biomedical and biological problems. The breadth of his research includes malaria diagnosis and treatment, cancer diagnosis, testing novel drugs for cancer treatment,

kidney disease, sepsis diagnosis, stem cell research, heart disease, liver disease, phytoplankton studies, aquatic wetland, food and soil studies, ancient materials along with fundamental studies into how light interacts with cells. He was appointed to the position of Professor in 2019. He has over 200 peer reviewed publications and 12 book chapters with a H index =59, i10 index 146 with over 11,500 citations (source Google Scholar author profile). He is Co-Chief Editor for the Elsevier journal Clinical Spectroscopy and editorial board member for Applied Spectroscopy. He is a current Director of the CLIRSPEC network and sits on the steering committee of the International Conference on Raman Spectroscopy (ICORS) and also on the steering committee for the International Conference on Advanced Raman Spectroscopy (ICAVS). He has a number of industry collaborators including Si-Ware and Perkin-Elmer. He has a strong focus on translating spectroscopy to real world problems through his large academic and commercial network.

## WILLIAM J. POEHLMAN AWARD

*Recognizing the Section of the Society, which has contributed the most towards accomplishing the goals and ideals of the Society during the preceding year*



### New York Capital Region Student Section

The section was chosen for its efforts to facilitate engagement via social events (video games, ice cream socials, scavenger hunts) and planned programming throughout the year, that balances both academic and social interaction among students.

The New York Capital Region student chapter of the Society for Applied Spectroscopy encompass universities and colleges in the Albany Area.

Whether you are a college freshman, or a graduate student with years of practical experience, there is a place for you as a member of the NYCR SAS!



## 2022 SAS SERVICE AWARDEES



**Andrew Whitley**  
President-Elect 2021  
President 2022  
Past President 2023



**Luisa Profeta**  
Newsletter Editor  
2020-2022

## SAS DISTINGUISHED SERVICE AWARD



**Robert J. Lascola**

Rob Lascola is a Senior Fellow Scientist and group leader for online monitoring at Savannah River National Laboratory in Aiken, SC, where he has worked since 1998. He received his B.S. with High Distinction from the University of Virginia, M.S. from the University of Colorado, and Ph.D. from the University of Wisconsin-Madison, all in Chemistry. His Ph.D. thesis work on nonlinear optical properties of charged fullerenes, done under the guidance of Prof. John Wright, was recognized with several awards, including the ACS Division of Analytical Chemistry Graduate Fellowship.

At SRNL, Rob's primary focus has been the development and installation of process analytical technologies to measure actinides, hydrogen isotopes, and process offgas composition in nuclear materials processing and radiological containment facilities. He also works with SRNL colleagues on diverse topics including actinide chemistry and processing flowsheet development, energy storage, and dissolution kinetics. He has co-authored over 60 papers and technical reports, and is proud to have been recognized both by SRNL and multiple production divisions at Savannah River Site for his contributions.

Rob has served SAS as President, Secretary, Governing Board member, Regional and Section Affairs Coordinator, and as a member of several committees. He has also been a SciX Program Chair, Forensics Section Chair/co-Chair, and session organizer. He enjoys mentoring and contributes to Coblenz Society and SAS outreach as well as early career programs affiliated with the Department of Energy. He also has volunteered for 25 years for the DOE National Science Bowl at the regional and national levels.

## SAS PRESIDENT'S AWARD



**Ed MacMillan**

*Awarded for recent extraordinary contributions in service to the  
Society for Applied Spectroscopy as Advertising Manager*

# COBLENTZ SOCIETY AWARDS

## COBLENTZ SOCIETY CLARA CRAVER AWARD

*This award is presented annually to an outstanding young molecular spectroscopist in the area of applied analytical vibrational spectroscopy. The work may include any aspect of infrared, and/or THz, and/or Raman spectroscopy in applied analytical vibrational spectroscopy and the winner may come from an academic, government lab, or industrial background.*



### **Ishan Barman**

Dr. Ishan Barman is an Associate Professor in the Department of Mechanical Engineering at the Johns Hopkins University with joint appointments in Oncology and Radiology. He graduated from Indian Institute of Technology (IIT), Kharagpur, in 2005 and moved to Massachusetts Institute of Technology (MIT) for his Ph.D., where he investigated transcutaneous blood analyte detection using Raman spectroscopy. His doctoral research established many of the experimental and computational methods that are now common to in vivo spectroscopic investigations, notably tissue turbidity correction, integration of non-imaging optical elements, and non-linear chemometric analysis. Continuing his academic journey at MIT, his postdoctoral research leveraged Raman and diffuse reflectance spectroscopy for the first real-time guidance of core needle breast biopsies and provided definitive validation of spectroscopy-based diagnosis of breast lesions with microcalcifications.

Dr. Barman joined the faculty at Johns Hopkins University in 2014 and was promoted to Associate Professor with tenure in 2019. His laboratory's primary objective is the development of transformative biophotonics technologies with the goal of disease detection at early, manageable stages, monitoring therapeutic effects and treatment outcomes, and guiding interventions. The optical tools generated from these investigations have been successfully adopted in diverse biomedical environments including automated histopathologic recognition of biopsy specimen, real-time diagnosis of middle ear pathology, and as a customized monoclonal antibody identification platform. Dr. Barman's recent breakthrough in the development of a surface-enhanced Raman spectroscopy platform for real-time, multiplexed detection of viruses in saliva has garnered significant attention. This technology has been licensed and is currently being commercialized through a startup company, RamanID.

His work has resulted in 120 peer-reviewed publications in journals such as Nature Materials, Nature Physics, Proceedings of National Academy of Sciences, Cancer Research, Angewandte Chemie, Advanced Materials and Nano Letters. His work has been prominently featured in leading scientific outlets such as Technology Review and Physics Today, as well as popular media platforms like The Wall Street Journal and CNN Newsroom.

In light of his research endeavors, Dr. Barman has received numerous prestigious awards, including the NIH MIRA Award for Established Investigators (2023), Oracle Research Fellow (2022), Emerging Leader in Molecular Spectroscopy Award (2019), Eastern Analytical Symposium (EAS) Young Investigator (2019), Johns Hopkins University Catalyst Award (2018), NIH Director's New Innovator Award (2017), Outstanding Young Engineer (OYE) from the Maryland Academy of Sciences (2016), Dr. Horace Furumoto Innovations Young Investigator Award from the American Society for Laser Medicine and Surgery (ASLMS) (2014), Gordon F. Kirkbright Bursary Award from the Association of British Spectroscopists (ABS) Trust (2011), and Tomas A. Hirschfeld Award from the Federation of Analytical Chemistry and Spectroscopy Societies (2010).

## COBLENTZ SOCIETY COBLENTZ AWARD

*The Coblentz Award is presented annually to an outstanding young molecular spectroscopist under the age of 40. This award is the Society's original award (first awarded in 1964), and is the complement of the Craver Award that recognizes young spectroscopists for efforts in applied analytical vibrational spectroscopy. The award is presented annually at the International Symposium on Molecular Spectroscopy (ISMS). Due to delays arising from COVID-19, the 2022 award will be presented in 2023 at SciX.*



### Wei Xiong

Professor Wei Xiong is a Professor and Kent Wilson Faculty Scholar in the Department of Chemistry and Biochemistry at the University of California, San Diego. Wei received his B.S. degree from Peking University, China, in 2006. He then joined Prof. Martin Zanni's group at the University of Wisconsin, Madison, and completed his Ph.D. degree in 2011. At Madison, Wei focused on developing novel 2D vibrational spectroscopy (transient 2D IR and heterodyne 2D SFG spectroscopy) to study molecules on solid-state material surfaces. Wei then moved to the University of Colorado, Boulder, in 2011, where he worked with Prof. Margaret Murnane and Henry Kapteyn to develop the table-top XUV source for ultrafast measurements and time-resolved photoelectron spectroscopy for nanoparticles. He joined the faculty at the University of California San Diego in 2014. At UCSD, Wei's research focuses on using and developing ultrafast nonlinear spectroscopic and imaging tools to reveal molecular structures and dynamics of materials, including ultrafast dynamics of polaritonic systems, guest molecule adsorptions in self-assembled materials, femtosecond charge transfer dynamics on organic material interfaces. He has specifically pioneered using and developing ultrafast multidimensional spectroscopy to reveal the dynamics and interactions between molecule polaritons. Wei earned many awards including the Coblentz Award, Sloan Research Fellow, JPC/PHYS Lectureship Award, DARPA Young Faculty Award, DARPA Director's Fellow, NSF CAREER Award, AFOSR Young Investigator Program Award. Wei has also been invited to give more than 80 invited talks at conferences and seminars in universities and research institutions, including several keynote/plenary/award talks.

## COBLENTZ SOCIETY WILLIAM G. FATELEY STUDENT AWARD

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



### Alexis Weber

Alexis is currently matriculating in the Ph.D. Program at the University at Albany, State University of New York. Working in Dr. Igor K. Lednev's lab, her research targets the development of the first universal tool for the identification and analysis of body fluid traces for forensic purposes and has the potential to revolutionize the crime scene investigation protocol. Alexis came to Albany after graduating from the University of New Haven with her Master of Science in Forensic Science in May 2019. Before pursuing her master's degree, Alexis graduated from the University of Central Florida with a degree in Forensic Science (B.S.), magna cum laude, as well as attaining a Chemistry minor.

During her undergraduate career, Alexis strived to maintain academic excellence; making the Dean's List or President's Honor Roll every semester while at the University of Central Florida. She also earned multiple awards during her time there, including the "W.W. McGee Forensic Science Award" and the University of Central Florida "Forensic Science Award," both awarded to students that display outstanding achievement in the forensic science bachelors' program. It was during this time that she first became involved in forensic science research. After completing her undergraduate degree, Alexis left Florida to continue her education at the University of New Haven where she obtained her master's degree under the advisement of Dr. Virginia Maxwell.

Read full biography at  
[scixconference.org/awards](https://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.*



### **Sevde Erkok**

Sevde Dogruer Erkok is a Ph.D. candidate in Professor Bruce McCord's trace laboratory at Florida International University (FIU). She is originally from Türkiye, where she obtained her bachelor's degree with honors in Teaching Chemistry, as the highest-ranked student. While pursuing her Ph.D., she received two master's degrees, one in Forensic Sciences and one in Analytical Chemistry.

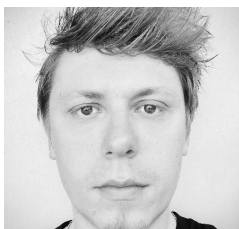
Before starting her Ph.D., she visited Dr. McCord's laboratory as a volunteer intern. She worked on the development of a method utilizing gold-silver nanostars to detect trace amounts of fentanyl in binary mixtures of both heroin and cocaine by portable Raman spectroscopy. Her current research mainly focuses on differentiating structurally similar fentanyl analogs with a theoretical and experimental analysis and detecting them in illicit drug mixtures by surface-enhanced Raman spectroscopy (SERS).



### **Danuta Liberda**

Danuta Liberda is currently a 3rd year PhD student in the Biomedical Sciences Programme at the SOLARIS National Synchrotron Radiation Centre, Jagiellonian University in Kraków. She obtained her MSc with a dissertation devoted to the application of chemometrics tools to analyze variance in high-performance liquid chromatography data.

Her interest in FT-IR spectroscopy started during her work as a technician in Dr. Tomasz Wrobel's project, devoted to pancreatic comprehensive histopathology based on IR chemical imaging. She was focusing on tissue measurements and their classification using machine learning tools, developing her knowledge in the data analysis field. After the end of the above project, she started working in the unique facility – Synchrotron SOLARIS – as the beamline scientist involved in CIRI (Chemical InfraRed Imaging) beamline construction.



### **Daniel Schäfer**

Daniel Schäfer is currently a second-year Ph.D. student in the group of Prof. Sebastian Schlücker at the University of Duisburg-Essen (UDE) in Germany. Born and raised in a small town close to the former industrial heart of Germany, the Ruhr metropolitan area, he achieved his B.Sc. and M.Sc. in chemistry at the UDE.

His research is focused on the SERS-based kinetic reaction monitoring of model reactions in heterogeneous catalytic systems. This work requires expertise in the wet chemical synthesis of hybrid Pt-coated gold nanorods (AuNR), optical spectroscopy (UV/Vis; Raman, SERS), TEM/EDX and chemical kinetics. He demonstrated that bimetallic Pt-coated AuNR catalysts enable hydrogen-based reductions that proceed via a metal-hydride transfer. Outside the lab, he is an animal lover and is active in cycling and skateboarding.



### **Thulya Chakkumpulakkal Puthanveetil**

Thulya is pursuing a joint PhD degree in analytical chemistry from Monash University, Australia, and the University of Bath, United Kingdom, under the guidance of Prof. Bayden R. Wood (Monash University), Dr. Paul De Bank (University of Bath), Dr. Keith Bambery (Australian Synchrotron), and Prof. Karen J. Edler (Lund University, Sweden).

In 2012, Thulya obtained her Bachelor of Science degree in Physics with minors in Chemistry and Mathematics from the University of Calicut, India. Following that, she earned her Master of Technology degree in Materials Science from the University of Mysore, India.

In her PhD, Thulya has been working on a highly multidiscipline project combining microfluidics, spectroscopy and machine modelling to develop new diagnostic tests for blood and water borne pathogens particularly focusing on malaria parasites, leishmania parasites and bacteria.

Read full biographies at [scixconference.org/awards](https://scixconference.org/awards)



# AES ELECTROPHORESIS SOCIETY AWARDS

## AES MID-CAREER AWARD

*Recognizes exceptional contributions to the field of electrophoresis, microfluidics, and related areas by an individual who is currently in the middle of their career.*



### **Robbyn K. Anand**

Robbyn K. Anand is the Suresh Faculty Fellow and Carlyle G. Caldwell Endowed Chair in Chemistry at Iowa State University. Her group has developed methods for circulating tumor cell analysis, electrokinetic enrichment and separation of chemical species within water-in-oil droplets, and more sensitive bioanalysis at arrays of wireless bipolar electrodes. Prof. Anand also founded the Midwest Retreat for Diversity in Chemistry - an annual event aimed at the retention of underrepresented groups in the chemical enterprise.

## AES LIFETIME ACHIEVEMENT AWARD

*The AES Lifetime Achievement Award is given for exceptional career contributions to the fields of Electrophoresis, Electrokinetics, and related areas*



### **James P. Landers**

James Landers is a Jefferson Scholars Fellow and Commonwealth Professor of Chemistry, Professor of Mechanical Engineering, and an Associate Professor of Pathology at the University of Virginia. He co-founded MicroLab Diagnostics in 2008 where he has served as a CSO. MicroLab entered into partnership with Lockheed Martin in 2008 in a project focused on delivering a microfluidic DNA analysis platform for forensic analysis. In 2010, MicroLab merged with ZyGEM Corp. to leverage the powerful suite of reagents they had developed and build on the company's synergies around nucleic acid extraction and detection. That company currently exists as MicroGEM International.

James received his Bachelor of Science degree in Biochemistry with a minor in Biomedicine at the University of Guelph in Ontario (Canada) in 1984. He earned his Ph.D. in Biochemistry from the same department in 1988. After a one-year post-doctoral fellowship at the Banting Institute at the University of Toronto's School of Medicine, he was awarded a Canadian Medical Research Council (MRC) Fellowship to study cancer biology and diagnostics under Dr. Thomas Spelsberg, a breast cancer biochemist at the Mayo Clinic. He launched and directed the Clinical Capillary Electrophoresis Facility in the Department of Lab Medicine and Pathology at Mayo developing clinical assays using capillary electrophoretic technology.

Research efforts have focused on generating rapid prototype microdevices for separations, DNA purification and DNA amplification, as well as devices that fluidically-integrate on-chip sample preparation with analysis. In addition to editing three editions of the Handbook of Capillary Electrophoresis, he has authored more than 265 peer-reviewed papers and 25 book chapters ranging from receptor biochemistry and capillary electrophoretic method development, to microchip fabrication and integrated microfluidic systems for application in the clinical and forensic arenas. This includes two chapters in the Tietz Handbook of Clinical Chemistry. He has edited three editions of the CRC Press Handbook of Capillary Electrophoresis, was the recipient of the 2008 Association for Lab Automation 'Innovative Technology of the Year' Award, and serves as the CoEditor-in-Chief for the journal *Analytica Chimica Acta* which currently has an impact factor of 6.58, and the recipient of the 2022 SCIEX Microscale Separations Innovation Medal and the 2023 AES Lifetime Award for Contributions to the Field of Electrophoresis.

## AES MID-CAREER AWARD

*The AES Student Award recognizes the most outstanding student paper submitted for the AES Annual Conference by a graduate student.*

### **Negar Farhang Doost**

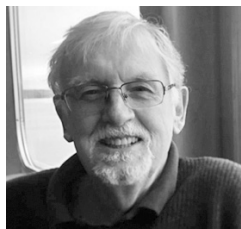
Dielectrophoresis as a detection tool for Rickettsial diseases



## ADDITIONAL AWARDS

### COBLENTZ SOCIETY CLARA CRAVER AWARD

*This award is presented annually to recognize an individual that has made significant contributions to the field of vibrational spectroscopy. The award was jointly established in 1975 by Optica (formerly OSA), the Coblentz Society, and the Society for Applied Spectroscopy to honor the unique contributions of Professor Ellis R. Lippincott. Among other contributions, 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.*



#### **Peter Griffiths**

Peter Griffiths was born in England and spent the first 25 years of his life there. After receiving a doctorate in Physical Chemistry from Oxford University in 1967, he spent the next two years doing postdoctoral research at the University of Maryland under the supervision of Ellis Lippincott. After brief stints with Digilab in Cambridge, MA and Sadtler Research Labs in Philadelphia, PA, he joined the faculty of Ohio University, reaching the rank of Distinguished Professor. After ten years, he moved to the University of California, Riverside before accepting the chairmanship of the Chemistry Department of the University of Idaho, from which he retired in 2008.

His principal research area has been analytical vibrational spectroscopy with particular emphasis on FT-IR spectroscopy with the occasional foray into Raman spectroscopy and gas, liquid and supercritical fluid chromatography. Among the specific topics that his research group has worked on are diffuse reflection spectroscopy, open-path atmospheric monitoring, and the interface of FT-IR spectrometers with various types of chromatographs (GC, HPLC and SFC). He has served as president of both the Coblentz Society and the Society for Applied Spectroscopy. He served on several editorial boards, including more than 30 years with Applied Spectroscopy. He was an Associate Editor of that journal from 1981 to 2009, the Editor-in-Chief from 2009 to 2012 and the Editor from 2012 to 2018.

He has co-authored over 300 papers and has written, co-authored or edited eleven books on various aspects of vibrational spectroscopy. He taught in a week-long course on the interpretation of IR and Raman spectra for over 30 years and acted as a consultant to several companies, law firms and organizations. His work has been recognized by several awards including the Coblentz Award (1975), the Spectroscopy Society of Pittsburgh Award (1985), the New York SAS Gold Medal in Spectroscopy (1995), the Fritz Prögl Medal of Austrian Society for Analytical Chemistry (1995), the Bomem Michelson Award (2003), the Gerald S. Birth Award for Outstanding Work in Near-Infrared Spectroscopy (2004) and the Anachem Award (2012). His selection as this year's Lippincott Awardee represents a marvelous way to ride off into the sunset.

## IRDG CHALMERS & DENT STUDENT TRAVEL AWARD



### **Benjamin Clarke**

Ben graduated from the University of Strathclyde with a first-class Master's degree in Pure and Applied Chemistry in June 2020. It was during his final year that he developed a growing interest in the use of nanotechnology coupled with spectroscopic techniques to solve biological problems. This interest influenced his decision to pursue a career in research by studying for a PhD. In October 2020 he began his PhD under the supervision of Professor Karen

Faulds and Professor Duncan Graham in the Centre of Nanometrology at the University of Strathclyde which is funded by the Engineering Physical Sciences Research Council (EPSRC) and Wasatch Photonics plc. Ben's project, in collaboration with Wasatch Photonics and the University of Edinburgh's School of Medicine, explores the use of SERS-Lateral Flow Immunoassays (LFIA) for the detection of Drug Induced Liver Injury (DILI) in a clinical environment. At this stage in his PhD, Ben is currently working on the development of a SERS-LFIA device which will detect cytokeratin-18, a biomarker associated with acute liver failure, from a single finger-prick of blood in under 30 minutes. This device will be assessed via clinical trials which will take place in late 2023. Ben has presented this research at Spring SciX 2022, British Pharmacology Society (BPS) Conference 2022, SAS/Coblentz Society 3-minute thesis and ICORS XXVII where he received an award for best poster presentation. The overall aim of his research further develops SERS for use in a clinical environment which will aid in efficient decision making when it comes to patient treatment.

## RSC JOSEPH BLACK PRIZE



### **Alexis Weber**

Alexis is currently matriculating in the Ph.D. Program at the University at Albany, State University of New York. Working in Dr. Igor K. Lednev's lab, her research targets the development of the first universal tool for the identification and analysis of body fluid traces for forensic purposes and has the potential to revolutionize the crime scene investigation protocol. Alexis came to Albany after graduating from the University of New Haven with her Master of Science in

Forensic Science in May 2019. Before pursuing her master's degree, Alexis graduated from the University of Central Florida with a degree in Forensic Science (B.S.), magna cum laude, as well as attaining a Chemistry minor.

During her undergraduate career, Alexis strived to maintain academic excellence; making the Dean's List or President's Honor Roll every semester while at the University of Central Florida. She also earned multiple awards during her time there, including the "W.W. McGee Forensic Science Award" and the University of Central Florida "Forensic Science Award," both awarded to students that display outstanding achievement in the forensic science bachelors' program. It was during this time that she first became involved in forensic science research. After completing her undergraduate degree, Alexis left Florida to continue her education at the University of New Haven where she obtained her master's degree under the advisement of Dr. Virginia Maxwell.

## SPECTROSCOPY MAGAZINE EMERGING LEADER IN MOLECULAR SPECTROSCOPY

*This award recognizes the achievements and aspirations of a talented young molecular spectroscopist who has made strides early in his or her career toward the advancement of molecular spectroscopy techniques and applications.*



### **Dmitry Kurouski**

Dmitry Kurouski is an assistant professor of chemistry at Texas A&M University. He earned his MS in Biochemistry from the Belarusian State University, in Belarus, and his PhD (Distinguished Dissertation) in Analytical Chemistry from SUNY Albany, NY, USA. After serving as a postdoctoral researcher in the laboratory of Professor Richard P. Van Duyne at Northwestern University, Kurouski joined Boehringer Ingelheim Pharmaceuticals, where he worked as a senior research scientist. In 2017, Kurouski joined the Biochemistry and Biophysics Department of Texas A&M University as an assistant professor.

Kurouski's research interests are focused on nanoscale characterization of biological and photocatalytic systems using tip-enhanced Raman spectroscopy (TERS) and atomic-force microscopy-infrared spectroscopy (AFM-IR). Specifically, the Kurouski group uses both nanoscopy methods to investigate the structural organization of amyloid oligomers—protein aggregates that are responsible for the onset and spread of neurodegenerative diseases. Recently reported findings by the Kurouski group demonstrated that lipids could uniquely alter the secondary structure of protein aggregates, which drastically changes their toxicity to neurons. These results demonstrate that lipids could play an important role in neurodegeneration.

The Kurouski group also investigates the mechanisms of plasmon-driven chemical reactions on mono- and bimetallic nanostructures. Their findings demonstrate that TERS can be used for a quantitative assessment of both yield and rates of plasmon-catalyzed reactions on such nanostructures. Using TERS, the group was able to determine the role of catalytic metals, such as platinum and palladium, in plasmon-driven reactions.

Kurouski also develops innovative methods for non-invasive sensing of plant health. His group showed that Raman spectroscopy can be used to detect and identify biotic and abiotic stresses in plants, probe nutritional composition of fruits and vegetables, and predict plant resistance to specific pathogens. These findings demonstrate that Raman sensors could be used directly in the field to monitor plant health.

The Kurouski group also has been advancing the forensic analysis of hair. Their research findings demonstrated that surface-enhanced Raman spectroscopy (SERS) could be used to detect and identify more than 30 individual colorants on hair. Thus, SERS-based analysis of hair colorants can be used to establish a connection between a suspect and a crime scene or demonstrate the absence of such connections.

## SPECTROSCOPY MAGAZINE EMERGING LEADER IN MOLECULAR SPECTROSCOPY

This award is for the Best Paper Published in *Applied Spectroscopy* on Laser Induced Breakdown Spectroscopy, 2022, Volume 76, Issue 8, August 2022, Pages 926-936.

### **Femtosecond Single-Pulse and Orthogonal Double-Pulse Laser-Induced Breakdown Spectroscopy (LIBS): Femtogram Mass Detection and Chemical Imaging with Micrometer Spatial Resolution**

Nikolaos Giannakaris, Anna Haider, Christoph M. Ahamer, Stefan Grünberger, Stefan Trautner and Johannes D. Pedarnig

*See previous listing (page 18) as this paper is also the SAS Meggers Award winner.*

## SPECTROSCOPY MAGAZINE EMERGING LEADER IN MOLECULAR SPECTROSCOPY

*No winner presented in 2023. This award is presented 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.*

# SCHEDULE-AT-A-GLANCE

## SUNDAY, OCTOBER 8

### 6:15 PM – 7:15 PM KEYNOTE PRESENTATION:

Fifty Years of FACSS and SciX Conferences:

The Remarkable Correspondence with Advances in Vibrational Spectroscopy

Peter Griffiths

Sierra 5

### 7:15 PM – 9:15 PM Welcome Mixer and SAS Sponsored Student Poster Session

Sierra 1

## MONDAY, OCTOBER 9

### 8:30 AM – 10:10 AM PARALLEL SESSIONS

<b>23ART01:</b> Student Research in Archaeological Chemistry	<i>Southern Pacific F</i>
<b>23ATOM03:</b> From Humble Beginnings – The Great Diversity of Glow Discharge Spectrometries	<i>Central Pacific A/B/C</i>
<b>23BIM06:</b> Spectroscopy and The Role it Plays in Commercialization of NextGen Therapeutics	<i>Sierra 2</i>
<b>23CHEM01:</b> Recent Advances in Chemometrics	<i>Southern Pacific E</i>
<b>23FORENS02:</b> Food Forensics	<i>Southern Pacific A/G</i>
<b>23IR02:</b> Celebrating Coblentz - NE/NE SAS ECR Student Prize Winners	<i>Sierra 5</i>
<b>23IR07:</b> Applications of Photothermal IR Spectroscopy and Imaging in the Life Sciences	<i>Sierra 3</i>
<b>23LIBS02:</b> LIBS Throughout the FACSS History	<i>Southern Pacific B/C</i>
<b>23PMA02:</b> Media Integrity in BioPharma	<i>Southern Pacific D</i>
<b>23RAM02:</b> SERS 1	<i>Cascade 3</i>
<b>23RAM15:</b> Raman in Regenerative Medicine	<i>Cascade 1</i>
<b>23SPSJ02:</b> 50 Years of UV Raman Spectroscopy	<i>Cascade 4</i>

**10:10 AM – 10:45 AM Poster Session and Break** *Nugget Foyer*

**10:45 AM – 11:00 AM Award Presentations** *Sierra 5*

**11:00 AM – 11:30 AM The Coblentz Society Coblentz Award: Wei Xiong** *Sierra 5*

**11:30 AM – 12:00 PM The Coblentz Society Clara Craver Award: Ishan Barman** *Sierra 5*

**12:00 PM – 1:30 PM Lunch on Own**

### 1:30 PM – 3:10 PM PARALLEL SESSIONS

<b>23AES02:</b> Electrokinetic Fundamentals	<i>Southern Pacific F</i>
<b>23ATOM08:</b> Edward Steers Memorial Award Symposium	<i>Central Pacific A/B/C</i>
<b>23AWD01:</b> The Coblentz Society Coblentz Award Symposium Honoring Wei Xiong	<i>Sierra 5</i>
<b>23CHEM02:</b> Chemometric Opportunities in Forensic Chemistry	<i>Southern Pacific D</i>
<b>23CTP/EARLY03:</b> Showcasing Career Paths in the Spectroscopic Sciences	<i>Sierra 2</i>
<b>23IR08:</b> Photothermal IR Spectroscopy and Imaging of Microplastics and Other Materials	<i>Sierra 3</i>
<b>23MASS01:</b> Early Career Researchers in Mass Spectrometry	<i>Southern Pacific A/G</i>
<b>23PAT02:</b> PAT Pharma/Biotech	<i>Southern Pacific E</i>
<b>23RAM01:</b> Emerging Raman	<i>Cascade 1</i>
<b>23RAM07:</b> ECR Raman	<i>Cascade 3</i>
<b>23SPECIAL03:</b> Microplastic Analysis - Standard Operating Procedures to Understand the Environmental and Health Threats	<i>Southern Pacific B/C</i>
<b>23SPR02:</b> 50 Years of Plasmonics	<i>Cascade 4</i>

## SCHEDULE-AT-A-GLANCE

**3:10 PM – 3:50 PM Poster Session/Break**

*Nugget Foyer*

### 3:50 PM – 5:30 PM PARALLEL SESSIONS

<b>23AES03:</b> Innovations in Device Fabrication and Applications	<i>Southern Pacific F</i>
<b>23ATOM05:</b> High-end ICP-MS Applications	<i>Central Pacific A/B/C</i>
<b>23AWD02:</b> The Coblenz Society Clara Craver Award Symposium Honoring Ishan Barman	<i>Sierra 5</i>
<b>23BIM01:</b> Machine and Deep Learning for Biomedical Diagnostics	<i>Sierra 2</i>
<b>23CHEM03:</b> Chemometrics Something Borrowed, Something New	<i>Southern Pacific E</i>
<b>23FORENS03:</b> Forensic Analysis in the Lab and at the Crime Scene	<i>Southern Pacific A/G</i>
<b>23IR03:</b> 140 Years of the Coblenz Society and the Infrared and Raman Discussion Group (IRDG)	<i>Sierra 3</i>
<b>23LIBS05:</b> LIBS for Nuclear Applications	<i>Southern Pacific B/C</i>
<b>23PMA01:</b> Vibrational Spectroscopy to Support Pharmaceutical Manufacturing	<i>Southern Pacific D</i>
<b>23RAM03:</b> SERS 2	<i>Cascade 3</i>
<b>23RAM13:</b> Nano Raman 1	<i>Cascade 1</i>
<b>23SPSJ01:</b> Higher Energy UV Spectroscopy	<i>Cascade 4</i>

**5:30 PM – 7:30 PM Exhibit Hall Reception**

*Nugget Ballroom*

## TUESDAY, OCTOBER 10

### 8:30 AM – 10:10 AM PARALLEL SESSIONS

<b>23AES05:</b> Early Career	<i>Southern Pacific F</i>
<b>23ATOM01:</b> ICP Time of Flight MS	<i>Central Pacific A/B/C</i>
<b>23AWD03:</b> Ellis R. Lippincott Award Symposium Honoring Peter Griffiths	<i>Sierra 5</i>
<b>23BIM04:</b> Celebrating Early Career Scientists in Biomedical and Bioanalytical Spectroscopy	<i>Sierra 2</i>
<b>23IR01:</b> Fluorescence and EEMS: Exploiting A New Approach for PAT and Monitoring	<i>Sierra 3</i>
<b>23MASS02:</b> Ion Mobility Separations: Instrumentation, Applications, and Methods	<i>Southern Pacific A/G</i>
<b>23PAT03:</b> Novel Process Analysis Technologies & Applications	<i>Southern Pacific E</i>
<b>23PMA04:</b> Nanomedicine Applications	<i>Southern Pacific D</i>
<b>23RAM10:</b> Low Frequency Raman	<i>Cascade 1</i>
<b>23SPR03:</b> Structuring Plasmonic Particles for Applications	<i>Cascade 4</i>

**10:10 AM – 10:45 AM Poster Session and Exhibits Viewing Break**

*Nugget Ballroom*

**10:45 AM – 11:00 AM Award Presentations**

*Sierra 5*

**11:00 AM – 11:30 AM FACSS Charles Mann Award for Applied Raman Spectroscopy: Juergen Popp**

*Sierra 5*

**11:30 AM – 12:00 PM The RSC Joseph Black Award: Mathew Horrocks**

*Sierra 5*

**12:00 PM – 1:30 PM Exhibits Viewing and Lunch**

*Nugget Ballroom*

### 1:30 PM – 3:10 PM PARALLEL SESSIONS

<b>23ART03:</b> Historic Perspective and Recent Advances in Art Analysis using Vibration Spectroscopy	<i>Southern Pacific F</i>
<b>23ATOM04:</b> Single Particle and Single Cell ICPMS	<i>Central Pacific A/B/C</i>
<b>23AWD04:</b> FACSS Charles Mann Award Symposium Honoring Juergen Popp	<i>Sierra 5</i>
<b>23CHEM04:</b> Chemometrics in Food and Agriculture	<i>Southern Pacific E</i>



## SCHEDULE-AT-A-GLANCE

<b>23CTP/EARLY02:</b> AMA Women in Analytical Sciences	Sierra 2
<b>23FORENS01:</b> Nuclear Forensics	Southern Pacific A/G
<b>23IR04:</b> Nanoscale IR in Bioscience	Sierra 3
<b>23LIBS01:</b> The New LIBS Generation	Southern Pacific B/C
<b>23PMA03:</b> Tackling Critical Pharmaceutical Challenges with Advanced Spectral Analyses	Southern Pacific D
<b>23RAM04:</b> SERS 3	Cascade 3
<b>23RAM09:</b> Spatially Offset Raman Spectroscopy	Cascade 1
<b>23SPSJ03:</b> Spectroscopy (Basic Spectroscopy)	Cascade 4
<b>3:10 PM – 3:50 PM</b> Poster Session and Exhibits Break	Nugget Ballroom
<b>3:50 PM – 5:30 PM PARALLEL SESSIONS</b>	
<b>23AES01:</b> Bioanalysis	Southern Pacific F
<b>23ATOM02:</b> Metallomics Based Applications	Central Pacific A/B/C
<b>23AWD05:</b> RSC Joseph Black Award Symposium Honoring Mathew Horrocks	Sierra 5
<b>23BIM03:</b> Point-of-Care Technologies for Biomedical Applications	Sierra 2
<b>23IR09:</b> Two-Dimensional Correlation Spectroscopy	Sierra 3
<b>23MASS03:</b> 50 Years in Mass Spectrometry	Southern Pacific A/G
<b>23PAT05:</b> PAT Coblenz: Machine Learning	Southern Pacific E
<b>23PMA07:</b> Vibrational Spectroscopy in Developing Biologics & Cell and Gene Therapy	Southern Pacific D
<b>23RAM06:</b> SERS – 50th Anniversary Chair Duncan Graham	Cascade 3
<b>23RAM12:</b> Raman Spectroscopy for Security and Forensics	Cascade 1
<b>23SPR01:</b> SPR Early Career Plasmonics Researchers	Cascade 4
<b>5:30 PM – 7:30 PM</b> Exhibitor-hosted Happy Hour	Chalet Terrace Room

## WEDNESDAY, OCTOBER 11

<b>8:30 AM – 10:10 AM PARALLEL SESSIONS</b>	
<b>23ART02:</b> Analysis of Exotic Materials from Mummies to Mars	Southern Pacific B/C
<b>23AES06:</b> AES Lifetime Achievement Award Symposium Honoring James Landers	Southern Pacific F
<b>23ATOM06:</b> Common Strategies for LA-ICP-MS and LIBS	Central Pacific A/B/C
<b>23BIM02:</b> Translating Multimodal Imaging Technologies into Routine Clinical Practice: Where do we Stand?	Sierra 2
<b>23FORENS04:</b> International Mail Security	Southern Pacific A/G
<b>23IR05:</b> Nanoscale IR Spectroscopy Theory and Applications	Sierra 3
<b>23IR10:</b> Instrumental advances for mid-IR spectroscopy	Sierra 5
<b>23PAT04:</b> In Situ Spectroscopy for industrial R&D	Southern Pacific E
<b>23PMA06:</b> Emerging Plasmonic Nanoparticles for Drugs and Pharmaceutical Analysis	Southern Pacific D
<b>23RAM11:</b> Raman Standards	Cascade 3
<b>23SPECIAL02:</b> Spectrochemical Acta B - Award Session	Cascade 1
<b>23SPSJ04:</b> NIR Spectroscopy (Applications)	Cascade 4
<b>10:10 AM – 10:45 AM</b> Poster Session and Exhibits Viewing Break	Nugget Ballroom

## SCHEDULE-AT-A-GLANCE

<b>10:45 AM – 11:00 AM</b>	<b>Award Presentations</b>	<i>Sierra 5</i>
<b>11:00 AM – 11:30 AM</b>	<b>NESAS and SAS Lester W. Strock Award: Maria Montes Bayon</b>	<i>Sierra 5</i>
<b>11:30 AM – 12:00 PM</b>	<b>AES Mid-Career Achievement Award: Robbyn Anand</b>	<i>Sierra 5</i>
<b>12:00 PM – 1:30 PM</b>	<b>Exhibits Viewing and Lunch</b>	<i>Nugget Ballroom</i>
<b>1:30 PM – 3:10 PM PARALLEL SESSIONS</b>		
<b>23AES07:</b> 50th Anniversary		<i>Southern Pacific F</i>
<b>23ATOM07:</b> Early Career in Atomic Spectroscopy		<i>Central Pacific A/B/C</i>
<b>23AWD06:</b> NESAS and SAS Lester W. Strock Award Symposium Honoring Maria Montes-Bayón		<i>Cascade 1</i>
<b>23AWD07:</b> AES Mid-Career Achievement Award Symposium Honoring Robbyn Anand		<i>Sierra 5</i>
<b>23BIM07:</b> Biomedical Spectroscopy and Imaging (CLIRSPEC)		<i>Sierra 2</i>
<b>23CHEM05:</b> Industrial/PAT Applications of Chemometrics		<i>Southern Pacific E</i>
<b>23IR12:</b> Mid-IR Sensing Schemes Beyond Absorbance Spectroscopy		<i>Sierra 3</i>
<b>23LIBS04:</b> LIBS for Mining, Geology and Space		<i>Southern Pacific B/C</i>
<b>23MASS04:</b> Understanding Protein Structure with Mass Spectrometry		<i>Southern Pacific A/G</i>
<b>23PMA08:</b> Small Molecule Analysis in Biopharma		<i>Southern Pacific D</i>
<b>23RAM05:</b> IRDG		<i>Cascade 3</i>
<b>23SPR05:</b> Plasmonics and Sensing		<i>Cascade 4</i>
<b>3:15 PM – 5:00 PM</b>	<b>Poster Session and Exhibits Closing Reception</b>	<i>Nugget Ballroom</i>

## THURSDAY, OCTOBER 12

### 8:30 AM – 10:10 AM PARALLEL SESSIONS

<b>23AES04:</b> Emerging Leaders		<i>Southern Pacific F</i>
<b>23ATOM09:</b> Laser Ablation Based Atomic Spectroscopies: Fundamental and Applications		<i>Central Pacific A/B/C</i>
<b>23BIM05:</b> Nanotheranostics: Diagnosis and Treatment of Disease Using Nanomaterials		<i>Sierra 2</i>
<b>23CHEM06:</b> Improvements in Field Sensing with Chemometrics		<i>Southern Pacific B/C</i>
<b>23CTP/EARLY01:</b> New Approaches in Instrumentation and Software Design		<i>Sierra 5</i>
<b>23FORENS06:</b> Pharma Forensics		<i>Southern Pacific A/G</i>
<b>23IR06:</b> Material Science: IR Nanospectroscopy Opens New Perspectives		<i>Sierra 3</i>
<b>23PAT01:</b> Looking 50 Years into the Future of PAT		<i>Southern Pacific E</i>
<b>23PMA05:</b> Measurement of Proteins and Modifications towards Precision Medicine		<i>Southern Pacific D</i>
<b>23RAM14:</b> Industrial Raman		<i>Cascade 1</i>
<b>23RAM16:</b> Nano Raman 2		<i>Cascade 3</i>
<b>23SPR04 :</b> Plasmonics and Catalysis		<i>Cascade 4</i>
<b>10:10 AM – 10:45 AM</b>	<b>Poster Session and Break</b>	<i>Nugget Foyer</i>
<b>10:45 AM – 11:00 AM</b>	<b>Award Presentations</b>	<i>Sierra 5</i>
<b>11:00 AM – 11:30 AM</b>	<b>SAS and Applied Spectroscopy William F. Meggers Award: Johannes Pedarnig</b>	<i>Sierra 5</i>
<b>11:30 AM – 12:00 PM</b>	<b>Spectroscopy's Emerging Leader in Molecular Spectroscopy: Dmitry Kuroski</b>	<i>Sierra 5</i>
<b>12:30 PM – 2:00 PM</b>	<b>Lunch on Own</b>	

## SCHEDULE-AT-A-GLANCE

### 1:30 PM – 3:10 PM PARALLEL SESSIONS

<b>23AWD08:</b> SAS and Applied Spectroscopy William F. Meggers Award Symposium Honoring Johannes Pedarnig	<i>Cascade 3</i>
<b>23AWD09:</b> Spectroscopy's Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Dmitry Kurouski	<i>Sierra 5</i>
<b>23FORENS05:</b> Early Career Research in Forensic Science	<i>Southern Pacific A/G</i>
<b>23IR11:</b> IR Frequency Combs	<i>Sierra 3</i>
<b>23IR13:</b> Applications of Optical- and AFM-Photothermal IR Spectroscopy	<i>Sierra 2</i>
<b>23LIBS03:</b> LIBS for Forensics and Security	<i>Southern Pacific B/C</i>
<b>23PAT06:</b> PAT in Petroleum and Refinery Industries	<i>Southern Pacific E</i>
<b>23PMA09:</b> Analysis of Proteins, Antibodies, Biologicals and Nucleic Acids	<i>Southern Pacific D</i>
<b>23RAM08:</b> Raman Imaging	<i>Cascade 1</i>
<b>23RAM17:</b> Bioanalytical Applications of Raman Spectroscopy	<i>Cascade 4</i>
<b>23RAM18:</b> SERS 4	<i>Central Pacific A/B/C</i>
<b>23SPECIAL01:</b> Skilled: Scientific Discoveries and Professional Lessons After Academia	<i>Southern Pacific F</i>

<b>3:40 PM – 4:20 PM</b>	<b>Poster Session and Break</b>	<i>Nugget Foyer</i>
<b>3:50 PM – 5:30 PM</b>	<b>FACSS Innovation Award Finalists Plenary Session</b>	<i>Sierra 5</i>
<b>7:00 PM</b>	<b>SciX Gala</b>	<i>Nugget Ballroom</i>

### FRIDAY, OCTOBER 13

<b>7:30 AM – 7:45 AM</b>	<b>Continental Breakfast</b>	<i>Sierra 5</i>
<b>7:45 AM – 8:00 AM</b>	<b>Announcement of 2023 FACSS Innovation Award Winner</b>	<i>Sierra 5</i>
<b>8:00 AM – 10:00 AM</b>	<b>Closing Plenary Session including Special Speakers and SciX 2024 Preview</b>	<i>Sierra 5</i>

# SHORT COURSES/WORKSHOPS

*Short courses are available for a separate registration fee.*

*Visit the registration desk to sign up. Space is limited and some courses may sell out or may be cancelled.*

## SUNDAY, OCTOBER 8

**9:00am- 5:00pm (Full Day)**

**Process Analytical Technology: Out of the Lab and into the Line (CSAS 105)** - James Rydzak

**9:00am- 5:00pm (2 Days)**

**Spectral Interpretation of Vibrational Spectra (CSAS 113)** - Peter Larkin / Mary Carrabba

**1:00pm- 5:00pm (Half Day)**

**How to Make Connections: Networking at Conferences and in Higher Education (CSAS 119)** - Alexis Weber

**Beginners Guide to Atomic Absorption and Emission Spectroscopy (SAS 109)** - Dula Amarasiriwardena

**Practical Vibrational Spectroscopy (CSAS 101)** - James de Haseth

## MONDAY, OCTOBER 9

**9:00am- 5:00pm (2 Days)**

**Spectral Interpretation of Vibrational Spectra (CSAS 113)** - Peter Larkin / Mary Carrabba

**9:00am- 12:00pm (2 Parts)**

**Modern Raman Microscopy for Applications in the Material and Life Sciences - Part I (CSAS 104)** - Alexander Rzhevskii

**Problems with FT-IR Spectra and How to Avoid Them - Part I (CSAS 103)** - Ellen Miseo /Jenni Briggs/ Jeff D'Agostino

**9am- 12pm (Half Day):**

**Spectral Searching (CSAS 102)** - James de Haseth

**1pm- 5pm (2 parts):**

**Modern Raman Microscopy for Applications in the Material and Life Sciences - Part I (CSAS 104)** - Alexander Rzhevskii

**Problems with FT-IR Spectra and How to Avoid Them - Part I (CSAS 103)** - Ellen Miseo /Jenni Briggs/ Jeff D'Agostino

**1pm- 5pm (Half Day):**

**Introduction to ICP-MS: Fundamentals, Best Practices and Tips and Tricks (SAS 110)** - Dula Amarasiriwardena

## TUESDAY, OCTOBER 10

**9:00am- 5:00pm (Full Day)**

**An Introduction to Quantitative Spectroscopic Analysis (SAS 107)** - Debbie Peru T

**Practical Raman Spectroscopy (CSAS 123)** - Tim Prusnick/Sarah Shidler

**9am- 12pm (Half Day):**

**Technologies and Applications for Miniature Optical Spectrometers and Spectroscopic Sensors (CSAS 118)** - Richard Crocombe

**LA-ICP-MS: Elemental Analysis of Incremental Tissues as an Indicator of Past Pollution Events (SAS 122)** - Dula Amarasiriwardena

**1pm- 5pm (Half Day):**

**Foreign Material Identification and Root Cause Analysis in Materials Manufacturing (SciX 125)** - Jinping Dong

**Multivariate Analysis for Beginners: Pre-processing and Data Analysis of Raman/IR Spectra in the Matlab Environment (CSIRDG 126)** - Cassio Lima

## WEDNESDAY, OCTOBER 11

**9:00am- 5:00pm (Full Day)**

**Using Fluorescence Spectroscopy & EEMs for Biopharmaceutical Analyses (CSAS 120)** - Linda Kidder /Alan Ryder

**Introduction to Data Analytics for the Analytical Chemist (SAS 121)** - Mary Kate Donais

**ABC to PMP: A Project Management Crash Course (CSAS 116)** - Luisa Profeta

**9am- 12pm (Half Day):**

**FTIR and Raman Spectroscopies Applied in Cosmetic and Beauty Industry (SciX 128)** - Samuel Gourion-Arsiquaud / Larry Senak

**What's in the Box – How Do Spectrometers Work (CSAS 124)** - Alex Scheeline / James de Haseth

**1pm- 5pm (Half Day):**

**Introduction to Microsystems: A Platform for Transforming Analysis Instruments to Sensor Scale Devices (SAS 127)** - Yasser Sabry

**Laser Fundamentals for Spectroscopy (CSAS 117)** - Rob Chimenti

# TECHNICAL PROGRAM – SUNDAY, OCTOBER 8, 2023

Welcome and Keynote Lecture | 6:00PM – 7:15PM | Sierra 5

## 23SUNKEY01: Keynote Session

(SUN-01.1) Fifty years of FACSS and SciX Conferences: The remarkable correspondence with advances in vibrational spectroscopy

Peter Griffiths, *Griffiths Consulting*

# TECHNICAL PROGRAM – MONDAY, OCTOBER 9, 2023

## Oral Symposia | 8:00AM – 10:10AM

### 23ART01: Student Research in

Archaeological Chemistry, Southern Pacific F

Chair: Juan Santiago, *Stanford University*

Co-Chair: Md Nazibul Islam, *Texas A&M University*

(ART-01.1) The Mobility of Fecal Stanols in Soils

AJ White, Varenka Lorenzi, Lora Stevens;  
*University of California, Berkeley, California State University Long Beach*

The Effects of Archaeological Fires on Volcanic Glass Shards: An Experimental Approach

(ART-01.2) Jayde N. Hirniak, Panagiotis Karkanis, Eamonn Needham, Eugene Smith, Christopher Campisano, Curtis Marean;  
*Arizona State University; American School of Classical Studies at Athens; University of Nevada, Las Vegas.*

(ART-01.3) The Application of Trace Metal Stable Isotopes to Hominid Physiology and Behavior

Renee Boucher, Linda Godfrey, Paul Koch;  
*University of California, Santa Cruz, Rutgers University, New Brunswick*

(ART-01.4) Paint Production in the Chaco World: Revealing Networks of Power from the Chemical to the Cosmological

Kelsey Hanson; *University Of Arizona*

(ART-01.5) Embodiment, Identity, and Infant feeding Practices in the Ancient Andes: Analysis of  $\delta^{13}\text{C}$  and  $\delta^{15}\text{N}$  in Serial Samples of Permanent Molars from Tiwanaku, Bolivia

Marcos de la Rosa-Martinez; *Arizona State University, School of Human Evolution and Social Change*

23ATOM03: From Humble Beginnings – The Great Diversity of Glow Discharge Spectrometries, Central Pacific A/B/C

Chair: R. Kenneth Marcus, *Clemson University*

(ATOM-03.1) A Long Way to Go - 50 Years of Permanent Progress from Glow Discharge Emission Spectroscopy to Glow Discharge Mass Spectrometry

Norbert Jakubowski; *Spetec GmbH*

(ATOM-03.2) Glow Discharge Optical Emission Spectroscopy from 1852 to the present - still going strong

Arne Bengtson; *Swerim AB*

(ATOM-03.3) Radiofrequency (Em)Powered Glow Discharge Spectrometry: Enabling novel analysis methods from materials to biological sciences

Gerardo Gamez, Harshit Agrawal, Rajendra Joshi, Hanuk Kwon; *Texas Tech University Dept. of Chemistry and Biochemistry*

(ATOM-03.4) New Developments and Strategies for Solution-Cathode Glow Discharge Atomic Emission Spectrometry

Steven Ray, Nicholas Hazel, Mitchell Stry;

*SUNY Buffalo Dept of Chemistry*

(ATOM-03.5) Mass Spectrometry of Solution Glow Discharges: Combined Atomic and Molecular (CAM) Ionization

R. Kenneth Marcus; *Clemson University*



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**23BIM06: Spectroscopy and The Role it Plays in Commercialization of NextGen Therapeutics**, Sierra 2

Chair: Linda Kidder, *HORIBA Scientific*

**(BIM-06.1) Estimating the optimal number of components in PARAFAC models of complex fluorescence data sets**

Helene Fog Froriep Halberg, Marta Bevilacqua, Åsmund Rinnan; *University of Copenhagen, Department of Food Science*

**(BIM-06.2) Assessment of Fluorescence Impact on Low-Level Detection in Drug Product**

Vladimir Villanueva-Lopez, David Wilsdon; *Worldwide Research and Development, Pfizer Inc.*

**(BIM-06.3) Making Chemical Imaging an Essential Part of Product Development**

Patrick Wray, Dimuthu Jayawickrama, Zoë Whalley, Gregory Lane, Lucy Hawarden, Venkata Bobba, David Trinkle, Elyse DiMaso, Gary McGeorge; *Bristol-Myers Squibb, The University of Birmingham, BMS.*

**(BIM-06.4) Multidimensional Fluorescence (A-TEEM) For the Characterization Of Challenging Samples - From AAVs To Exosomes**

Jeffrey Julien, Linda Kidder, Adam Gilmore; *Horiba Instruments Incorporated*

**(BIM-06.5) Using Polarized Excitation Emission Matrix (pEEM) for monitoring protein conjugation reactions.**

Alan Ryder; *Nanoscale Biophotonics Laboratory, University Of Galway.*

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**23CHEM01: Recent Advances in Chemometrics**, Southern Pacific E

Chair: Peter Harrington, *Harrington Center for Intelligent Instrumentation*

**(CHEM-01.1) Uncovering Chemical Information using Virtual Reality**

John Kalivas, Jordan Peper; *Idaho State University*

**(CHEM-01.2) Graphing a New Path Forward: Network Analysis in Chemometrics**

Caelin Celani, William Gilbraith, Karl S. Booksh; *University of Delaware, Savannah River National Laboratory*

**(CHEM-01.3) Analysis of the Electrochemical Depolymerization of Lignin using Chemometrics**

Gobind Sah, John Staser, Peter Harrington; *Ohio University, Harrington Center for Intelligent Instrumentation.*

**(CHEM-01.4) Simple Procedure to Synthesize Data for Machine Learning**

Peter Harrington; *Harrington Center for Intelligent Instrumentation*

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**23FORENS02: Food Forensics**, Southern Pacific A/G

Chair: Luis Rodriguez-Saona; *The Ohio State University*

**(FORENS-02.1) Potential of LIBS in Food Analysis**

Ismail Boyaci; *OHIO STATE UNIVERSITY*

**(FORENS-02.2) Optical Trade Space Analysis for Handheld Near-Infrared Spectroscopic Sensors**

Christopher Ball, Siyu Yao, Luis Rodriguez-Saona; *The Ohio State University*

**(FORENS-02.3) Bright Path for Spectroscopy Devices to Safeguard Foods**

Luis Rodriguez-Saona; *The Ohio State University*

**(FORENS-02.4) Near-infrared spectrometers: Overview of state-of-the-art instrumentation**

John Gilmore; *Hamamatsu Photonics*

**(FORENS-02.5) Microplastics in our drinking water - does the container really matter?**

Julie Chen-Nguyen, Sanga Kim, Eunah Lee; *HORIBA Scientific*

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**23IR07: Applications of Photothermal IR Spectroscopy and Imaging in the Life Sciences**, Sierra 3

Chair: Rohith Reddy; *University of Houston*

(IR-07.1) **Advances in Cancer Tissue Analysis using Photothermal Mid-infrared Spectroscopic Imaging**

Chalapathi-Charan Gajjala, Ragib Ishrak, Xinyu Wu, Reza Reihani, Sharmin Afrose, David Mayerich, Rohith Reddy; *University of Houston*

(IR-07.2) **Probing metabolic heterogeneities within microbial populations at single-cell level with O-PTIR imaging**

Cassio Lima, Howbeer Muhamadali, Royston Goodacre; *University of Liverpool*

(IR-07.3) **Spatially Resolved Photothermal Infrared Spectroscopy of Antiparallel Amyloid Aggregates in Cerebral Amyloid Angiopathy**

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**23LIBS02: LIBS Throughout the FACSS History**, Southern Pacific B/C

Chair: Hunter Andrews; *Oak Ridge National Laboratory*

(LIBS-02.1) **Excitation temperature with Boltzmann plot: Significance, accuracy and correct use**

Bruno Bousquet, Vincent Gardette, Vincent Motto-Ros, Rosalba Gaudioso, Marcella Dell'Aglio, Alessandro De Giacomo; *University Of Bordeaux, Université de Lyon, ILM, University of Bari, CNR-IFN*

(LIBS-02.2) **The Evolution of LIBS Calibration Curves**

Matthieu Baudalet; *University Of Central Florida*

(LIBS-02.3) **Isotopic LIBS**

Richard Russo, Jhanis Gonzalez, George Chan; *Applied Spectra, Inc., Lawrence Berkeley National Laboratory*

(LIBS-02.4) **Improved Data Processing for Accurate Plasma Diagnostics and Calibration-Free LIBS**

Igor Gornushkin; *BAM*

(LIBS-02.5) **Coupling Microwave Excitation with Laser Induced Breakdown Spectroscopy: Wave of the Future or Doomed Approach?**

Avanjeet Ghosh; *The University Of Alabama*

(IR-07.4) **High-Resolution Infrared And Raman Microscopy Applied To Brain Hippocampal Sections Of A Transgenic Mouse Model of Tauopathy**

Francesca Palombo, Hao Meng, Jessica Mansfield, Michelle Bailey, Francesco Tamagnini, Nick Stone; *University Of Exeter, University Of Reading*

(IR-07.5) **Multiplexed Mapping of Endogenous Synthesis and Exogenous Uptake of Fatty Acids by Optical Photothermal Infrared Microscopy**

Sydney Shuster, Hannah Castillo, Caitlin Davis; *Yale University*

Steven Ray, Kelsey Williams, Buddhika Kumara; *SUNY Buffalo Dept of Chemistry, The State University Of New York at Buffalo*

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**23RAM02: SERS 1**, Cascade 3

Chair: Roy Goodacre; *University of Liverpool*  
Co-Chair: Zac Schultz; *The Ohio State University*

Co-Chair: Sian Sloan Dennison; *University of Strathclyde*

(RAM-02.1) -Withdrawn

(RAM-02.2) **Surface-Enhanced Raman Spectroscopy (SERS)-Assisted Gradient Detection in a Gut-on-a-Chip Fluidic Device**  
Alexis Lebrun, Antoine Girard, Flavie Lavoie-Cardinal, Denis Boudreau ; *Université Laval*

(RAM-02.3) **Deep Learning-enabled Classification of Extracellular Vesicles Using SERS**

Colin Hisey; *The Ohio State University*

(RAM-02.4) **SERS Investigation of the Impact of Common Nanoparticle Surfactants on the Transfer of Hot-Carriers**  
Chelsea Goetzman, Zachary Schultz; *Savannah River National Lab, The Ohio State University*

(RAM-02.5) **SERS of cells: from status to physiological process**

**Janina Kneipp**, Cecilia Spedalieri, Yiqing Feng; *Humboldt Universität Zu Berlin*

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**23RAM15: Raman in Regenerative Medicine**, Cascade 1

Chair: Ioan Notingher; *University of Nottingham*

Co-Chair: Max Dooley; *University of Nottingham*

(RAM-15.1) **Raman Spectroscopy For In Vivo Longitudinal Monitoring Of Rodent Models**

**Martin Aage Barsøe Hedegaard**, Anders Runge Walther, Elzbieta Stepula, Nicholas Ditzel, Moustapha Kassem, Morten Østergaard Andersen, Mads Sylvest Bergholt; *University of Southern Denmark, King's College London, Odense University Hospital and University of Southern Denmark*

(RAM-15.2) **Imaging Topical Drug Delivery With Stimulated Raman Scattering Microscopy**

**Natalie Belsey**, Dimitrios Tsikritsis, Vasundhara Tyagi, Panagiota Zarnpi, Anukrati Goel, Jean-Luc Vorng, Alex Dexter, Tao Chen, Richard Guy; *National Physical Laboratory, University of Bath, University of Surrey*

(RAM-15.3) **Optimisation Of Spatially Offset Raman Spectroscopy For Quantification Of The Fibrotic Tissue Response**

**Max Dooley**, Ioan Notingher; *University of Nottingham*

(RAM-15.4) **Detection of the early response of viral infection to cell by Raman spectroscopy**

**Keita Iwasaki**, Momoko Imai, Rheta Elkhaira, Hidetoshi Sato; *Kwansei Gakuin University*

(RAM-15.5) **A non-destructive Raman quantification of fatty acid in non-alcoholic fatty liver organoids**

**Sanghoon Cho**, Hoeil Chung; *Hanyang University*

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**23SPECIAL03: Microplastic Analysis - Standard Operating Procedures to**

**Understand the Environmental and Health Threats**, Southern Pacific B/C

Chair: Andrew Whitley, *HORIBA*

Co-Chair: Andrew Patterson, *HORIBA*

(SPEC-03.1) **Current Status Of Microplastics Analysis Solutions: A California-Based Perspective**

**Leah Thornton Hampton**; *Southern California Coastal Water Research Project (SCCWRP)*

(SPEC-03.2) **Analysis of microplastics in drinking water and other clean waters by vibrational spectroscopies – methodology challenges and opportunities for rationalizing the debate through harmonization & ISO normalization**

**Nizar Benismail**; *Nestle Waters*

(SPEC-03.3) **Automated identification of micron-scale microplastic particles identification using optical photothermal infrared spectroscopy (O-PTIR) and Raman**

**Craig Prater**, Eoghan Dillon, Andrew Stuart, Austin Tisor, Jay Anderson, Mustafa Kansiz, Frank Weston, Kevin Kjoller; *Photothermal Spectroscopy Corp, PerkinElmer*

(SPEC-03.4) **Stimulated Raman Scattering Analysis of Nanoplastics in Flow: High Sensitivity Enables Multi-Parameter Analysis**

**Maximilian Huber**, Liron Zada, Freek Ariese, Natalia Ivleva; *Technical University of Munich - Institute of Water Chemistry, Vrije Universiteit Amsterdam, LaserLaB Amsterdam, Department of Physics and Astronomy*

(SPEC-03.5) **Characterization of select table salts for microplastics using Raman spectroscopy**

**Andrew Patterson**, Nikita Kovalyov, Bijan Jafari; *Eurofins*

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**23SPSJ02: 50 Years of UV Raman Spectroscopy**, Cascade 4

Chair: Igor Lednev, *University at Albany, SUNY*

Co-Chair: Barbara Rossi, *Elettra Sincrotrone Trieste*

(SPSJ-02.1) **Deep-UV Raman Study of Exosomes for Cancer Diagnosis and Monitoring**

Sila Jin, Yeonju Park, Jongmin Park, **Young Mee Jung**; *Kangwon National University, University At Albany.*

(SPSJ-02.2) **Advanced Instrumentation for DUV Raman Microscopy: Finer, Faster, and Brighter**  
**Atsushi Taguchi**; *Hokkaido University*

(SPSJ-02.3) **Electron-phonon coupling in linear sp-carbon chains unveiled by UV resonance Raman spectroscopy.**  
**Carlo S. Casari**; *Politecnico di Milano*

(SPSJ-02.4) **Modeling Resonance Raman in Complex Environments**  
Chiara Cappelli, **Sara Gomez**, *Scuola Normale Superiore*

(SPSJ-02.5) **Deep UV Resonance Raman spectroscopy for selective characterization of biological specimens**  
**Barbara Rossi**, Fatima Matroodi, Denis Rajnovic, Alessandro Marcello, Lamyaa Almeahmadi, Igor Lednev; *Elettra Sincrotrone Trieste, Elettra, Elettra-Sincrotrone And Icgeb, ICGEB, Massachusetts Institute of Technology (MIT), University at Albany, SUNY.*

## TECHNICAL PROGRAM – MONDAY, OCTOBER 9, 2023

**Awards and Plenary Lectures | 10:45AM – 12:00PM | Sierra 5**

**Plenary Sessions: The Coblenz Society  
Coblenz Award; Wei Xiong**

(PLEN-L1.1) **Ultrafast Dynamics of Molecular Polaritons: How Can A Photonic Cavity Modify Molecular Dynamics?**  
**Wei Xiong**; *University of California, San Diego*

**Plenary Sessions: The Coblenz Society  
Clara Craver Award; Ishan Barman**

(PLEN-L1.2) **From Spectroscopy to Solutions: Transformative Biophotonics in Disease Detection and Monitoring**  
**Ishan Barman**; *Johns Hopkins University*

## TECHNICAL PROGRAM – MONDAY, OCTOBER 9, 2023

**Oral Symposia | 1:30 PM - 3:10PM**

**23AES02: Electrokinetic Fundamentals,**  
Southern Pacific F  
Chair: Rafael Davalos, *Virginia Tech*  
Co-Chair: Alaleh Vaghef Koodehi, *Rochester Institute of Technology*

(AES-02.1) **Microscale Bioseparations Combining Linear And Nonlinear Electrokinetic Effects**

**Blanca H. Lapizco-Encinas**; *Rochester Institute of Technology*

(AES-02.2) **Zeta-potential as a biomarker in red blood cell (RBC) physiology**

**Erin Henslee**; *Wake Forest University*

(AES-02.3) **Synthesis of Bacterial Cellulose under AC electric fields**

**Rodrigo Martinez-Duarte**, Sindora Baddam; *Clemson University*

(AES-02.4) **Monte Carlo Simulation of Polymer Electrophoretic Transport through Polydisperse Nanoscale Pores via Entropic Trapping**

**Sourav Bandyopadhyay**, Victor Ugaz; *TAMU, Texas A&M University*

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**23ATOM08: Edward Steers Memorial Award Symposium,** Central Pacific A/B/C  
Chair: Gerardo Gamez, *Texas Tech University Dept. of Chemistry and Biochemistry*  
Co-Chair: Peter Robinson, *MassCare Ltd*

(ATOM-08.1) **In Memory of Professor Edward Steers – His Achievements and His Legacy**

**Peter Robinson**; *MassCare Ltd*

(ATOM-08.2) **Investigation of matrix independent calibration of oxygen in GD-OES**

**Volker Hoffmann**, Gebel Bernhard, Thomas Gemming, Rene Heller, *IFW Dresden, HZDR*

(ATOM-08.3) **Glow-Discharge Optical Emission Coded Aperture Spectral Imaging Elemental Mapping**

**Harshit Agrawal**, Rajendra Joshi, Hanuk Kwon, Gerardo Gamez, *Texas Tech University*

(ATOM-08.4) **GDOES investigation on the W/Be erosion/deposition and D retention at the first wall of the nuclear fusion devices**

**Eduard Grigore**, Cristian Ruset, Flaviu Baiasu, Corneliu Porosnicu, Matej Mayer, Stepan Krat, Anna Widdowson, Jari Likonen, Michael Analytis, Ruediger Meihnsner, JET contributors, *National Institute For Laser, Plasma And Radiation Physics, Max-Planck-Institut für Plasmaphysik, Garching, Germany, Euratom/UKAEA, Culham Science Centre, Abingdon, UK*

(ATOM-08.5) **Analyte Solution-to-Plasma transfer in the Solution Cathode Glow Discharge**

**Jaime Orejas**, Yinchexi Zhang, Cristian Soto-Gancedo, Luis Javier Fernández-Menéndez, Nicholas Hazel, Steven Ray, Jorge Pisonero, Nerea Bordel, *Universidad De Oviedo, SUNY Buffalo Dept of Chemistry*

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**23AWD01: The Coblentz Society Coblentz Award Symposium Honoring Wei Xiong**, Sierra 5

Chair: Wei Xiong, *University of California, San Diego*

(AWD-01.1) **Moving towards transient 2D IR: Mapping structure and dynamics with site-specific vibrational probe pairs**

**Matthew Tucker**, *University Of Nevada Reno*

(AWD-01.2) **Absorber-Specific Dynamics in Vibration-Cavity Polaritons**

**Adam Dunkelberger**, *Us Naval Research Laboratory*

(AWD-01.3) **Energy transport control under strong light-matter interactions**

**Raphael Ribeiro**, Gustavo Aroeira, Enes Suyabatmaz, *Emory University*

(AWD-01.4) **Ultrafast energy relaxation in carbon nanotube exciton-polariton microcavities**

**Minjung Son**, Michael Arnold, Martin Zanni, *Boston University, University of Wisconsin-Madison*

(AWD-01.5) **New Experimental Platforms for Polariton Reaction Dynamics**

**Marissa Weichman**, *Princeton University*

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**23CHEM02: Chemometric Opportunities in Forensic Chemistry**, Southern Pacific D  
Chair: Ruth Smith, *Michigan State University*

(CHEM-02.1) **Ignitable Liquid Analysis by DART-MS and Chemometrics**

**Mengliang Zhang**, Shruthi Perna, Ngee Sing Chong, *Middle Tennessee State University*

(CHEM-02.2) **Elucidation of the Effect of Heat and Sun Exposures on Hair Colored by Permanent and Semi-Permanent Colorants Using Surface Enhanced Raman Spectroscopy (SERS)**

**Dmitry Kurouski**, Aidan Holman, Mackenzi Peterson, *Texas A&M University*

(CHEM-02.3) **Expert Algorithm for Substance Identification (EASI) Applied to the Mass Spectra of Seized Drugs**

**Glen Jackson**, Alexandra Adeoye, Isabel Galvez-Valencia, *West Virginia University*

(CHEM-02.4) **The application of Raman spectroscopy to estimate the time since deposition of bloodstains aged under environmental conditions**

**Alexis Weber**, Igor Lednev, *University at Albany, SUNY*

(CHEM-02.5) **Non-Destructive And Rapid Monitoring Of Cannabinoid Degradation In Hemp Inflorescence During Storage: Kinetic Modeling Using A Time-Based Approach**  
**Cameron Jordan**, Ms. Siyu Yao, Silvia De Lamo Castellvi, Christopher Ball, M. Monica Giusti, Luis Rodriguez-saona, *The Ohio State University*

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**23CTP/EARLY03: Showcasing Career Paths in the Spectroscopic Sciences (Sponsored by SAS Early Career),** Sierra 2  
Chair: Fay Nicolson, *Dana-farber Cancer Institute / Harvard Medical School*  
Co-Chair: Samuel Mabbott, *Texas A&M University*

(CTP-03.1) **Between two worlds: from researcher to professor**  
Andrea Locke, *Vanderbilt University Biophotonics Center*

(CTP-03.2) **Moving out of academia – Setting up, financing and scaling our university spin out CanSense**  
Cerys Mitchell, *Cansense Limited*

(CTP-03.3) **Harvesting the Benefits and Overcoming the Challenges of a Multi-Cultural Career**  
Amandine Calvet, *Boehringer Ingelheim Pharma GmbH & Co.KG*

(CTP-03.4) **The Experiments Never End: Building a Career in Research Translation and Commercialization**  
Steven Asiala, *University Of Notre Dame*

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**23IR08: Photothermal IR Spectroscopy and Imaging of Microplastics and Other Materials,** Sierra 3  
Chair: Curtis Marcott, *Light Light Solutions*  
Co-Chair: Minghe Li, *Boehringer-Ingelheim Pharmaceuticals*

(IR-08.1) **Materials for Inhaled Aerosol Treatment of Disease: PTIR Microscopy for Bioequivalence and Improving Therapeutic Index**  
Mark Banaszak Holl, Dipesh Khanal, Sheikh Tanzina Haque, Blessy Joseph, Hak-Kim Chan, *The University of Alabama at Birmingham, University of Sydney*

(IR-08.2) **Surely It's Just a Phase: Probing Solid and Semi-Solid Atmospheric Particles from Urban Haze to Algal Blooms to Microplastics with Photothermal Infrared Plus Raman Spectroscopy**  
Andrew Ault, *University Of Michigan*

(IR-08.3) **Simultaneous SERS & SEIRA with Single Molecule Detection – The Application and Characterization of Plasmonically Resonant Structures with Sub-Micron Optical Photothermal Infrared and Simultaneous Raman spectroscopy**

Mustafa Kansiz, Deepthy Kavungal, Felix Richter, Mark Anderson, Hatice Altug, *Photothermal Spectroscopy Corp., EPFL, CALTECH/JPL/NASA*

(IR-08.4) **Vibrational spectroscopic detection of microplastics in water using diverse microplastics-capturing media**  
Yunjung Kim, Sanghoon Cho, Sangjae Kim, Hoeil Chung, *Hanyang University*

(IR-08.5) **Overcoming fluorescence in Raman when measuring weathered/oxidized microplastics, using sub-micron optical photothermal infrared**  
Jay Anderson, Mustafa Kansiz, Eoghan Dillon, Frank Weston, *Photothermal Spectroscopy Corp,*

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**23MASS01: Early Career Researchers in Mass Spectrometry,** Southern Pacific A/G  
Chair: Gabe Nagy, *University of Utah*  
Co-Chair: Chris Chouinard, *Clemson*

(MASS-01.1) **Developing a Bioanalytical Toolbox for Human Milk Oligosaccharide Characterization**  
Sanaz Habibi, David Williamson, Gabe Nagy, *University of Utah*

(MASS-01.2) **From Solution to the Gas Phase: An Examination of Protein Charging in Electrospray**  
Elyssia Gallagher, Michael Cordes, Alexis Edwards, Madeline Bannon, *Baylor University*

(MASS-01.3) **Coupling Tandem MS and IM<sup>n</sup> for Mass and Structure Selective Analysis of Biomolecular Complexes**  
Varun Gadkari, Rowan Matney, *University Of Minnesota - Twin Cities*

(MASS-01.4) **Multimodal Mass Spectrometry Imaging Approaches for Probing Complex Biological Systems.**  
Elizabeth Neumann, *University of California at Davis*

(MASS-01.5) **Dissociation Patterns of Ionic Liquid Cations: A Survey of Common Structures and Substituents**  
Amanda Patrick, *Mississippi State University*

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**23PAT02: PAT Pharma/Biotech**, Southern Pacific E  
Chair: Hossein Hamed, *Biogen*

(PAT-02.1) **In-situ FTIR and Raman in Fermentations of Crop Protection Active Ingredients**  
Michael Bishop, David Archer, David Ferial-Gervasio, Stefanie Casada, Jeremy McFadden, Bryon Herbert, *Corteva Agriscience*

(PAT-02.2) **Getting more "eyes" on your process: the value proposition of PAT for early-phased development**  
Sayyeda Zeenat Razvi, Zhenqi (Pete) Shi, *Genentech*

(PAT-02.3) **Optimizing Critical Harvest Process Variables using Real Time Particle and Spectroscopic Measurements**  
Jim Cronin, *Mettler Toledo Autochem*

(PAT-02.4) -Withdrawn    Type text here

(PAT-02.5) **Optimizing Pharmaceutical Process Performance using Advanced Process Control and Process Analytical Technologies (PAT)**

Claudia Corredor, Aparajith Bhaskar, Gregory Lane, Dimuthu Jayawickrama, Sandra Roberts, Brian Breza, *BMS, Applied Materials*

**23PMA02: Media Integrity in BioPharma**, Southern Pacific D  
Chair: Alan Ryder, *Nanoscale Biophotonics Laboratory, University Of Galway*

(PMA-02.1) **Implementation of a control strategy insuring low impact of cell culture media quality on bioprocesses**  
Amandine Calvet, *Boehringer Ingelheim Pharma GmbH & Co.KG*

(PMA-02.2) **Automated determination of trace metals in biopharmaceutical samples of complex matrix using seaFAST preparation system coupled to inductively coupled plasma mass spectrometry**  
Qiang Tu, Chengbei Li, Wendy Zhong, Hillary A. Schuessler, *Merck & Co., Inc.*

(PMA-02.3) -Withdrawn

(PMA-02.4) **Comprehensive Metals Mass Balance in CHO Cell Processes**  
Cameron Stouffer, Sarah Wysor, R. Kenneth Marcus, *Clemson University*,

(PMA-02.5) **Optimal Spectral Resolution for Solids and Liquids Using FTIR and Other Infrared Spectrometers: Results from Database studies**  
Timothy Johnson, Brenda Forland, Kendall Hughey, Michael Wilhelm, Olivia Williams, Benjamin Cappello, Connor Gaspar, Tanya Myers, *Pacific Northwest National Laboratory*,

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**23RAM01: Emerging Raman**, Cascade 1  
Chair: Pavel Matousek, *Rutherford Appleton Laboratory*  
Co-Chair: Bhavya Sharma, *University Of Tennessee*

(RAM-01.1) **In Vivo Surface-Enhanced Transmission Raman Spectroscopy: Toward Photosafe Localization of Deep-Seated Lesions**

**Li Lin**, Jian Ye, *Shanghai Jiao Tong University*

(RAM-01.2) **Swept Source NIR Raman Spectroscopy for Distributed Multi-Point Sensing Using an Optical Fiber Network**

**Nili Persits**, Dahlia Dry, Rajeev Ram, *MIT*

(RAM-01.3) **Efficient Optical Plasmonic Tweezer-Controlled Surface-Enhanced Raman Spectroscopy For Single-Molecule Studies In Solution**

**Jinqing Huang**, *The Hong Kong University Of Science And Technology*

(RAM-01.4) **Wearable Microfluidic Devices for Sweat Analysis**

**Limei Tian**, *Texas A&M University*

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**23RAM07: ECR Raman**, Cascade 3

Chair: Bhavya Sharma, *University Of Tennessee*

Co-Chair: Sian Sloan-Dennison, *University of Strathclyde*

(RAM-07.1) **Investigating the structure of non-crystalline macromolecular assemblies and aggregates using Raman Spectroscopy**

**David Punihaole**, *University Of Vermont*

(RAM-07.2) **Imaging Though – Advances in Transmission Raman for Non-Invasive Whole Animal Imaging**

**Benjamin Gardner**, Alexandra Vaideanu, Ryan Mellor, Ijeoma Uchegbu, Andreas Schatzlein, Pavel Matousek, Nick Stone, *University Of Exeter*

(RAM-07.3) **Developing Surface-Enhanced Raman Spectroscopy Methods For Quantification Of Complex Analyte Mixtures In Plant-Based Extracts**

**Stephanie Zaleski**, *California State University East Bay*

(RAM-07.4) **Multiplex Cellular Imaging Using Stimulated Raman Scattering Microscopy and Spectral Phasor Analysis**

**William Tipping**, Ewan Hislop, Liam Wilson, Henry Braddick, Nicholas Tomkinson, Karen Faulds, Duncan Graham, *The University Of Strathclyde*

(RAM-07.5) **Scanning Ion-Conductance Microscopy for Tip-Enhanced Raman Spectroscopy**

**Naihao Chiang**, *University of Houston*

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**23SPR02: 50 Years of Plasmonics**, Cascade 4  
Chair: Amanda Haes, *University Of Iowa*

(SPR-02.1) **Plasmonics as a strategy for the design and sensitive readout of immunodiagnostic platforms by surface-enhanced Raman scattering: It's not only about limits of detection**

**Marc Porter**, *University Of Utah*

(SPR-02.2) **A plasmonic tongue to predict maple syrup quality from sap**

**Jean-Francois Masson**, Simon Forest, Juklien Coutu, Issraa Beniani, Zhe Si Yu, Morgan Craig, *Universite de Montreal*

(SPR-02.3) **Development of SERS Sensing Platform for TSH Detection: From Buffer Solution to Patient Samples**

**Piyush Raj**, Peng Zheng, Lintong Wu, Takayuki Mizutani, Miklos Szabo, William Hanson, Ishan Barman, *Johns Hopkins University*

(SPR-02.4) **Janus MOF-based Micromotors as Sensors**

**Eric Languirand**, Matthew Collins, Errie Gibson Parrilla, *Languirand*

# TECHNICAL PROGRAM – MONDAY, OCTOBER 9, 2023

## Oral Symposia | 3:50PM – 5:30PM

### **23AES03: Innovations in Device Fabrication and Applications**, Southern Pacific F

Chair: Alex Hyler, *Cytorecovery*

Co-Chair: Olivia Ernst, *Microscale*

*Bioseparations Laboratory and Biomedical Engineering Department, Rochester Institute of Technology, 160 Lomb*

#### **(AES-03.1) Advanced 3D Printing for High Resolution Microfluidic Devices**

**Greg Nordin**, Dallin Miner, Mawla Boaks, Matthew Viglione, *Brigham Young University*

#### **(AES-03.2) Enhancing Accessibility and Reproducibility in Zeta Potential Measurements: A Novel Approach with Commercial Microfluidic Chips and Open-Source Workflows**

**Jonathan Cottet**, Josephine Oshodi, Ada Erus, Ariel Furst, Cullen Buie, *MIT*

#### **(AES-03.3) -Withdrawn**

#### **(AES-03.4) Improving Device Design For Low-Frequency Alternating Current Electrokinetic Separations**

**Nuzhet Nihaar Nasir Ahamed**, Carlos A. Mendiola-Escobedo, Victor H. Perez-Gonzalez, Blanca H. Lapizco-Encinas, *Rochester Institute of Technology, Microscale Bioseparations Laboratory and Biomedical Engineering Department*

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### **23ATOM05: High-end ICP-MS**

**Applications**, Central Pacific A/B/C

Chair: Frank Vanhaecke, *Ghent University*

Co-Chair: Thibaut Van Acker

#### **(ATOM-05.1) Evaluation of fs-LA-ICP-TOFMS for multi-matrix analysis with high spatial resolution**

**Jorge Pisonero**, Cristian Soto, Ana Mendez, Jaime Orejas, Nerea Bordel, Ines García, Alex Calón, Jennifer Linares, Esteban Avigliano, Antonia Cepedal, *University Of Oviedo*

#### **(ATOM-05.2) The Power of a Multi-Modal Platform Based on ICP-MS to Provide New Insights into the Fractionation of Titania Particles in Food Samples**

**David Ojeda**, Malvinder Singh, Dorota Bartczak, Paul Hancock, Heidi Goenaga-Infante, *LGC*

#### **(ATOM-05.3) Stretching the boundaries of high-precision isotopic analysis using multi-collector ICP-MS**

**Frank Vanhaecke**, Lana Abou-Zeid, Eduardo Bolea-Fernandez, Marta Costas-Rodriguez, José Ignacio Garcia-Alonso, Steven Goderis, Kasper Hobin, Sara Lauwens, Björn Meermann, Katerina Rodiouchkina, Ana Rua Ibarz, Laura Suarez-Criado, Ir. Thibaut Van Acker, *Ghent University*

#### **(ATOM-05.4) Data processing tool for automated calculation of isotope ratios from transient signals - IsoCor**

**Dariya Tukhmetova**, Jan Lisec, Jochen Vogl, Björn Meermann, *Federal Institute for Materials Research and Testing (BAM)*

#### **(ATOM-05.5) Single-cell ICP-TOF-MS as a powerful tool to investigate the elemental chemical profile of snow algae and their responses to phosphorus starvation**

**Silvana Ruella Oliveira**, Helen Feord, Cícero A. Lopes Júnior, Ravi S. Peters, Liane G. Benning, Björn Meermann, *Federal Institute For Materials Research And Testing - BAM, Division 1.1, Inorganic Trace Analysis*

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### **23AWD02: The Coblentz Society Clara Craver Award Symposium Honoring Ishan Barman**, Sierra 5

Chair: Ishan Barman, *Johns Hopkins University*

#### **(AWD-02.1) Chemical imaging: fit for purpose instruments**

**Rohit Bhargava**, Sudipta Mukherjee, Kianoush Falahkheirkhah, Yamuna Phal,

Anirudha Rao, Ruo-Jing Ho, Kevin Yeh, Seth Kenkel, *University of Illinois at Urbana-Champaign*

(AWD-02.2) **Innovation of far-ultraviolet spectroscopy in condensed phase**

Yukihiro Ozaki, *School Of Biological And Environmental Science*

(AWD-02.3) **Spectroscopic Marker vs. Biomarker for Disease Diagnostics and Forensics**

Igor Lednev, *University at Albany, SUNY*

(AWD-02.4) **SERS Immunoassay quantifications at ultra-low concentrations**  
Alexandre Brolo

(AWD-02.5) **Bridging the Gap from Whole Body to Subcellular Level using Fluorinated Probes for MRI and Raman Microscopy**

Renzo Vanna, Cristina Chirizzi, Carlo Morasso, Matteo Tommasini, Fabio Corsi, Linda Chaabane, Francesca Baldelli Bombelli, Pierangelo Metrangolo, *IFN- CNR / Politecnico di Milano*

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**23BIM01: Machine and Deep Learning for Biomedical Diagnostics, Sierra 2**

Chair: Thomas Bocklitz, *Leibniz-ipht*

Co-Chair: Oleg Ryabchykov, *Leibniz Institute of Photonic Technology (IPHT)*

(BIM-01.1) **Machine learning for pathology detection along with macromolecular orientation using FT-IR bioimaging**

Tomasz Wrobel, *Jagiellonian University*

(BIM-01.2) **Using machine learning for the processing and modeling of vibrational spectral data**

Oleg Ryabchykov, MSc Azadeh Mokari, Rola Houhou, Ute Neugebauer, Juergen Popp, Thomas Bocklitz, *Leibniz Institute of Photonic Technology (IPHT)*

(BIM-01.3) **Standardizing Raman Line Illumination Microscopy Data to Investigate Hydrogel-Mediated Reprogramming of Cancer Stem Cells**

Jean-emmanuel Clément, Zannatul Ferdous, Masumi Tsuda, Shinya Tanaka, Jian Ping

Gong, Thomas Bocklitz, Katsumasa Fujita, Tamiki Komatsuzaki, *Hokkaido University*

(BIM-01.4) **Volterra based Explainable Artificial intelligence (XAI) methods for spectroscopy and imaging.**

Jhonatan Contreras, Thomas Bocklitz, *Leibniz-ipht*

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**23CHEM03: Chemometrics Something Borrowed, Something New, Southern Pacific E**

Chair: Federico Marini, *University Of Rome "la Sapienza"*

(CHEM-03.1) **DIAGNOSIS AND CORRECTION METHODS FOR SPECTRAL INTERFERENCE IN THE FRAMEWORK OF LIBS IMAGING**

Ludovic Duponchel, Vincent Motto-Ros, *University Of Lille*

(CHEM-03.2) **Screening Trans Fatty Acids in Butter Using a Portable MIR Spectrometer Combined with Multivariate Analysis.**

Celeste Aurora Matos Gonzalez, Luis Rodriguez-Saona, *The Ohio State University*

(CHEM-03.3) **Labeled Baseline Correction of NIR Spectra via Regularized Least Squares**

Erik Andries, Ramin Nikzad-Langerodi, *Central New Mexico Community College*

(CHEM-03.4) **Class modeling: something old, something new...**

Federico Marini, *University Of Rome "la Sapienza"*

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**23FORENS03: Forensic Analysis in the Lab and at the Crime Scene, Southern Pacific A/G**

Chair: Igor Lednev, *University at Albany, SUNY*

Co-Chair: Marisia Fikiet, *University of New Haven*

(FORENS-03.1) **Forensic Science R&D Funding Programs at the National Institute of Justice**

Gregory Dutton, *National Institute Of Justice*



(FORENS-03.2) **Validation of the Fast Blue BB (FBBB) Colorimetric Test for the Detection of delta-9- tetrahydrocannabinol ( $\Delta^9$ -THC) in Oral Fluid**

Jose Almirall, *Robert Gorziza, Nicole Valdes, Florida International University*

(FORENS-03.3) **Probing Phototransformation of Saliva Stain with Steady State Fluorescence Spectroscopy**  
Entesar Al-hetlani, *Igor Lednev, Kuwait University*

(FORENS-03.4) **Streamlining Decision-making Processes at the Crime Scene and the Laboratory by Incorporating Fast Screening Tools into Current Gunshot Residue Workflows.**

Tatiana Trejos, *Luis Arroyo, Kourtney Dalzell, Leah Thomas, Madison Lindung, Thomas Ledergerber, West Virginia University*

(FORENS-03.5) **Multi-Element Analysis of Inorganic Gunshot Residues via Single Particle Inductively Coupled Plasma Mass Spectrometry**

Sarah Szakas, *Alexander Gundlach-Graham, Iowa State University*

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**23IR03: 140 Years of the Coblenz Society and the Infrared and Raman Discussion Group (IRDG), Sierra 3**

Chair: John Waslyk, *Bristol Myers Squibb*  
Co-Chair: Ashley Love, *University Of Nottingham*

(IR-03.1) **The Interplay Between Spectrometer Development (Lab And Portable) And Professional Spectroscopic Societies**

Richard Crocombe, *Crocombe Spectroscopic Consulting*

(IR-03.2) **"You Ought to be in Pictures": The Emergence of Infrared Chemical Imaging**  
Linda Kidder, *E. Neil Lewis, HORIBA Scientific*

(IR-03.3) **Closing The Loop In The Pulp And Paper Industry - A Process Intensification Approach For Chemical Recovery**

Karin Wieland, *Miranda Eisenköck, Barbara Weiß, Anna Katharina Schwaiger, Wolfgang Anton Fuchs, Bernhard Lendl, Michael Harasek, Martin Kraft, Competence Center Chase GmbH*

(IR-03.4) **A retrospect of spectroscopic studies on dipyrrophenazine - from Queens University Belfast to Los Lamos to the University of Otago New Zealand**  
Keith Gordon, *University Of Otago*

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**23LIBS05: LIBS for Nuclear Applications, Southern Pacific B/C**

Chair: Kyle Hartig, *University of Florida*  
Co-Chair: Hunter Andrews, *ORNL*

(LIBS-05.1) **Recent advances in laser-based sensing for nuclear safety and security applications**

Milos Burger, *University Of Michigan*

(LIBS-05.2) **Effects of atmospheric turbulence on remote isotope sensing for nuclear security applications**

Changmin Kim, Boyu Zhang, Jose Chirinos, Xianglei Mao, Vassilia Zorba, *Lawrence Berkeley National Lab & Uc Berkeley*

(LIBS-05.3) **Bulk Aerosol and Single Particle Dynamics in Femtosecond Laser Filaments for Aerosol Sensing**

Kyle Latty, *Kyle Hartig, University Of Florida*

(LIBS-05.4) **Detection and Analysis of Light Isotopes in Nuclear Materials using Laser Induced Breakdown Spectroscopy**

Elizabeth Kautz, *Annie Xu, Ajay Harilal, Mathew Polek, Arun Devaraj, Andrew Casella, David Senor, Sivanandan Harilal, North Carolina State University*

(LIBS-05.5) **Calibration, chemometrics, and mapping of rare earth elements with laser-induced breakdown spectroscopy**

Daniel Diaz, *Amir Fayyaz, David Hahn, University Of Arizona*

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**23PMA01: Vibrational Spectroscopy to Support Pharmaceutical Manufacturing, Southern Pacific D**

Chair: Patrick Wray, *Bristol-Myers Squibb*  
Co-Chair: Sergei Kazarian, *Imperial College London*

(PMA-01.1) **Studying Monoclonal Antibody Aggregation Under Flow Using Attenuated Total Reflection Fourier Transform Infrared Spectroscopic Imaging**  
**Céline van Haaren**, Bernadette Byrne, Sergei Kazarian, *Imperial College London*

(PMA-01.2) **Process Related Particulate Analysis In Pharmaceutical Manufacture**  
**Don Clark**, *Pfizer Ltd*

(PMA-01.3) **Spectroscopic Applications for Pharmaceutical Development**  
**John Wasyluk**, Robert Wethman, Ming Huang, *Bristol Myers Squibb*

(PMA-01.4) **Spectroscopic Imaging Of Multi-Material 3D Printed Pharmaceutical Dosage Forms**  
**Zoë Whalley**, *The University Of Birmingham*

(PMA-01.5) **Machine Learning and Data Rich Process Analytical Technology (PAT) for Enhancing Biocatalysis**  
**Joseph Smith**, *Merck & Co.*

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**23RAM03: SERS 2**, Cascade 3  
Chair: Zac Schultz, *Ohio State University*  
Co-Chair: Sian Sloan-Dennison, *University of Strathclyde*  
Co-Chair: Roy Goodacre, *University of Liverpool*

(RAM-03.1) **Applications of Surface-Enhanced Raman Spectroscopy in Environmental Pollutant Detection**  
**Huiyuan Guo**, *Binghamton University*

(RAM-03.2) **Detection of Multiple Foodborne Pathogens by SERS**  
**Hayleigh May**, Royston Goodacre, Duncan Graham, Karen Faulds, *University Of Strathclyde*

(RAM-03.3) **Revealing the Multiplexing Potential of SERS Nanoparticles for Molecular Imaging of Cancer**  
**Olga Eremina**, Alexander Czaja, Augusta Fernando, Cristina Zavaleta, *University Of Southern California*

(RAM-03.4) **Raman and SERS of liquid biopsy biofluids for cancer diagnostics: focus on extracellular vesicles (EVs)**  
**Randy Carney**, *UC Davis*

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**23RAM13: Nano Raman 1**, Cascade 1  
Chair: Andrew Whitely, *HORIBA*  
Co-Chair: Andrey Krayev, *HORIBA*

(RAM-13.1) **TERS Origins and the Next Generation**

**Volker Deckert**, *Friedrich Schiller University Jena*

(RAM-13.2) **Nanoimprinted pyramid scanning probe for nanoscale optical mapping**

**Junze Zhou**, Edward Barnard, Keiko Munechika, Adam Schwartzberg, Alexander Weber-Bargioni, *Lawrence Berkeley National Laboratory*

(RAM-13.3) **TERS/TEPL imaging of the moiré domains in transition metal dichalcogenide bilayers**

**Thomas Darlington**, Yinjie Guo, Emanuil Yanev, Kevin Kwock, Cory Dean, P. James Schuck, *Columbia University*

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**23SPSJ01: Higher Energy UV Spectroscopy**, Cascade 4  
Chair: Yusuke Morisawa, *Kindai University*  
Co-Chair: Ichiro Tanabe, *Rikkyo University*

(SPSJ-01.1) **A study on electronic structure and transition of saccharides by ATR-FUV and UVRR spectroscopy**  
**Kosuke Hashimoto**, Fatima Matroodi, Mariagrazia Tortora, Barbara Rossi, Yusuke Morisawa, Yukihiro Ozaki, Hidetoshi Sato, *Kwansei Gakuin University*

(SPSJ-01.2) **-Withdrawn**

(SPSJ-01.3) **SPR sensing in far and- deep-ultraviolet regions**

**Ichiro Tanabe**, *Rikkyo University*

(SPSJ-01.4) **Enabling Label Free Biosensing With Ultraviolet Plasmonics Engineered Native Fluorescence.**

**Yunshan Wang**, *University Of Utah*

(SPSJ-01.5) **Electronic states of water in “Water-in-Salts” and “Hydrate-melts” electrolytes.**

**Yusuke Morisawa**, *Kindai University*

## TECHNICAL PROGRAM – TUESDAY, OCTOBER 10, 2023

### Oral Symposia | 8:00AM – 10:10AM

**23AES05: Early Career**, Southern Pacific F

Chair: Blanca Lapizco-Encinas, *Rochester*

*Institute of Technology*

Co-Chair: Zach Gagnon, *Texas A&M*

*University*

**On-Chip Multichannel Cytometry For Phenotypic Monitoring Of Microfluidic Separations**

(AES-05.1) **Karina Torres-Castro**, Javad Jarmoshti, Carlos Honrado, Nathan S. Swami  
*University of Virginia*

**Exploring The Use Of Low-Frequency Alternating Current Potentials In Insulator-Based Electrokinetic Separations**

(AES-05.2) **Nuzhet Nihaar Nasir Ahamed**, Carlos A. Mendiola-Escobedo, Olivia D. Ernst, Victor H. Perez-Gonzalez, Blanca H. Lapizco-Encinas *Microscale Bioseparations Laboratory and Biomedical Engineering Department, Rochester Institute of Technology, School of Engineering and Sciences, Tecnologico de Monterrey, Monterrey, Nuevo Leon 64849, Mexico, Microscale Bioseparations Laboratory and Biomedical Engineering Department, Rochester Institute of Technology, 160 Lomb, School of Engineering and Sciences, Tecnologico de Monterrey, Monterrey, Nuevo Leon 64849, Mexico, Rochester Institute of Technology*

**Exploring the Insulating Properties of Paper Fibers for Enhanced Electrokinetic Applications in Sample Purification and Liquid Handling**

(AES-05.3) **Md Nazibul Islam**, *Texas A&M University*

**A Numerical Approach to Understanding the Effect of Impedance on High-Frequency Dielectrophoresis Applications**

(AES-05.4) **Josie Duncan**, *Virginia Tech*

**Deep eutectic solvent-based separations for amino acid analysis via CE**

(AES-05.5) **Jessica Torres**, Christopher Harrison, Karen Campos, *San Diego State University*

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**23ATOM01: ICP Time of Flight MS**, Central Pacific A/B/C

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

(ATOM-01.1) **Capabilities Of a Downwards Pointing ICP-TOFMS For Nanoparticle and Cell Characterization**

**Detlef Günther**, Sandro Fazzolari, Guanghui Niu, Thomas Vonderach, Alexander Gundlach-Graham, *Department Of Chemistry And Applied Biosciences Iowa State University*

(ATOM-01.2) **The Origins of Noisy Single-Particle ICP-TOFMS Data and How to Use It**

**Alexander Gundlach-Graham**, Raven Buckman, Hark Karkee, Sarah Szakas, *Iowa State University*

(ATOM-01.3) **Expanding the Elemental Coverage by Combining LIBS with ICP-TOF-MS for High-Speed Imaging**

**C. Derrick Quarles**, Benjamin Manard, Hunter Andrews, Tyler L. Spano, Joseph A. Petrus, Cole R. Hexel, *Elemental Scientific Inc., Oak Ridge National Laboratory*

(ATOM-01.4) **Automated Elemental and Isotopic Analysis of Particles with Single-Particle Inductively Coupled Plasma-Time of Flight-Mass Spectrometry**

**Veronica Bradley**, Benjamin Manard, Brian Sanders, Amber Webb, Lyndsey Hendriks, Hunter Andrews  
*Oak Ridge National Laboratory, TOFWERK,*

(ATOM-01.5) **Accurate Classification And Quantification Of Engineered And Natural Titanium Submicron Particles Using Single-particle ICP-TOFMS**

**Hark Karkee**, Alexander Gundlach-Graham  
*Iowa State university*

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**23AWD03: Ellis R. Lippincott Award Symposium Honoring Peter Griffiths**, Sierra 5

Chair: Peter Griffiths, *Griffiths Consulting*

(AWD-03.1) **Fourier transform spectroscopy and the evolution of infrared imaging: From theory to fast, sensitive measurements**

**Rohit Bhargava**, *University of Illinois at Urbana-Champaign*

(AWD-03.2) **ATR-FTIR Spectroscopic Imaging for the Analysis of Biopharmaceuticals**

**Sergei Kazarian**, *Imperial College London*

(AWD-03.3) **Infrared determination of total particulate mass in mine dust samples: Are cluster models worth the trouble?**

**Andrew Weakley**, David Parks, Arthur Miller, *Weakley Consulting, National Institute of Occupational Safety and Health*

(AWD-03.4) **Quo vadis in process Raman spectroscopy**

**Ian Lewis**, Maryann Cuellar, Justin Moretto, Karen Esmonde-White, Scott Sutherland, Shajeel Haider, Sean Gilliam, Randy Benedict, Joel Patrow, David Strachan, Herve Lucas, Carsten Uerpmann, *Endress+Hauser Optical Analysis, Endress+Hauser, Endress+Hauser Process Analysis Support, SARL*

(AWD-03.5) **Sampling for Field Studies: A Mixed Bag**

**James de Haset**, Franklin Barton, *Infrared & Raman Courses, Inc., LLS Instruments, Inc*

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**23BIM04: Celebrating Early Career Scientists in Biomedical and Bioanalytical Spectroscopy**, Sierra 2

Chair: Fay Nicolson, *Dana-farber Cancer Insitute / Harvard Medical School*

(BIM-04.1) **Spatially Offset Raman Spectroscopy Of Biological Tissue – What Can We Get Out Of It?**

**Sara Mosca**, Megha Mehta, William Skinner, Benjamin Gardner, Francesca Palombo, Nick Stone, Pavel Matousek *Ral, Stfc, Uki, University Of Exeter, Rutherford Appleton Laboratory*

(BIM-04.2) **Harnessing DNA Hairpin Assemblies for Enhanced Signal Amplification in Point-of-Care Diagnostics**  
**Samuel Mabbott**, *Texas A&M University*

(BIM-04.3) **Raman spectroscopy for culture-free bacteria detection**

**Andrea Locke**, Anna Rourke-Funderburg, Timothy Yokley, *Vanderbilt University Biophotonics Center, Vanderbilt University*

(BIM-04.4) **Improving Colorectal Cancer early detection with the CanSense-CRC Blood Test**

**Cerys Mitchell**, Charles Brilliant, Nafiseh Badiei, Nerissa Thomas, Freya Woods, Peter Dunstan, Dean Harris *Cansense Limited, Swansea Universit*

(BIM-04.5) **New Approaches to Process Analytical Technologies in the Monitoring, Optimization and Scale-Up of Flow Chemical Processes**

**Ashley Love**, *University Of Nottingham*

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**23IR01: Fluorescence and EEMS: Exploiting A New Approach for PAT and Monitoring**, Sierra 3

Chair: Alan Ryder, *Nanoscale Biophotonics Laboratory, University Of Galway*  
Co-Chair: Ashley Love, *University Of Nottingham*

(IR-01.1) **Polarized Excitation Emission Matrix (pEEM) spectroscopy: another dimension for protein analysis.**

**Alan Ryder**, *Nanoscale Biophotonics Laboratory, University Of Galway*

(IR-01.2) **SCALABLE CONTINUOUS PHOTOCHEMICAL & ELECTROCHEMICAL REACTIONS:**

**REACTORS AND PAT CHALLENGES:  
FROM PICOSECONDS TO TONNES.**

**Ashley Love**, *University Of Nottingham*

(IR-01.3) **Measuring Protein-polymer nanoparticle interactions using polarized Excitation Emission Matrix (pEEM) spectroscopy.**

**Matheus de Castro**, Alan Ryder, *University of Galway, Nanoscale Biophotonics Laboratory, University Of Galway.*

(IR-01.4) **Advanced deep UV Raman and fluorescence instruments for industrial process analysis and cleaning verification**  
Rohit Bhartia, Ray Reid, Ken Nguyen, Quoc Nguyen, **William Hug**, *Photon Systems, Inc.*

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**23MASS02: Ion Mobility Separations: Instrumentation, Applications, and Methods**, Southern Pacific A/G

Chair: Chris Chouinard, *Clemson University*

(MASS-02.1) **Clinical Applications of Advanced Ion Mobility Mass Spectrometry**

**Ahmed Hamid**, Orobola Olajide, Kimberly Kartowikromo, Yuyan Yi, Jingyi Zheng, *Auburn University*

(MASS-02.2) **Improved Analysis of Small Molecule Drugs using High Resolution Ion Mobility-Mass Spectrometry Approaches**

Ralph Aderorho, **Christopher Chouinard**, *Clemson University*

(MASS-02.3) **Fingerprinting the Unique Lipidome of Membrane Proteins Using Liquid Chromatography, Ion Mobility Spectrometry and Mass Spectrometry**

**Jack Ryan**, Yun Zhu, Melanie Odenkirk, Arthur Laganowsky, Erin Baker, *University Of North Carolina At Chapel Hill, Texas A&M University, University of Arizona*

(MASS-02.4) **Real-time metabolomics of mammalian cell-based biotechnology using mass spectrometry**

**Bart Pander**, Luke Johnston, Tessa Moses, Sophie Bennet, Lorna Eades, Juraj Bella, Karl Burgess, *University of Edinburgh*

(MASS-02.5) **Towards Portable Elemental and Isotopic Analysis with Differential Mobility Coupled to Mass Spectrometry**

**Jacob Shelley**, Garrett MacLean, Ifeoluwa Ayodeji, Sunil Badal, Alexandra Keidel, Theresa Evans-Nguyen, *Rensselaer Polytechnic Institute, University of South Florida,*

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**23PAT03: Novel Process Analysis Technologies & Applications**, Southern Pacific E

Chair: Shawn Chen, *Dow*

(PAT-03.1) **Real-Time Monitoring of Polymer Manufacturing Process Using Optical Spectroscopy.**

**Arindom Saha**, *tec5USA, Inc.*

(PAT-03.2) **Real-time Online Nanoparticle Size Monitoring During Wet Bead Milling With a Microdilution Device**

**Nick Koumakis**, Carl Schuurmans, Remy Van Tuijn, Marko Verbeek, Michiel Damen, Rut Besseling, Ad Gerich, *InProcess-LSP*

(PAT-03.3) **In Situ Infrared Spectroscopy of a Cementitious Material**

**Mark Rickard**, Kyoung moo Koh, Stephane Costeux, *DuPont*

(PAT-03.4) **Solid-state Raman - the ideal process analytical technology for monitoring & control of industrial fermentation processes**

**Brian Marquardt**, John Richmond, Thomas Dearing, *MarqMetrix Inc.*

(PAT-03.5) **Fiber spectroscopy in-line for PAT by different methods in 0.3-16µm range**

**Viacheslav Artyushenko**, *Art Photonics Gmbh*

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**23PMA04: Nanomedicine Applications**, Southern Pacific D

Chair: Zahra Rattray, *University Of Strathclyde*

(PMA-04.1) **Analytical Pipelines for Profiling Nanomedicine Biological Interactions**

Karim Daramy, MS Panida Punnabhum, Callum Davidson, Ms Rand Abdulrahman, **Zahra Rattray**, *University Of Strathclyde*



**(PMA-04.2) Field Flow Fractionation Applications For The Analysis Of Nanomaterials For Health**

**Panida Punnabhum**, Karim Daramy, Callum Davidson, Ms Rand Abdulrahman, Zahra Rattray, *University of Strathclyde*

**(PMA-04.3) Orthogonal Pipelines for Lipid Nanoparticle Evaluation**

**Callum Davidson**, Rand Abdulrahman, Panida Punnabhum, Yvonne Perrie, Zahra Rattray, *University of Strathclyde*

**(PMA-04.4) Investigating the Impact of Shear Flow on Polymeric Nanoparticle-Protein Interactions**

**Karim Daramy**, Panida Punnabhum, Yvonne Perrie, Zahra Rattray, *University of Strathclyde*

**(PMA-04.5) Raman Spectroscopy Characterization Methods for CVD-grown Graphene in Biosensors Applications**

**Elizabeth Legge**, Andrew Pollard, Andrew Wain, *National Physical Laboratory*

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**23RAM10: Low Frequency Raman**, Cascade 1

Chair: Robert Chimenti, *Texas A&M University*

**(RAM-10.1) THE BOSN PEAK AND HETEROGENEITIES IN LIQUIDS AND DISORDER SOLIDS**

**Alexei Sokolov**, *University of Tennessee*

**(RAM-10.2) -Withdrawn**

**(RAM-10.3) Kinetic Study of Rheology-Modified Interpenetrating Polymer Network (IPN) Resins Using Ultra-Low Frequency Raman**

**Alexandra Lehman-Chong**, Robert Chimenti, Jianwei Tu, Samuel Lofland, Joseph F. Stanzone, III, *Rowan University*

**(RAM-10.4) Catching nucleation in action by Raman and terahertz Raman spectroscopies**

**Mark Christie**, Jan Sefcik, Karen Faulds, *University Of Strathclyde*

**(RAM-10.5) Size effects in nanoparticles of WO<sub>3</sub>, Y<sub>2</sub>O<sub>3</sub>, and TiO<sub>2</sub>: quantum confinement**

**Sergey Mamedov**, *HORIBA Scientific*

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**23SPR03: Structuring Plasmonic Particles for Applications**, Cascade 4

Chair: Matthew Sheldon, *Texas A&M University*

**(SPR-03.1) Broad Spectral Range Linear and Circular Dichroism Responses of Gold and Aluminum Nanostructures**

**Jennifer Shumaker-Parry**, *University of Utah*

**(SPR-03.2) Tunable Gold and Aluminum Nanocrescents as a Platform for Circular Dichroism Spectroscopy**

**Anh Nguyen**, Jennifer Shumaker-Parry, *The University Of Utah*

**(SPR-03.3) A Novel Method for the Synthesis of Core-Satellite Plasmonic Nanostructures for Single Particle SERS and CARS**

**Sanjun Fan**, Brian Scarpitti, Zachary Schultz, *department of chemistry and biochemistry, The Ohio State University*

**(SPR-03.4) Polydopamine as a Versatile Tool to Develop Surface Enhanced Raman Scattering Substrates**

**Ahmed Mahmoud**, Alexandra Teixeira, Maria Sousa-Silva, Antonio Fernández, Sara Abalde-Cela, Lorena Diéguez, *NL - International Iberian Nanotechnology Laboratory (INL), RUBYnanomed LDA, Centro de Estudios Superiores Aloya*

## **TECHNICAL PROGRAM – TUESDAY, OCTOBER 10, 2023**

### **Awards and Plenary Lectures | 10:45AM – 12:00PM | Sierra 5**

**Plenary Sessions: FACSS Charles Mann Award for Applied Raman Spectroscopy; Juergen Popp**

**(PLEN-L2.1) Applied Raman spectroscopy for clinical diagnosis and therapy to fulfill currently unmet medical needs**

**Juergen Popp**, *Leibniz Institute of Photonic Technology*

**Plenary Sessions: RSC Joseph Black Award;**  
**Mathew Horrocks**

(PLEN-L2.2) **Visualizing neuroscience at the single-molecule level**

**Mathew Horrocks**, *The University of Edinburgh*

## TECHNICAL PROGRAM – TUESDAY, OCTOBER 9, 2023

### Oral Symposia | 1:30 PM - 3:10PM

**23ART03: Historic Perspective and Recent Advances in Art Analysis using Vibration Spectroscopy**, Southern Pacific F

Chair: Marc Vermeulen, *The National Archives*

(ART03.1) **Tales of Art and Raman Spectroscopy**

**Anastasia Rousaki**, *Ghent University, Raman Spectroscopy Research Group, Department of Chemistry*

(ART03.2) **A Well of Information: Mutli-Technical Studies of Della Robbia's Christ and the Samaritan Woman**

**Alicia McGeachy**, Elena Mars, Colleen Snyder, Gwen DePolo, Adrienne Gendron, Beth Edelstein, Marc Vermeulen, Marc Walton, *The Metropolitan Museum of Art, The University of Arizona, The Cleveland Museum of Art, Northwestern University, Harvard Art Museums, The National Archives, M+ Museum*

(ART03.2) **Innovations for rapid x-ray fluorescence and infrared chemical imaging of cultural heritage objects**

**Thomas Tague**, Michael Beauchaine, *Bruker Scientific, Llc, Bruker Nano*

(ART03.4) **Development Of Advanced Micro-SORS For Heritage Science**

**Alberto Lux**, Alessandra Botteon, Marco Realini, Pavel Matousek, Pietro Strobba, Claudia Conti, *CNR-ISPC, Rutherford Appleton Laboratory, University Of Cincinnati*

(ART03.5) **Using Vibrational Spectroscopic Imaging Techniques to Visualize Subsurfaces in Cultural Heritage Studies**

**Marc Vermeulen**, *The National Archives*

Co-Chair: Derrick Quarles, *Elemental Scientific, Inc.*

(ATOM-04.1) **Overcoming interferences in single event-ICP-MS**

**Martin Resano**, Maite Aramendía, Flávio Nakadi, Antonio Bazo, Raúl Garde, Javier Resano, Juan Carlos García-Mesa, Elisa Vereda Alonso, *Universidad De Zaragoza, Universidad de Málaga, University of Oviedo*

(ATOM-04.2) **Novel tools for the characterisation of micro- and nanostructures in biology and the environment**

**David Clases**, Thomas Lockwood, Lukas Schlatt, Marko Simic, Christian Neuper, Christian Hill, Raquel Gonzalez De Vega, *University Of Graz, University of Technology Sydney, Nu Instruments, Brave Analytics*

(ATOM-04.3) **Real-Life Applications of Single-Cell ICP-Mass Spectrometry in the Biomedical Sciences**

**Eduardo Bolea-Fernandez**, Tong Liu, Rinus Dejonghe, Mina Nikolić, Olivier De Wever, Kevin Braeckmans, Frank Vanhaecke, *University of Zaragoza, aGhent University, Department of Chemistry, Atomic & Mass Spectrometry (A&MS) research unit*

(ATOM-04.4) **Considerations for the Measurement of Individual Atmospheric Mineral Dust Particles Entrapped in Glacial Ice Cores by Single Particle Inductively Coupled Plasma Time of Flight Mass Spectrometry**

**Madeleine Lomax-Vogt**, Stanislav Kutuzov, Susan Welch, Lucas Carter, Paolo Gabrielli, Jonas Wielinski, Greg Lowry, Ryan Sullivan, John Olesik, *The Ohio State University, Italian Glaciological Committee, Carnegie Mellon University*

**23ATOM04: Single Particle and Single Cell ICPMS**, Central Pacific A/B/C

Chair: Antonio Montoro, *NIST*

(ATOM-04.5) **Comparison of Direct and Indirect Measures of Transport Efficiency in Single Particle ICP-MS**

**Antonio Montoro Bustos**, Karen Murphy, Lee Yu, Monique Johnson, Michael Winchester, *NIST*

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**23AWD04: FACSS Charles Mann Award Symposium Honoring Juergen Popp**, Sierra 5

Chair: Juergen Popp, *Leibniz Institute of Photonic Technology*

(AWD-04.1) **FLIM in Surgical Oncology**  
**Laura Marcu**, *University of California Davis*

(AWD-04.2) **Ultraviolet Raman spectroscopy as a novel approach for testing the stability of mRNA vaccine in situ**

**Igor Lednev**, Lamyaa Almeahmadi, Sergei Reverdatto, Vladimir Ermolenkov, Alexander Shekhtman, *University at Albany, SUNY, University of Albany*

(AWD-04.3) **The Wonderful Land of Miniaturization in Near-Infrared Spectroscopy**

**Christian Huck**, *University Of Innsbruck, Institute Of Analytical Chemistry*

(AWD-04.4) **Spectroscopic Approaches to Biomedical Analysis**

**Duncan Graham**, Waleed Hassanain, William Tipping, Sian Sloan-Dennison, Karen Faulds *Spring SciX, University of Strathclyde*

(AWD-04.5) **Strategies for the Successful Implementation of Molecular Spectroscopy Across the Biopharmaceutical Value Chain**

**Andrew Whitley**, Linda Kidder, Sean Travers, Jeffrey Julien, *HORIBA*

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**23CHEM04: Chemometrics in Food and Agriculture**, Southern Pacific E

Chair: Mengliang Zhang, *Middle Tennessee State University*

(CHEM-04.1) **Authentication of Edible Oils Using an Infrared Spectral Library and Digital Sample Sets for Calibrated and Uncalibrated Adulterants**

**Barry Lavine**, DIsio Sota-Uba, Collin White, Karl S. Booksh, *Oklahoma State University, University of Delaware*

(CHEM-04.2) **Infrared Solutions for Rapid Sensing of Food Contaminants**

**Luis Rodriguez-saona**, *The Ohio State University*

(CHEM-04.3) **Use Of Chemometrics And Factorial Multivariate Analysis Of Variance For Identification Of The Impact of Genetics, Environment, Management, And Processing On Plant Food Composition**  
**James Harnly**, *US Department of Agriculture*

(CHEM-04.4) **Detection of Insect Infestation of Milled Grain-Focus on Tribolium castaneum**

**Rabi Musah**, Amy Osborne, Samira Beyramysoltan, *University At Albany-SUNY, GSK*

(CHEM-04.5) **Application of Self-Optimizing Support Vector Classifier-Radial Basis Function for Multivariate Classification of Maca Metabolomic Mass Spectral Profiles from China and Peru**

**Qudus Thanni**, Peter Harrington, *Ohio University*

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**23CTP/EARLY02: AMA: Women in Analytical Sciences**, Sierra 2

Chair: Andrea Locke, *Vanderbilt University Biophotonics Center*

(CTP-02.1) **An Imaging Chemist in a Cancer Biology World: (Scientific) Imagination, Life is Your Creation**

**Fay Nicolson**, *Dana-farber Cancer Insitute / Harvard Medical School*

(CTP-02.2) **A Scientific Journey From Scotland To Silicon Valley**

**Kristy McKeating**, *Google*

(CTP-02.3) **From Small Town to Big City: One Girl's Journey**

**Cristina Zavaleta**, *University Of Southern California*

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**23FORENS01: Nuclear Forensics**, Southern Pacific A/G

Chair: Robert Lascola, *Savannah River National Laboratory*

**(FORENS-01.1) Sensor fusion, experimental design, and chemometrics for monitoring uranium(VI) in the presence of lanthanides and corrosion products**

Luke Sadergaski, Hunter Andrews, Brandon Wilson, *Oak Ridge National Laboratory*

**(FORENS-01.2) On-Line Monitoring of Nitric Acid Concentration in Advanced Nuclear Fuel Reprocessing**

Catriona McFarlan, Alison Nordon, Mark Sarsfield, Robin Taylor, *University of Strathclyde, National Nuclear Laboratory, Sellafield, UK*

**(FORENS-01.3) Quantifying Dense Multicomponent Slurries with In-line ATR-FTIR and Raman Spectroscopy: A Hanford Case Study**

Rupanjali Prasad, Steven Crouse, Ronald Rousseau, Martha Grover, *Georgia Tech*

**(FORENS-01.4) Online Monitoring of Hydrogen Processing using Hollow Core Waveguide-Based Raman Spectroscopy**

John Kelly, Robert Lascola, *Savannah River National Laboratory*

**(FORENS-01.5) Cascading optical processes and their impacts on spectroscopic characterization of nanoscale or larger materials**

Dongmao Zhang, *Mississippi State University*

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**23IR04: Nanoscale IR in Bioscience**, Sierra 3

Chair: F. Simone Ruggeri, *Wagenigen University*

**(IR-04.1) Lipids Uniquely Alter the Secondary Structure and Toxicity of Amyloid beta 1-42 Aggregates.**

Dmitry Kurouski, *Mississippi State University*

**(IR-04.2) Effect of Co-Incubation with RNA on the Formation of Alphasynuclein Aggregates**

Antonia Intze, Jakob Rupert, Maria Eleonora Temperini, Raffaella Polito, Elsa Zacco, Gian Gaetano Tartaglia, Michele Ortolani, Valeria Giliberti, *Sapienza University Of Rome*,

*Centre for Human Technologies, Istituto Italiano di Tecnologia*

**(IR-04.3) Investigating the bacterial protein quality control system with AFM-IR nanospectroscopy**

Wouter Duverger, Grigoria Tsaka, Katerina Konstantoulea, Ladan Khodaparast, Laleh Khodaparast, Nikolaos Louros, Joost Schymkowitz, Frederic Rousseau, *Catholic University Leuven / Flemish Institute of Biotechnology*

**(IR-04.4) IR nanospectroscopy to investigate biomaterials: where do we stand?**

Ariane Deniset-besseau, Jérémie Mathurin, Margaux Petay, Dominique Bazin, Alexandre Dazzi, *Université Paris-saclay*

**(IR-04.5) Nanoscale Hyperspectral IR Characterization of Amyloid Proteins via IR PiFM**

Sung Park, Derek Nowak, Padraic O'Reilly *Molecular Vista*,

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**23LIBS01: The New LIBS Generation**,

Southern Pacific B/C

Chair: Hunter Andrews, *Oak Ridge National Laboratory*

**(LIBS-01.1) 3D Mapping of Uranium Absorption and Migration in Ex-vivo Human Skin with Femtosecond-LIBS and LA-ICP-MS**

Gregory Hull, Brian Jun, Jennifer Harris, Jeremy Inglis, *Los Alamos National Laboratory*,

**(LIBS-01.2) Nebulization-assisted LIBS as a potential tool for online analysis of liquids including complex halogen-containing samples**

Cristina Méndez-lópez, Luis Javier Fernández-Menéndez, Cristina González-Gago, Jorge Pisonero, Nerea Bordel, *Department Of Physics, University Of Oviedo*

**(LIBS-01.3) Optical Spectroscopy of Laser-Induced Plutonium Plasmas**

Emily Kwapis, Eliel Villa-Aleman, Kyle Hartig, *University Of Florida, Savannah River National Laboratory*

**(LIBS-01.4) Overview of LIBS Research at Oak Ridge National Laboratory**

**Hunter Andrews**, *Oak Ridge National Laboratory*

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**23PMA03: Tackling Critical Pharmaceutical Challenges with Advanced Spectral Analyses**, Southern Pacific D

Chair: Lydia Breckenridge, *Bristol Myers Squibb*

Co- Chair: Steve Bouffard, *Agilent Technologies*

**(PMA-03.1) Transmission Raman Spectroscopy Evaluating Process Induced Phase Transformation at Drug Substance/Drug Product Interface**

**Michelle Raikes**, Matthew McKay, Christian Reichardt, *Boehringer Ingelheim Pharmaceuticals*,

**(PMA-03.2) From Powder Pediatric In-Use Samples To Multi-Dose Tablets, Method Development And Validation Approaches For TRS In Drug Product**

**Greg Doddridge**, Yemin Liu, Eddie Hong, David Tan, Anh Nguyen, *Abbvie, The University Of Utah*

**(PMA-03.3) Leveraging the Versatility of Atomic Spectroscopy for Pharmaceutical Analysis**

**Lydia Breckenridge**, Sharla Wood, *Bristol Myers Squibb*

**(PMA-03.4) Advanced Imaging Methods For Studying Structure Morphology And Excipients Solid State Transformations In Pharmaceutical Multiparticulate Formulations**

**Elizabeth Legge**, Mark Stewart, Lourdes Contreras, Hannah Zhang, Dimitrios Tsikritsis, Natalie Belsey, Mark McAllister, John Richard Murphy, Ken Mingard, Caterina Minelli, *National Physical Laboratory, Pfizer Ltd, U.K.*

**(PMA-03.5) Use of High-Throughput Raman Spectroscopy for Tablet Coating PAT**

**Mark Kemper**, Shaun Fraser, Colin Couper, *Tornado Spectral Systems, Inc.*

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**23RAM04: SERS 3, Cascade 3**

Chair: Sian Sloan-Dennison, *University of Strathclyde*

Co-Chair: Royston Goodacre, *University of Liverpool*

**(RAM-04.1) Point Of Care Detection Of Drug Induced Liver Injury Using SERS-Based Lateral Flow Testing**

**Sian Sloan-Dennison**, Benjamin Clark, Kathleen Scullion, Paul Fineran, Joanne Mair, Dieter Bingemann, Cicely Rathmell, Jonathan Faircloth, David Creasey, James Dear, Karen Faulds, Duncan Graham, *University of Strathclyde, University of Edinburgh, Wasatch Photonics*

**(RAM-04.2) Neurotransmitter Sensing With Nanosensors for Dynamic Near Infrared Surface Enhanced Raman Spectroscopy**

**Ryma Boudries**, *Université de Montréal*

**(RAM-04.3) Ambient Focusing Ion Funnel-assisted Electrospray Deposition (ESD) of Gold Nanoparticles for Uniform and Highly Sensitive Surface-enhanced Raman Scattering (SERS)**

**Royston Goodacre**, Baris Akbali, Barry Smith, Cedric Boisdon, Boonphop Chaisrihwun, Kanet Wongravee, Tirayut Vilaivan, Cassio Lima, Chen-Han Huang, Tsan-Yao Chen, Simon Maher, *University of Liverpool, Chulalongkorn University, National Central University, National Tsing Hua University*

**(RAM-04.4) Dual SERS/colorimetric - RPA sensing platform for antibiotic resistance diagnosis**

**Waleed Hassanain**, Christopher Johnson, Karen Faulds, Neil Keegan, Duncan Graham, *University of Strathclyde, Newcastle University*

**(RAM-04.5) Colloidal SERS: The Do's and The Don'ts**

**Priyanka Dey**, *University of Portsmouth, UK*

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**23RAM09: Spatially Offset Raman Spectroscopy, Cascade 1**

Chair: Bhavya Sharma, *University Of Tennessee*

**(RAM-09.1) Imaging and Localisation of Nanoparticles in Tissue Using Surface Enhanced Spatially Offset Raman Spectroscopy**



**Karen Faulds**, Duncan Graham, Matthew Berry, Samantha McCabe, Sian Sloan-Dennison, Stacey Laing, Neil Shand, *University of Strathclyde*

(RAM-09.2) **Comparison of resonant and non-resonant reporter for the selection of brightest gold nanoparticles for Surface-enhanced Raman spectroscopy.**

**Megha Mehta**, *University Of Exeter*

(RAM-09.3) **Detecting changes in tissue hydration across different skin tones: a phantom study**

**Trevor Voss**, Anita Mahadevan-Jansen, *Vanderbilt University*,

(RAM-09.4) **SORS and SESORS how deep can we realistically sample?**

**Nick Stone**, Benjamin Gardner, Sara Mosca, Priyanka Dey, Megha Mehta, William Skinner, Francesca Palombo, Pavel Matousek, *University of Exeter, Ral, Stfc, Ukri, University of Portsmouth, UK*

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**23SPSJ03: NIR Spectroscopy (Basic Spectroscopy)**, Cascade 4

Chair: Akifumi Ikehata, *Food Research Institute, Naro*

Co-Chair: Krzysztof Bec, *University Of Innsbruck*

(SPSJ-03.1) **Interference Effects On Light-scattering Properties In Dense Colloidal Suspensions**

## TECHNICAL PROGRAM – TUESDAY, OCTOBER 9, 2023

### Oral Symposia | 3:50PM – 5:30PM

**23AES01: Bioanalysis**, Southern Pacific F

Chair: Juan Santiago, *Stanford University*

Co-Chair: Md Nazibul Islam, *Texas A&M University*

(AES-01.1) **Candida auris infection detection by dielectrophoresis**

**Negar Farhang Doost**, Soumya K Srivastava, Tagbo Niepa, *Shimane University, West Virginia University, Niepa*

(AES-01.2) **Device optimization for electrokinetic separation of microparticles**

**Hirovuki Fujii**, Hyeonwoo Na, Koyata Nishikawa, Kazumichi Kobayashi, Masao Watanabe, *Hokkaido University*

(SPSJ-03.2) **Sophisticated approach of NIR spectroscopy to agricultural and forest products**

**Satoru Tsuchikawa**, Te Ma, Tetsuya Inagaki, *Nagoya University*,

(SPSJ-03.3) **Combination of Near-infrared Spectroscopy with Other Fast Spectroscopic Methods to Improve Discrimination of Geographical Origins of Agricultural Products**

**Hoeil Chung**, Seongsoo Jeong, *Hanyang University*

(SPSJ-03.4) **Chemical Interpretation of Meaningful Variables in Chemometric Models by Theoretical Simulation - The Case of NIR Analysis of Pharmaceuticals**  
**Krzysztof Bec**, Justyna Grabska, Christian Huck, *University of Innsbruck*

(SPSJ-03.5) **Investigation on protein hydration and hydrogen bond network of water molecules induced by the secondary structural changes of proteins using near-infrared spectroscopy**

**Mika Ishigaki**, *Shimane University*

**Alaleh Vaghef Koodehi**, Patricia Cyr, Blanca H. Lapizco-Encinas, *Rochester Institute of Technology*,

(AES-01.3) **The electrical properties and morphology of selected Candida strains**  
**Rodrigo Martinez-duarte**, Cora Bisbee, Max Vogel, Emma Barnett, Carly Hammond, Alexandra Smith, Alicia Baldwin, Aaron Toler, Michelle Propp, Shivam Yadav, Erin Henslee, *Clemson University, Wake Forest University*

(AES-01.4) **Characterization of Human Mesenchymal Stem Cells' Electrical**

**Properties using Light-Induced  
Dielectrophoresis**

**Kiara Lacy**, Samuel Salib, Mary Tran, Tunglin Tsai, Rominna Valentine, Herdeline Ardoña, Tayloria N.G. Adams, *University Of California Irvine*

**(AES-01.5) Dielectric Characterization of Various Cells under Microgravity**

**Sai Deepika Reddy Yaram**, Soumya K Srivastava, *West Virginia University*

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**23ATOM02: Metallomics Based**

**Applications**, Central Pacific A/B/C

Chair: Derrick Qurles, *Elemental Scientific*

**(ATOM-02.1) Multimodal Approaches for Fully Quantitative Elemental Bioimaging Using Synchrotron Based X-ray Fluorescence Microscopy (SXFM) and LA-ICP-TOF-MS**

**Keith Macrenaris**, Andrew Crawford, David Zee, Qiaoling Jin, Thomas O'Halloran, *Michigan State University, Northwestern University, Argonne National Laboratory*

**(ATOM-02.2) Elemental Analysis in Biological Material**

**Martina Ralle**, Sophia Miller, *Oregon Health And Science University*

**(ATOM-02.3) Fluorine mapping in biological and geological specimens by LA-ICP-MS**

**Raquel Gonzalez De Vega**, David Clases, John Parnell, Jörg Feldmann, *University Of Graz, University of Aberdeen*

**(ATOM-02.4) Screening of Bromine Species in Enzymatically Digested DNA Samples Using a Fast and Automated Separation and Quantification IC-ICP-MS Method**

**Catharina Erbacher**, Nils Flothkötter, Marcel Macke, Derrick Quarles Jr., Michael Sperling, Jens Müller, Uwe Karst, *University of Münster, Elemental Scientific*

**(ATOM-02.5) Optimization of Quantification in Single Cell ICP-MS**

**Alexander Köhrer**, Matthias Elinkmann, C. Derrick Quarles, Michael Sperling, Uwe Karst, *University Of Münster*

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**23AWD05: RSC Joseph Black Award Symposium Honoring Mathew Horrocks,**

Sierra 5

Chair: Mathew Horrocks, *University Of Edinburgh, School Of Chemistry*

**(AWD-05.1) Using Peptides to Look at Proteins: Developing Peptide-based Imaging Modalities**

**Zuzanna Konieczna**, Fabio De Moliner, Lorena Mendive-Tapia, Zoe Gidden, Katie Morris, Takeshi Kaizuka, Marc Vendrell, Mathew Horrocks, *University Of Edinburgh*

**(AWD-05.2) -Withdrawn**

**(AWD-05.3) Surface enhanced Raman sensors for monitoring responses of tissue models derived from stem cells.**

**Colin Campbell**, William Skinner, Bilgi Kip, Peter Robinson, Mariska Simpson, Robert Gray, *University Of Edinburgh, University of Exeter, MassCare Ltd,*

**(AWD-05.4) High-Resolution Imaging of CSF Circulation in the Brain Parenchyma and Meninges**

**Juan Alberto Varela**, *University Of St Andrews*

**(AWD-05.5) Nano Single-molecule Two-color Aggregate Pull-down (Nano-STAPull) Technique: Highly Specific and Sensitive Detection for Early Stage Oligomeric Species in Neurodegenerative Diseases**

**Ji-Eun Lee**, Rebecca Saleeb, Craig Leighton, Judi O'Shaughnessy, Kiani Jeacock, Alexandre Chappard, Robyn Cumberland, Sarah Ball, Margaret Sunde, David Clarke, Kristin Piché, Jacob McPhail, Ariel Louwrier, Rachel Angers, Sonia Gandhi, Patrick Downy, Tilo Kunath, Mathew Horrocks, *The University of Edinburgh, The University of Sydney, Stressmarq Biosciences Inc., UCB Biopharma S.P.R.L., 1) The Francis Crick Institute, 2) UCL Queen Square Institute of Neurology, 3) 8Aligning Science Across Parkinson's (ASA)*

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**23BIM03: Point-of-Care Technologies for Biomedical Applications**, Sierra 2

Chair: Karina Weber, *Leibniz Institute Of Photonic Technology, Albert-Einstein-Straße 9, 07745 Jena, Germany*

**(BIM-03.1) Novel blood diagnostics using Raman spectroscopy at the point-of-care**  
Anja Silge, Anuradha Ramoji, Aikaterini Pistiki, Ute Neugebauer, Iwan Schie, Richard Grohs, Alexander Wiede, Uwe Glaser, Oleg Ryabchykov, Franziska Hornung, Karina Weber, Stefanie Deinhardt-Emmer, Bettina Löffler, Juergen Popp, *Leibniz Institute of Photonic Technology, Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller University, Ernst-Abbe-Hochschule, University of Applied Sciences, Fachbereich Medizintechnik und Biotechnologie, Carl-Zeiss-Promena, Jena University Hospital, Institute of Medical Microbiology, and Center for Infectious Diseases and Infection Control*

**(BIM-03.2) Visible-, Near-Infrared and Raman Spectroscopic Imaging Data Fusion for Point-of-Care Diagnostics**  
Christian Huck, *University Of Innsbruck, Institute Of Analytical Chemistry*

**(BIM-03.3) AI-enabled detector array for deeper vision and sensing beyond the limit**  
Saif Islam, Laura Marcu, *Univ of California Davis*

**(BIM-03.4) Towards Determining Amyloid Fibril Structures Using Experimental Constraints from Raman Spectroscopy**  
Madeline Harper, Uma Nudurupati, Riley Workman, Taras Lakoba, Delaney Nelson, Nicholas Perez, Yangguang Ou, David Punihaole, *University of California Davis, University of Vermont, Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch*

**(BIM-03.5) Rapid diagnosis of fibromyalgia disorder and other rheumatologic syndromes by portable mid-infrared spectroscopy combined with chemometric analysis**  
Shreya Nuguri, Luis Rodriguez-saona, *The Ohio State University*

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**23IR09: Two-Dimensional Correlation Spectroscopy, Sierra 3**

Chair: Young Mee Jung, *Kangwon National University, South Korea*  
Co-Chair: Isao Noda, *University of Delaware*

**(IR-09.1) Enhanced Spectral Resolution and 2D-COS**  
Isao Noda, *University of Delaware*

**(IR-09.2) Characterization of Silicone Rubber under Electrical, Chemical, and Thermal Stress**  
Kavin Darshan, Aruna Kumarasiri, Mosfeq Uddin, Harpreet Kaur, Rajkumar Padmawar, Dennis Hore, *ASAssoft, University of Victoria,*

**(IR-09.3) Investigation of bread staling by handheld NIR spectroscopy in tandem with 2D-COS and MCR-ALS analysis**  
Heinz Siesler, Marina De Gea Neves, Isao Noda, *Department of Physical Chemistry, University Duisburg-Essen, University of Delaware*

**(IR-09.4) Quantum Cascade Laser Microscopy And Two-Dimensional Correlation Algorithms: A Powerful Combination For The Characterization Of Therapeutic Proteins**  
Belinda Pastrana, Elizabeth Culyba, Sherly Nieves, Steve Sazinsky, Eduardo Canto, Isao Noda, *Protein Dynamic Solutions, Inc. Verseau Therapeutics, Inc, Auxilio Mutuo Hospital, University of Delaware*

**(IR-09.5) Polarized Raman Microscope Studies of Spherulites in Thin PHA Films as a Means to Further Characterize Crystallization Mechanisms**  
Fran Adar, Isao Noda, *HORIBA Scientific, University of Delaware*

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**23MASS03: 50 Years in Mass Spectrometry, Southern Pacific A/G**  
Chair: Benjamin Garcia, *Washington University School Of Medicine In St. Louis*

**(MASS-03.1) Development of new tools for RNA modification analysis by MS**  
Benjamin Garcia, *Washington University School Of Medicine In St. Louis*

**(MASS-03.2) The glycomics of food**  
Carlito Lebrilla, *University Of California, Davis*

(MASS-03.3) **Unraveling the Spatial Lipidome Using Gas-phase Ion/ion Reactions**  
**Boone Prentice**, *University Of Florida*

(MASS-03.4) **Functional Group-selective Ion-molecule Reactions in Structural Characterization of Drug Metabolites and Degradation Products by Tandem Mass Spectrometry**  
**Hilkka Kenttamaa**, *Purdue University*

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**23PAT05: PAT Coblenz: Machine Learning**, Southern Pacific E  
Chair: James Rydzak, *Specere Consulting*  
Co-Chair: Barry Wise, *Eigenvector Research, Inc.*

(PAT-05.1) **Getting "lean" on monitoring your process: the value proposition of "machine learning" for early-phased development**  
**Zhenqi (Pete) Shi**, *Senior Principal Scientist*

(PAT-05.2) **Evaluation of Machine Learning Techniques for PAT applications**  
**Larry McDermott**, Gregory McLaughlin, Meredith Brown, Massoud Ghasemzadeh-Barvarz, Rajesh Morampudi, Sean Daughtry, *Vertex Pharmaceuticals*

(PAT-05.3) **Machine Learning Based Vision System For Tablet Elegance**  
**Yong Mei**, *Pfizer*

(PAT-05.4) **Locally Weighted Regression Revisited**  
**Barry M Wise**, Sean Roginski, Lyle W Lawrence, Donal O'Sullivan, Bob Roginski, *Eigenvector Research, Inc.*

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**23PMA07: Vibrational Spectroscopy in Developing Biologics & Cell and Gene Therapy**, Southern Pacific D  
Chair: Kevin Dahl, *Particlese*

(PMA-07.1) **Investigating The Physicochemical Properties Of Lipid Nanoparticles In Protein Containing Media**

**Rand Abdulrahman**, Panida Punnabhum, Callum Davidson, Karim Daramy, Yvonne Perrie, Zahra Rattray, *University Of Strathclyde*

(PMA-07.2) **Microbiology in minutes for the Pharmaceutical Industry: Could Raman spectroscopy be the solution to this challenge ?**

**Markus Lankers**, Oliver Valet, *MIBIC GmbH & Co KG*,

(PMA-07.3) **Real-time Monitoring of Protein Capture Chromatography Load Phase and Break-through Detection using High Throughput Process Raman Spectroscopy**  
**Shaun Fraser**, Mark Kemper, Colin Couper, *Tornado Spectral Systems*

(PMA-07.4) **The Intricacy of In-line Monitoring of Tween 80 in Protein Formulations**  
**Gregory Webster**, *Abbvie*

(PMA-07.5) **Opportunities and Challenges of Process Analytical Technology (PAT) in Bioprocessing 4.0**  
**Dhanuka Wasalathanthri**, *Bristol-Myers Squibb*

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**23RAM06: SERS – 50th Anniversary**, Cascade 3  
Chair: Duncan Graham, *University Of Strathclyde*

(RAM-06.1) **50 years of SERS and Scix**  
**Duncan Graham**, *University Of Strathclyde*

(RAM-06.2) **What We Learn from SERS**  
**Janina Kneipp**, *Humboldt Universität Zu Berlin*

(RAM-06.3) **SERS as a Healthcare Diagnostic Tool: Are We There Yet?**  
**Marc Porter**, *University Of Utah*

(RAM-06.4) **In vivo SERS biosensing for human health monitoring**  
**Bhavva Sharma**, *University Of Tennessee*

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**23RAM12: Raman Spectroscopy for Security and Forensics Purposes**, Cascade 1  
Chair: Igor Lednev, *University at Albany, SUNY*

Co-Chair: Lamyaa Almeahmadi, *Massachusetts Institute of Technology (MIT)*

**(RAM-12.1) Spectroscopic Analysis of Liquids and Airborne Particles**

**Karina Weber**, Dana Cialla-May, Juergen Popp, *Leibniz Institute Of Photonic Technology*,

**(RAM-12.2) Raman Spectroscopy as a Universal test for Body Fluid Identification: Method Validation vs. False Positives**

**Luis Perez Almodovar**, Igor Lednev, Lenka Halamkova, Marisia Fikiet, *University at Albany, SUNY, Texas Tech University, University of New Haven*

**(RAM-12.3) -Withdrawn**

**(RAM-12.4) Application of Raman Spectroscopy to the Forensic Analysis of Drugs**

**Sergey Mamedov**, *HORIBA Scientific*

**(RAM-12.5) Effect of Temperature and Time on the Stability of Drugs Contaminated Fingermarks Probed by Raman Spectroscopy**

**Mohamed O. Amin**, **Entesar Al-hetlani**, Igor

Lednev, *Kuwait University, University at Albany, SUNY*

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**23SPR01: Early Career Plasmonics**

**Researchers**, Cascade 4

Chair: Jean-Francois Masson, *Universite de Montreal*

**(SPR-01.1) Plasmonic Heating of Metallic Nanostructures: Comparing Bulk and Surface Temperatures**

**Gregory Wallace**, Jodie Fergusson, Amritpal Singh, Ewen Smith, Tell Tuttle, Karen Faulds, Duncan Graham, *University of Strathclyde*

**(SPR-01.2) Using Plasmonic Fibre Nanosensors to Probe Chemical Dynamics Essential for Cell Physiology**

**Malama Chisanga**, Haiyan Wu, Jean-Francois Masson, *University of Montreal*

**(SPR-01.3) From Water to Whisky: Golden Opportunities in Analysis with Plasmonic Particles**

Jennifer Gracie, Justin R Sperling, Alasdair W Clark, **William Peveler**, *University of Glasgow*

**(SPR-01.4) Highly ordered nanostars-based solid substrate for ultrasensitive SERS**

**Alexandre Chicharo**, Alexandra Teixeira, Maria Relvas, Marta Aranda-Palomer, Jérôme Borme, Lorena Diéguez, Sara Abalde-Cela, *INL - International Iberian Nanotechnology Laboratory*

**(SPR-01.5) Characterization of Mycobacterium Tuberculosis – Bacillus Calmette-Guerin Using Surface Enhanced Raman Spectroscopy**

**Timothy Yokley**, Andrea Locke, *Vanderbilt University*

## TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 11, 2023

### Oral Symposia | 8:00AM – 10:10AM

**23ART02: Analysis of Exotic Materials from Mummies to Mars**, Southern Pacific B/C

Chair: Mary Kate Donais, *ACS DAC*

**(ART02.1) Unravelling the Secrets of Egyptian Mummification using Vibrational Spectroscopy**

**Bayden Wood**, Janet Davey, Callum Gassner, Ankit Dodla, Magdalena Giergiel, *Monash*

*University, Victorian Institute of Forensic Science*,

**(ART02.2) Exotic Hardwood Species Classification using Network Guided Classification Schemes**

**William Gilbraith**, Karl S. Booksh, Caelin Celani, *Savannah River National Laboratory, University of Delaware*



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(ART02.3) **Making GANes in Wine Detection for Archaeological Ceramics**  
Vernon Stafford, Rachel Sparks, David Jenkins, *University of Tennessee, Knoxville*

(ART02.4) -Withdrawn

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**23AES06: AES Lifetime Achievement Award Symposium Honoring James Landers**, Southern Pacific F  
Chair: Christopher Easley, *Auburn University*

(AES-06.1) **High resolution DNA separation as the backbone for a portable genotyping system for human identification.**  
James Landers, *UVA*

(AES-06.2) **Using Electrical Circuit Analogies to Design Plug-and-Play 3D-Printed Pneumatic Logic Gates and Oscillators for Microfluidic Flow Control**  
Christopher Easley, Joanne Seow, Md Mohibullah, *Auburn University*

(AES-06.3) **Microfluidic Analytical Systems For Assaying Dynamic Cellular Secretions**  
Michael Roper, *Florida State University*

(AES-06.4) **Use of Electroosmotic Flow in Brain Tissue for Biochemical Measurements**  
Stephen Weber, Tingyuan Xu, *University Of Pittsburgh*,

(AES-06.5) **Bioanalytical applications of microchip electrophoresis**  
Susan Lunte, *University Of Kansas*

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**23ATOM06: Common Strategies for LA-ICP-MS and LIBS**, Central Pacific A/B/C  
Chair: Matthieu Baudalet, *University Of Central Florida*  
Co-Chair: Mauro Martinez, *Icahn School Of Medicine At Mount Sinai*

(ATOM-06.1) **LIBS and Visible/Near Infrared Spectroscopy on Mars**  
Valerie Payre *University of Iowa*

(ATOM-06.2) **New approaches of laser induced breakdown spectroscopy (LIBS) for imaging in medicine.**  
Mauro Martinez, Manish Arora, Christine Austin, *Icahn School Of Medicine At Mount Sinai*

(ATOM-06.3) **Synthesis and characterization of matrix-matched standard for laser-ablation-based analysis of hair**  
Matthieu Baudalet, Kaitlyn Bonilla, Charlene Harris, Chloe Phillips, *University Of Central Florida*

(ATOM-06.4) **Analysis of lithium-ion battery materials by Laser-Induced Breakdown Spectroscopy (LIBS) and Laser Ablation-Inductively Coupled Plasma Mass Spectrometry (LA-ICPMS)**  
C. Derrick Quarles, Ross Coenen, *Elemental Scientific, Inc.*

(ATOM-06.5) **Detection of uranium in complex matrices via laser-based sampling**  
Benjamin Manard, Hunter Andrews, C. Derrick Quarles, Tyler Spano, Daniel Dunlap, Veronica Bradley, N. Alex Zirakparvar, Cole Hexel, *Oak Ridge National Laboratory, Elemental Scientific, Inc.*

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**23BIM02: Translating Multimodal Imaging Technologies into Routine Clinical Practice: Where do we Stand?**, Sierra 2  
Chair: Juergen Popp, *Leibniz Institute of Photonic Technology*

(BIM-02.1) **Realizing the utility of infrared spectroscopic imaging for cancer pathology**  
Rohit Bhargava, Kevin Yeh, Kianoush Falahkheirkhah, *University of Illinois at Urbana-Champaign*,

(BIM-02.2) **Challenges and opportunity in translating in vivo Raman spectroscopy for clinical applications**  
Anita Mahadevan-Jansen, *Vanderbilt University*

(BIM-02.3) **Intraoperative tumor characterization via multimodal imaging**  
Juergen Popp, *Leibniz Institute of Photonic Technology*

(BIM-02.4) **In vivo bond-selective imaging by en-face detected mid-infrared photothermal microscopy**  
Mingsheng Li, Hongli Ni, Jiaze Yin, Hongjian He, Yuhao Yuan, Guo Chen, Ji-Xin Cheng, *Boston University*

(BIM-02.5) **Single-cell mid-IR Spectroscopy of the Disease Affected Neurons in Brain Tissue using Fluorescence-Detected Photothermal Imaging**  
Aleksandr Razumtcev, Aris Polyzos, Hans Bechtel, Garth Simpson, *Purdue University*, *Lawrence Berkeley National Laboratory*

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**23FORENS04: International Mail Security**, Southern Pacific A/G  
Chair: Adam Lanzarotta, *Us Food And Drug Administration*  
Co-Chair: Bhavik Vyas, *University at Albany*

(FORENS-04.1) **Analysis of FDA-Regulated Products for Drugs at International Mail Facilities**  
Sara Kern, Adam Lanzarotta, JaCinta Batson, Michael Thatcher, Martin Kimani, Lisa Lorenz, Brian Boyd, Melissa Collins, Anvi Patel, Julio Arrecis, Kelsey Griffin, Fernando Gonzalez, Gregory Howe, Morgan Hudson-Davis, Mark Loh, Flavia Morales, Megan Sterling, Allison Reimer, Anthony Wetherby, Muhammad Altaf, David Laguerre, Donna LaGarde, Valerie Toomey, *Us Food And Drug Administration*

(FORENS-04.2) **Statistical Tools to Identify Reliable Discriminating Ions of Structurally Similar Fentanyl Analogs**  
Isaac Willis, Victoria L. McGuffin, Ruth Smith, *Michigan State University*

(FORENS-04.3) **Chemical Authentication and Determination of Composition of Counterfeit Drug Products**  
Scott Huffman, *Bristol Myers Squibb*

(FORENS-04.4) **Integration of LC-MS and DART-MS in Routine Investigations of Suspected Counterfeit Pharmaceutical Drug Products and Product Quality Complaints**  
Mark Wang, Scott Huffman, Ravi Kalyanaraman, *Bristol Myers Squibb*

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**23IR05: Nanoscale IR Spectroscopy Theory and Applications**, Sierra 3  
Chair: Andrea Centrone, *Nist*

(IR-05.1) **NULL-DEFLECTION SCANNING PROBE INFRARED (NDIR) SPECTROSCOPIC IMAGING: FROM ANALYTICAL MODELS TO APPLICATIONS**  
Seth Kenkel, Rohit Bhargava, *University of Illinois at Urbana-Champaign*

(IR-05.2) -Withdrawn

(IR-05.3) **Understanding Cantilever Transduction Efficiency and Spatial Resolution in Nanoscale Infrared Microscopy**  
JEFFREY SCHWARTZ, Georges Pavlidis, Andrea Centrone, *University of Maryland & NIST*, *University of Connecticut & NIST*

(IR-05.4) **Spectroscopy and Imaging of Optical Near-fields on Individual Plasmonic Nanoparticles via Visible PiFM**  
Sung Park, Derek Nowak, *Molecular Vista*

(IR-05.5) **Photothermal Nanoscale Mid-IR Imaging - the Good, the Bad, the Ugly**  
Georg Ramer, Ufuk Yilmaz, Lena Neubauer, Nikolaus Hondl, Elisabeth Holub, Yide Zhang, A. Catarina V. D. dos Santos, Bernhard Lendl, *TU Wien*

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**23IR10: Instrumental Advances for Mid-IR Spectroscopy**, Sierra 5  
Chair: Young Jong Lee, *National Institute Of Standards And Technology*  
Co-Chair: Bernhard Lendl, *Technische Universität Wien*

(IR-10.1) **Towards mid-IR photothermal lens spectroscopy for the analysis of liquids**  
Gustavo Vinicius Bassi Lukasiewicz, Elizandra Sehn, Alicja Dabrowska, Hongtu Cheng, *UTFPR / TU Wien*, *Technische Universität Wien*

(IR-10.2) **High-Sensitivity Infrared Absorption Spectroscopy for Aqueous Protein Solutions**

**Seongmin Kim**, Yow-Ren Chang, Young Jong Lee, *National Institute of Standards And Technology*

(IR-10.3) **Reading In-Between Spectra: Exploiting Laser-Based Mid-Infrared Spectroscopy with Chemometrics As A Tool to Study Continuous Unfolding of Proteins**  
**Shilpa Vijayakumar**, Andreas Schwaighofer, Georg Ramer, Bernhard Lendl, *Technische Universität Vienna*

(IR-10.4) **Capillary Absorption Spectrometer (CAS) with Gas Chromatograph and Reactor for High Sensitivity Compound Specific Isotope Analysis**

**Jason Kriesel**, Emre Ozen, Kaori Emerson-Shurilla, Andrew Fahrland, *OKSI / Guiding Photonics, OKSI*

(IR-10.5) **High-Speed Infrared Spectroscopy and Analysis in Combustion Studies Using Swept-Wavelength External Cavity Quantum Cascade Lasers**

**Mark Phillips**, Austin Butler, Nick Glumac, Michael DeMagistris, Morgan Ruesch, Andrea Zambon, Neeraj Sinha, *University Of Arizona, University of Illinois at Urbana-Champaign, Combustion Research and Flow Technology, Inc. (CRAFT Tech)*

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**23PAT04: In Situ Spectroscopy for industrial R&D**, Southern Pacific E  
Chair: Mark Rickard, *DuPont*

(PAT-04.1) **Optimization-Based Strategies for Spectral Analysis and Kinetic Modeling**

**Xiaoyun Chen**, Thomas Krumpolc, Daniel Trahan, Lorenz Biegler, Michael Wang, *Dow, Carnegie Mellon University*

(PAT-04.2) **In Situ IR Study on Polyurethane Reactions**

**William Wang**, Lin Liu, Jake Grewe, *Lubrizol*

(PAT-04.3) **Mesoporous Materials and Mid-Infrared Spectroscopy for the Trace Monitoring of Contaminants in Process Analytical Technology**

**Felix Frank**, Bettina Baumgartner, Mattias Verstuyft, Nuria Teigell Beneitez, Dominik Wacht, Mauro David, Elsa Traxler, Borislav Hinkov, Dries Van Thourhout, Bernhard Lendl,

*Tu Wien, Utrecht University, Ghent University-imec*

(PAT-04.4) **Measurement of Nitrogen-Containing Compounds and Oxyanions in Industrial Wastewater using High-Throughput Raman Spectroscopy**

Colin Couper, **Shaun Fraser**, Mark Kemper, *Tornado Spectral Systems*

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**23PMA06: Emerging Plasmonic Nanoparticles for Drugs and Pharmaceutical Analysis**, Southern Pacific D  
Chair: Malama Chisanga, *Universite de Montreal*

(PMA-06.1) **Functionalized SERS sensors for the detection and quantitative analysis of narcotics**

**Li-lin Tay**, *National Research Council Canada*

(PMA-06.2) **SERS Biosensors for Early Diagnosis and Treatment Guidance in Plants**

**Pietro Strobbia**, *University Of Cincinnati*

(PMA-06.3) **Tailoring The Nanoparticle Surface For The SERS Detection Of Drugs And Biological Analytes**

**Chiara Deriu**, Laura Fabris, *Politecnico di Torino*

(PMA-06.4) - Withdrawn

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**23RAM11: Raman Standards**, Cascade 3  
Chair: Aaron Urbas, *National Institute of Standards and Technology*

(RAM-11.1) **Semiconducting Nanowires for Metrological Calibration of Spatial Resolution in Raman Microscopy**

**Sebastian Wood**, *National Physical Laboratory*

(RAM-11.2) **Raman Data with CHARISMA**  
**Enrique Lozano**, *ELODIZ Ltd*

**(RAM-11.3) The Influence of Molecular Structure on the Raman Spectral Pattern and Reproducibility of Per- and Polyfluoroalkyl Substances in Liquid Extracts**

**Seo Won Cho**, Christina Remucal, Haoran Wei, *University of Wisconsin-Madison*

**(RAM-11.4) Renewal, Revision and Modernization of the ASTM E13.08 Raman Spectroscopy Standards**

**Li-lin Tay** *National Research Council Canada*

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**23SPECIAL02: Spectrochimica Acta B - Award Session, Cascade 1**

Chair: Alessandro De Giacomo, *University of Bari*

**(SPEC-02.1) Novel types of biomedical ICP-MS applications**

**Frank Vanhaecke**, Lana Abou-Zeid, Eduardo Bolea-Fernandez, Marta Costas-Rodriguez, Rinus Dejonghe, Rosa Grigoryan, Kasper Hobin, Tong Liu, Mina Nikolic, Kaj Sullivan, Ir. Thibaut Van Acker, Tom Van Helden, *Ghent University, University Of Zaragoza, University of Vigo*

**(SPEC-02.2) A Compilation of Landmark Publications in Analytical Atomic Spectrometry**

**George Chan**, Gary Hieftje, Nicolás Omenetto, *Lawrence Berkeley National Laboratory, Indiana University, University of Florida*

**(SPEC-02.3) Advances On Micro Laser Induced Breakdown Spectroscopy And Micro X-Ray Fluorescence Mineralogical And Elemental Quantitative Imaging**

**Cecile Fabre**, Kimberly Trebus, Alexandre Tarantola, Jean Cauzid, Vincent Motto-Ros, Panagiotis Voudouris, *Georessources, Carleton University, ILM, University of Athens*

**(SPEC-02.4) The Crucial Role of Molecular Emissions on LIBS Differentiation of Organic Compounds of Interest in Astrobiology under a Mars Simulated Atmosphere**

**Javier Laserna**, Laura Garcia-Gomez, Tomas Delgado, Francisco Javier Fortes, Luisa Cabalin, *Universidad de Malaga*

**(SPEC-02.5) Quantification of Major Elements in Rocks and Soils on Mars with SuperCam Laser-Induced Breakdown Spectroscopy (LIBS)**

**Ryan Anderson**, Paolo Pilleri, Travis Gabriel, Olivier Forni, Agnes Cousin, Roger Wiens, Sam Clegg, Jens Frydenvang, Ann Ollila, Susanne Schröder, Olivier Beyssac, Erin Gibbons, David Vogt, Elise Clavé, Jose-Antonio Manrique, Carey Leggett IV, Raymond Newell, Joseph Sarrao, Sylvestre Maurice, Shiv Sharma, The SuperCam Team, *Usgs Astrogeology, Institut de Recherche en Astrophysique et Planetologie, Purdue University, Los Alamos National Laboratory, University of Copenhagen, Deutsches Zentrum für Luft- und Raumfahrt, Université Pierre et Marie Curie, McGill University, Universidad de Valladolid, University of Hawaii*

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**23SPSJ04: NIR Spectroscopy (Applications), Cascade 4**

Chair: Christian W. Huck, *University Of Innsbruck, Institute Of Analytical Chemistry*  
Co-Chair: Mika Ishigaki, *Shimane University*

**(SPSJ-04.1) Handheld NIR spectroscopy: a non-destructive, rapid and informative technique for quality control in the materials- and life-sciences**

**Heinz Siesler**, Marina De Gea Neves, Hui Yan, *Department of Physical Chemistry, University Duisburg-Essen, Jiangsu University of Science and Technology*

**(SPSJ-04.2) Near-infrared spectral pattern classification of glycolytic reactions using oscillating reactions of yeast extracts**

**Akifumi Ikehata**, Miho Sesumi, *Food Research Institute*

**(SPSJ-04.3) Hyperspectral image data analytics with deep learning fusion-nets**

**Bosoon Park**, Taesung Shin, *U.S. Department of Agriculture, Agricultural Research Service, USDA, ARS*

**(SPSJ-04.4) Unleashing the Potential: Overcoming Hurdles to Make Vibrational Spectroscopy a Routine Diagnostic Tool**

**Bayden Wood**, John Adegoke, Karin Jandeleit-Dahm, Diana Bedolla, Phil Heraud, Adele Kinces, Keith Dias, *Monash University*

(SPSJ-04.5) Miniaturized NIR in Natural Products and Food Analysis - From Mechanistic Understanding to Framework Optimization

Justyna Grabska, Krzysztof Bec, Christian Huck, *University of Innsbruck*

## TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 11, 2023

### Awards and Plenary Lectures | 10:45AM – 12:00PM | Sierra 5

Plenary Sessions: NESAS and SAS Lester W. Strock Award; Maria Montes Bayon

(PLEN-L3.1) ICP-MS BASED STRATEGIES IN BIOMEDICINE: EXPANDING THE BOUNDARIES  
Maria Montes-Bayon, *University Of Oviedo*

Plenary Sessions: AES Mid-Career Achievement Award; Robbyn Anand

(PLEN-L3.2) Electrokinetic Enrichment of Analytes Integrated with Label-Free Electrochemical Sensing - Scale-up and Scaling Laws

Beatrise Berzina, Sungu Kim, Umesha Peramune, Kumar Saurabh, Sommer Osman, Echo Claus, Sanduni Devasinghe, Md Ruhul Amin, Madison Strait, Baskar Ganapathysubramanian, Robbyn Anand, *Iowa State University, Stanford University*

## TECHNICAL PROGRAM – WEDNESDAY, OCTOBER 9, 2023

### Oral Symposia | 1:30PM – 3:10PM

23AES07: 50th Anniversary, Southern Pacific F

Chair: Tayloria Adams, *University of California Irvine*

Co-Chair: Erin Henslee, *Wake Forest University*

(AES-07.1) Isotachophoresis theory and its application to sample preparation of nucleic acids

Juan Santiago, Ashwin Ramachandran, Charles Blanluet, Diego Huyke, Alexandre Avaro, *Stanford University*

(AES-07.2) Contactless Dielectrophoresis: History and Future Directions

Rafael Davalos, Josie Ducan, *Virginia Tech*

(AES-07.3) A History of Dielectrophoresis for Cell Characterization and Sorting

Lisa Flanagan, *University of California, Irvine*

(AES-07.4) Understanding Nonlinear Electrophoretic Effects in Microfluidic Devices

Blanca H. Lapizco-Encinas, *University of California, Irvine*

(AES-07.5) Women in Electrokinetics

Erin Henslee, Tayloria N.G. Adams, *Wake Forest University, University of California Irvine*

23ATOM07: Early Career in Atomic Spectroscopy, Central Pacific A/B/C

Chair: Benjamin Manard, *Oak Ridge National Laboratory*

(ATOM-07.1) Matrix-Matched Calibration Approaches for Quantitative Mapping of Various C-based Samples Using LA-ICP-MS

Ana Lores Padin, Ir. Thibaut Van Acker, Beatriz Fernández, Ana Rua Ibarz, Rosario Pereiro, Frank Vanhaecke, *Ghent University, University of Oviedo*



(ATOM-07.2) **An Early Career Perspective on Laser Ablation Plasma Spectroscopy for Nuclear Security Applications**  
Kyle Hartig, Emily Kwapis, Kyle Latty, Justin Borrero, *Univeristy Of Florida*

(ATOM-07.3) **Small Particles, Big Challenges: Comprehensive Multi-Elemental Analysis Of Discrete Samples Using ICP-TOFMS**  
Lyndsey Hendriks, *TOFWERK*

(ATOM-07.4) **Utilization of atomic spectroscopy at National Labs – an early career’s perspective**  
Benjamin Manard, *Oak Ridge National Laboratory*

(ATOM-07.5) **Building your own fs/ns-LIBS system - from desperation to success and everything in between**  
Cristina Méndez-lópez, Luis Javier Fernández-Menéndez, Cristina González-Gago, Jorge Pisonero, Nerea Bordel, *University Of Oviedo*,

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**23AWD06: NESAS and SAS Lester W. Strock Award Symposium Honoring Maria Montes-Bayón**, Cascade 1  
Chair: Maria Montes-Bayón, *University Of Oviedo*

(AWD-06.1) **A Personal Retrospective on the Analysis of Small Objects: Nanoparticles and Individual Cells**  
Jörg Bettmer, *University Of Oviedo*

(AWD-06.2) **Exploration Of A Nitrogen Plasma For The Analysis Of Laser-Generated Aerosols**  
Detlef Günther, Dylan Kaeser, Bodo Hattendorf, Joachim Koch, *Department Of Chemistry And Applied Biosciences*

(AWD-06.3) **Microwave-Enabled Ionization and Chemistries for Mass Spectrometry Analysis**  
Steven Ray, *SUNY Buffalo Dept of Chemistry*

(AWD-06.4) **Analysis of unconventional elements via ICP-MS: Targeting Carbon and Fluorine**  
Raquel Gonzalez De Vega, Jörg Feldmann, David Clases, *University Of Graz*

(AWD-06.5) **The Role of Data Analysis in Analytical Chemistry**  
Juris Meija, *NRC*

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**23AWD07: AES Mid-Career Achievement Award Symposium Honoring Robbyn Anand**, Sierra 5  
Chair: Robbyn Anand, *Iowa State University*

(AWD-07.1) **Simplified Valve Control and Droplet Merging System for Sampling and Multiplexed Secretion Assays from Ex Vivo Adipose Tissue**  
Christopher Easley, Andresa Bezerra, Md Moniruzzaman, Sabita Dangol, *Auburn University*,

(AWD-07.2) **Computationally Modeling Electrokinetic Phenomena: Complex Geometries and Small Electric Double Layers**  
Baskar Ganapathysubramanian, *Iowa State University*

(AWD-07.3) **Increasing Sensitivity and Selectivity of miRNA Analyses with Thermal Gel Electrophoresis**  
Thomas Linz, Mario Cornejo, *Wayne State University*

(AWD-07.4) **Characterizing micro- and nanoplastics in human body fluids with dielectrophoresis**  
Alexandra Ros, Timothy Long, Shulin Bu, *Arizona State University*

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**23BIM07: Biomedical Spectroscopy and Imaging (CLIRSPEC)**, Sierra 2  
Chair: Nike Stone, *University of Exeter*  
Co-Chair: Olga Eremina, *University Of Southern California*

(BIM-07.1) **A Comprehensive Strategy for SERS Multiplex Imaging and Analysis of the Tumor Microenvironment**  
Chrysafis Andreou, Konstantinos Plakas, Naxhije Berisha, Mathieu Gigoux, Suchetan Pal, Taha Merghoub, Michael Detty, Mortiz Kircher, *University Of Cyprus, University of Buffalo, Memorial Sloan Kettering Cancer*

*Center, Indian Institute Of Technology–Bhilai,  
Weill Cornell Medical School*

**(BIM-07.2) Cutting-Edge Biomarkers  
Discovery for Early Diagnosis of Central  
Sensitivity Syndromes Using Surface-  
Enhanced Raman Spectroscopy (SERS) and  
FTIR-Microscope**

**Haona Bao**, Siyu Yao, Silvia De Lamo  
Castellvi, Chelsea Goetzman, Zachary Schultz,  
Luis Rodriguez-saona, *The Ohio State  
University, Savannah River National Lab*

**(BIM-07.3) Characterization of Vaginal  
Fluid and Vaginal Lactobacillus using  
Raman Spectroscopy and Surface-Enhanced  
Raman Spectroscopy**

**Anna Rourke-Funderburg**, Andrea Locke,  
*Vanderbilt University*

**(BIM-07.4) Deep UV Raman spectroscopy  
for probing active eukaryotic viruses**

**Denis Rajnovic**, Fatima Matroodi, Igor  
Lednev, Lamyaa Almeahadi, Barbara Rossi,  
Claudio Masciovecchio, Alessandro Marcello,  
*Elettra-sincrotrone And ICGEB, University at  
Albany, SUNY*

**(BIM-07.5) Pharmacokinetic and  
Pharmacodynamic Tomography with  
Coherent Raman Imaging**

**Dandan Tu**, Conor Evans, *Massachusetts  
General Hospital, Wellman Center For  
Photomedicine, Mass. General Hospital,  
Harvard Medical School*

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**23CHEM05: Industrial/PAT Applications of  
Chemometrics**, Southern Pacific E

Chair: Brandye Smith-Goettler, *Merck & Co.,  
Inc*

**(CHEM-05.1) Comparison Of 3-Way And 2-  
Way Multivariate Models For The  
Assessment Of Data Generated By  
Multidimensional Fluorescence A-TEEM  
Method**

**Brad Swarbick**, *KAX Group Pty Ltd*

**(CHEM-05.2) External Variable Augmented  
Iterative Optimization Technology (EVA-  
IOT): A Minimal Calibration Robust  
Modeling Approach to Monitor Continuous  
Pharmaceutical Powder Streams**

**Natasha Velez-Silva**, Adam Rish, Carl  
Anderson, James K. Drennen, III, *Duquesne  
University*

**(CHEM-05.3) Demonstration of Novel Model  
Diagnostic Based on Net Analyte Signal for  
Iterative Optimization Technology  
Algorithms**

**Adam Rish**, Natasha Velez-Silva, Samuel  
Henson, Md. Nahid Hasan, James Drennen,  
Carl Anderson, *Duquesne University*

**(CHEM-05.4) Calibration-Free Blend  
Uniformity Monitoring and Active  
Pharmaceutical Ingredient Potency  
Detection: The Role of Iterative  
Optimization Technology in Continuous  
Manufacturing Systems**

**Samuel Henson**, Adam Rish, James Drennen,  
Carl Anderson, *Duquesne University*

**(CHEM-05.5) Integrating digital capabilities  
and data analytics for rapid resolution of  
manufacturing inefficiencies**

**Brandye Smith-Goettler**, *Merck & Co., Inc*

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**23IR12: Mid-IR Sensing Schemes Beyond  
Absorbance Spectroscopy**, Sierra 3

Chair: Bernhard Lendl, *Technische Universität  
Wien*

**(IR-12.1) Mid-Infrared Dispersion  
Spectroscopy – A New Avenue for Liquid  
Phase Analysis**

**Alicja Dabrowska**, Andreas Schwaighofer,  
Bernhard Lendl, *Technische Universität Wien*,

**(IR-12.2) IR Refraction Spectroscopy**

**Thomas Mayerhoefer**, Vladimir Ivanovski,  
Juergen Popp, *Leibniz Institute Of Photonic  
Technology, Ss. Cyril and Methodius  
University*

**(IR-12.3) Comparison of Attenuated Total  
Reflectance (ATR) to Reflectance Fourier  
Transform Infrared (FTIR) Spectra of  
Explosives for Real-Time FTIR -  
Differential Scanning Calorimetry (DSC)  
Measurements**

**Gregory Klunder**, Batikan Koroglu, Keith  
Coffee, Ana Racoveanu, Alan Burnham, John  
Reynolds, *Lawrence Livermore National  
Laboratory*

(IR-12.4) **High-Sensitivity IR Spectroscopy of Protein Drugs at Low Concentrations**  
**Young Jong Lee**, Seongmin Kim, *National Institute Of Standards And Technology*

(IR-12.5) **Non-Invasive Glucose Monitoring Techniques using QCL-IR Lasers**  
**Edeline Fotheringham**, Brock Koren, Taylor Stathopoulos, *DRS-Daylight Solutions*

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**23LIBS04: LIBS for Mining, Geology and Space**, Southern Pacific B/C  
Chair : Andressa Adame, *Institut National De La Recherche Scientifique (INRS)*  
Co-Chair: Aissa Harhira, *National Research Council Canada*

(LIBS-04.1) **SuperCam Laser-Induced Breakdown Spectroscopy (LIBS) Results from Jezero Crater, Mars**  
**Ryan Anderson**, Roger Wiens, Sylvestre Maurice, Arya Udry, Olivier Beyssac, Elise Clavé, Ann Ollila, Baptiste Chide, Benjamin Weiss, Shiv Sharma, The SuperCam Team, *USGS Astrogeology, Purdue University, IRAP, University of Nevada Las Vegas, Université Pierre et Marie Curie, DLR, Los Alamos National Laboratory, Massachusetts Institute of Technology, University of Hawaii*

(LIBS-04.2) **Analysis of Earthen-based Materials using LIBS**  
**Aissa Harhira**, Josette El Haddad, Paul Bouchard, Francis Vanier, Elton Soares de Lima Filho, Christian Padioleau, André Beauchesne, Antoine Hamel, Francis Boismenu, Daniel Gagnon, Mohamad Sabsabi, *National Research Council Canada*

(LIBS-04.3) **Validation of Laser-Induced Breakdown Spectroscopy assisted by Laser-Induced Fluorescence (LIBS-LIF) for the measurements of platinum and palladium in solid ore**  
Ismail Elhamdaoui, **Andressa Adame**, *Inrs*

(LIBS-04.4) **LIBS Analysis of Aerosolized Lithium Brines**  
**David Day**, Morgan Jennings, Agustin Loureiro, *Sciaps*

(LIBS-04.5) **Recent ChemCam Observations on the Curiosity Mars Rover**

**Sam Clegg**, The ChemCam Science Team, *Los Alamos National Laboratory*

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**23MASS04: Understanding Protein Structure with Mass Spectrometry**, Southern Pacific A/G  
Chair: Jared Shaw, *University Of Nebraska Lincoln*

(MASS-04.1) **Dissecting hierarchical organization of proteins and lipids organization in the membrane**  
**Kallol Gupta**, *Yale University*

(MASS-04.2) **Mass Spectrometric Characterization of Chemically and Natively Unfolded Proteins**  
**Ian Webb**, *Iupui*

(MASS-04.3) **Protein Complex Heterogeneity and Structure Revealed by Native Mass Spectrometry with Electron Capture Charge Reduction and Surface Induced Dissociation**  
**Jared Shaw**, Sophie Harvey, Chen Du, Vicki Wysocki, *University Of Nebraska Lincoln, The Ohio State University*

(MASS-04.4) **Marriage Between Native Mass Spectrometry and Cryo-EM for Structural Analysis of Membrane Proteins**  
**Weijing Liu**, Christopher Mullen, Donggyun Kim, Vadim Cherezov, Gregory Dodge, Barbara Imperiali, Hiruni Jayasekera, Michael Marty, Rosa Viner, *Thermo Fisher Scientific, University of Southern California, Massachusetts Institute of Technology, University of Arizona*

(MASS-04.5)

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**23PMA08: Small Molecule Analysis in Biopharma**, Southern Pacific D  
Chair: Karl Burgess, *University of Edinburgh*  
Co-Chair: Katherine Hollywood, *University Of Manchester*

**(PMA-08.1) An Automated Workflow For Global Metabolomics Of Complex Biological Samples**

Martina Pičmanová, Tessa Moses, Joan Cortada-Garcia, Ms Georgina Barrett, Hannah Florance, Sufyan Pandor, Karl Burgess, James Hutton Institute, Lonza, University of Edinburgh, Agilent Technologies

**(PMA-08.2) An Analytical Platform for Real-Time Monitoring of Biopharmaceutical Manufacturing Processes and Integration of a Raman Platform**

Maikel Gaitkoski, Noemi Dorival Garcia, Jonathan Bones, NIBRT,

**(PMA-08.3) Raman Spectroscopy to Detect Lentivirus in Living Human Cells**

Rheta Elkhaira, Keita Iwasaki, Kosuke Hashimoto, Hidetoshi Sato, Kwansei Gakuin University

**(PMA-08.4) Application of real-time metabolomics to CHO cell optimisation**

Luke Johnston, Mark Rendall, Jeff Keen, Karl Burgess, University Of Edinburgh, FUJIFILM Diosynth Biotechnologies

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**23RAM05: IRDG, Cascade 3**

Chair: Karen Faulds, University of Strathclyde

**(RAM-05.1) Exploring Pharmaceutical Formulation Structure Using 3D Raman Chemical Images**

Liam Davison-Gates, Don Clark, Fiona Clarke, Andrew Ewing, Pfizer

**(RAM-05.2) Enzyme-Activated Biorthogonal Raman Probes For Targeted Tumor Imaging**

Swati Tanwar, Behnaz, Piyush Raj, Aruna Singh, Lintong Wu, Dian Respati Arifin, Michael T McMahon, Jeff W.M. Bulte, Ishan Barman, Johns Hopkins University

**(RAM-05.3) Understanding Molecule-Metal Interactions through SERS**

Laura Fabris, Chiara Deriu, Shaila Thakur, Kaleigh M. R. Scher, Politecnico di Torino, Rutgers University

**(RAM-05.4) Design and Fabrication of Porous Silicon Nanoparticle Paper-based Sensor**

Huijin An, Rabeb Layouni, Sharon Weiss, Andrea Locke, Vanderbilt University

**(RAM-05.5) Transforming Healthcare Pathways By Screening Multiple Biomarkers Via SERS-Lateral Flow Immunoassays**

Benjamin Clark, Sian Sloan-Dennison, Kathleen Scullion, Karen Faulds, Duncan Graham, James Dear, Paul Fineran, Joanne Mair, David Creasey, Cicely Rathmell, Dieter Bingemann, Jonathan Faircloth, University Of Strathclyde, University of Edinburgh, Wasatch Photonics

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**23SPR05: Plasmonics and Sensing, Cascade 4**

Chair: Jennifer Shumaker-Parry, University of Utah

**(SPR-05.1) Probing SERS intensity fluctuations with high-speed acquisitions**

Alexandre Brolo, Nathan Lindquist, University of Victoria, Bethel Univesity

**(SPR-05.2) Detecting Fentanyl Analogs by Combining Surface-Enhanced Raman Spectroscopy (SERS) and Paper Spray Mass Spectrometry (PS-MS).**

Sevde Dogruer Erkok, Roxanne Gallois, Leon Leegwater, Pascal Camoiras Gonzalez, Arian van Asten, Bruce McCord, Florida International University, ENS of Lyon, University of Amsterdam

**(SPR-05.3) Towards Point-of-Care Methods for the Detection of Different Biomarkers in Blood Samples Using a Surface Plasmon Resonance (SPR) Sensor**

Caroline Dubois, Jean-Francois Masson, Danny Brouard, Jonathan Robidoux, Université de Montréal, Héma-Québec

(SPR-05.4) -Withdrawn

# TECHNICAL PROGRAM – THURSDAY, OCTOBER 12, 2023

Oral Symposia | 8:30AM – 10:10AM

## **23AES04: Emerging Leaders, Southern Pacific F**

Chair: Lisa Flanagan, *University of California, Irvine*

Co-Chair: Alan Jiang, *University of California, Irvine*

### **(AES-04.1) Paper-based Microchip Electrophoresis for Point-of-Care Infectious Disease Testing**

Yi Yang, **Ran An**, *University of Houston*

### **(AES-04.2) Electrokinetic Isolation of Protein Complexes from Single Cancer Cells**

Edgar E. Ruiz Bello, **Julea Vlassakis**, *Rice University*

### **(AES-04.3) On the use of nonlinear electrokinetics for cell separations**

**Alaleh Vaghef Koodehi**, Curran Dillis, Adrian Lomeli Martin, Blanca H. Lapizco-Encinas, Olivia D. Ernst, *Rochester Institute of Technology*

### **(AES-04.4) Integrated on-chip nucleic acid purification using isotachopheresis for sequencing applications**

**Crystal Han**, *San Jose State University*

### **(AES-04.5) Examining the biological properties of DEP-sorted mesenchymal stem cells (MSCs)**

**Alonso Stephany**, Zuri rashad, Sune Terbush, Kiara Lacy, Tayloria Adams, *UC Irvine*

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## **23ATOM09: Laser Ablation Based Atomic Spectroscopies: Fundamental and Applications, Central Pacific A/B/C**

Chair: Jorge Pisonero, *University of Oviedo*

Co-Chair: Ana Lores Padin, *University of Ghent*

### **(ATOM-09.1) Advancing microplastics characterization with laser ablation-single particle-inductively coupled plasma-mass spectrometry**

**Thibaut Van Acker**, Ana Rua Ibarz, Frank Vanhaecke, Eduardo Bolea-Fernandez, *Ghent University*

### **(ATOM-09.2) Single spot Rb-Sr isochron dating of micas by LA-MC-ICP-MS/MS**

**Alicia Cruz-Urbe**, Cemil Arkula, Grant Craig, Claudia Bouman Joshua Garber, *University Of Maine, ThermoFisher Scientific Bremen GmbH™, The Pennsylvania State University, Bence Paul, Elemental Scientific Lasers*

### **(ATOM-09.3) High Fidelity Imaging Of Earth Materials By Laser Ablation Inductively Coupled Plasma Time Of Flight Mass Spectrometry**

**John Cottle**, Andrew Kylander-Clark, Ciaran O'Connor, Robert Hutchinson, Lukas Schlatt, Phil Shaw *Nu Instruments, University Of California Santa Barbara, Elemental Scientific Lasers*

### **(ATOM-09.4) Fast full-elemental LA-ICP-MS: Using TOF-ICP-MS to easily gain a deep understanding of samples in a matter of minutes**

**Lukas Schlatt**, Phil Shaw, *Nu Instruments*

### **(ATOM-09.5) Dual-Comb Absorption Spectroscopy of Molecular Species in a Laser-Produced Plasma**

**Ryan Rhoades**, Ryland Wala, Jason Jones, John McCauley, Reagan Weeks, Sivanandan Harilal, Jeremy Yeak, Opiclah, Mark Phillips, *University of Arizona, Pacific Northwest National laboratory*

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## **23BIM05: Nanotheranostics: Diagnosis and Treatment of Disease Using Nanomaterials, Sierra 2**

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

### **(BIM-05.1) Endoscopic Surface Enhanced Spatially Offset Raman Spectroscopy for the Detection of Colorectal Cancer**

**Fay Nicolson**, Dana-farber Bohdan Andreiuk, Eunah Lee, Andrew Whitley, Scott Rudder, Samuel Mabbott, Kevin Haigis, *HORIBA Scientific, Texas A&m University, Cancer Insitute / Harvard Medical School, Optosigma*

### **(BIM-05.2) Novel Surface Modification and Time-Resolved Reading of Mn-Doped**



**Nanocrystal Signal Reporter for Enhanced Bioassay Sensitivity**

**Bryan Lee**, Gita Kharal, Benjamin Sreenan, Claire Lin, Xiaoshan Zhu, *University Of Nevada, Reno*

**(BIM-05.3) Point of care testing of blood coagulation using a smartphone**

Weiming Xu, Majed Althumayri, Amin Mohammad, **Hatice Ceylan Koydemir**, *Texas A&M University*

**(BIM-05.4) Automating the Design of a Catalytic SERS Sensor for the Detection of Disease Biomarkers**

**Steven Quarin**, Amanda Macke, Ruxandra Dima, Pietro Strobbia, *University Of Cincinnati*

**Combining Nanoparticle Photothermal Therapy with Surface-Enhanced Raman Scattering (SERS) Temperature Feedback**

**(BIM-05.5) William Skinner**, Renata L. Sala, Kamil Sokolowski, Oren A. Scherman, Jeremy J. Baumberg, Benjamin Gardner, Pavel Matousek, Nick Stone, *University of Exeter*

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**23CHEM06: Improvements in Field Sensing with Chemometrics**, Southern Pacific B/C  
Chair: Caelin Celani, *University of Delaware*

**(CHEM-06.1) A Comparison of 3 Chemical Tools for Identifying the Geographic Region of Pinus ponderosa**

**Erin McClure-Price**, Pamela McClure, Edgar Espinoza, James A. Jordan, Ty Coplen, *US Fish and Wildlife Forensics Laboratory, US Geological Survey*

**(CHEM-06.2) Portable Instrumentation - Inside the Black Box**

**Suzanne Schreyer**, *Rigaku Analytical Devices*

**(CHEM-06.3) Field studies of monumental paintings: exploring the trade-off between high spatial sampling at lower spectral resolution and range versus lower spatial sampling and higher spectral resolution and range for materials identification and chemical mapping**

**Roxanne Radpour**, John Delaney, *National Gallery Of Art, Ioanna Kakoulli, University of California, Los Angeles*

**(CHEM-06.4) Surface enhanced Raman scattering (SERS) sensors: combining machine learning and nanosciences**

**Jean-Francois Masson**, *Universite de Montreal*

**(CHEM-06.5) Using X-ray diffraction for the development of a reference methodology to validate chemometric models for quantifying respirable quartz by infrared spectroscopy**

**Rachel Walker**, Cody Wolfe, Milan Yekich, Emanuele Cauda, *National Institute For Occupational Safety And Health*

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**23CTP/EARLY01: New Approaches in Instrumentation and Software Design**, Sierra 5

Chair: Alexis Weber, *University at Albany*  
Co-Chair: Francis Esmonde-White, *Esmonde-White Technologies, LLC*

**(CTP-01.1) Determination of Broadband-Light Atomic Absorption through Interferometric Spectrometry with a Spatial Heterodyne Spectrometer**

**Yi You**, Xunyu Li, Jens Riedel, *Federal Institute For Materials Research And Testing (bam)*

**(CTP-01.2) Developing real-time solutions for quantification of protein in edible insect powders**

**Silvia De Lamo Castellvi**, Carmen Mendez, Celeste Aurora Matos Gonzalez, Yalan Wu, Luis Rodriguez-saona, *The Ohio State University, The Ohio State University-Universitat Rovira i Virgili*,

**(CTP-01.3) Portable Shifted Excitation Raman Difference Spectroscopy -Capability for On-Site Analysis on Solids, Liquids and Gases**

**Martin Maiwald**, Kay Sowoidnich, André Müller, Bernd Sumpf, *Ferdinand-Braun-Institut*

**(CTP-01.4) Single-particle analysis using time-of-flight-ICP-MS – What can we do with this new dimension?**

**Lukas Schlatt**, Phil Shaw, *Nu Instruments*

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**23FORENS06: Pharma Forensics, Southern Pacific A/G**  
Chair: Ravi Kalyanaraman, *Bristol-Myers Squibb*  
Co-Chair: Scott Huffman, *Bristol-Myers Squibb*

(FORENS-06.1) **Multirange Vibrational Spectroscopy for Pharmaceutical Forensics**  
**Mike Bradley**, Robert Heintz, Stephan Woods, *Thermo Fisher Scientific*

(FORENS-06.2) **What's In The Bottle? Real Patient Complaints Submitted to FIT**  
**Brittany Handzo**, Scott Huffman, Ravi Kalyanaraman, *Bristol Myers Squibb*

(FORENS-06.3) **Oh Pharmaceutical Forensic Microscopy, Where Art Thou Come From?**  
**Dale Purcell**, *Chemical Microscopy, LLC*

(FORENS-06.4) **Sourcing Foreign Or Extraneous Matter Using The Particle Approach**  
**Craig Schwandt**, *McCrone Associates, Inc.*

(FORENS-06.5) **Microscopy Tool Ideas In Parenteral Pharmaceutical Environment**  
**David R Martinez Wolcott**, *Bristol Myers Squibb*

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**23IR06: Material Science: IR Nanospectroscopy Opens New Perspectives, Sierra 3**  
Chair: Ariane Deniset-Besseau, *National Institute of Standards and Technology*  
Co-Chair: Georg Ramer, *University of Illinois*

(IR-06.1) **Nanoscale Insight into Paint Degradation Mechanisms**  
**Suzanne Morsch**, Stuart Lyon, Claudio Di Lullo, *University Of Manchester, AkzoNobel*

(IR-06.2) **Travelling thru time with IR nano-spectroscopy**  
**Jérémie Mathurin**, Laure Bejach, Emmanuel Dartois, Cecile Jean Duprat, Alexandre Dazzi, Ariane Deniset-besseau, Keyron Hickman-Lewis, *Institut De Chimie Physique, CNRS, Université Paris-Saclay, National History Museum London*

(IR-06.3) **Probing Phonon Polaritons of Hexagonal Boron Nitride in the Aqueous**

**Phase With Liquid-phase Peak Force Infrared Microscopy**  
**Xiaoji Xu**, *Lehigh University*

(IR-06.4) **Poking into the nano-World: Infrared Nanospectroscopy for Chemical and Structural Analysis of Nanoplastics**  
**Clementina Vitali**, Hans-Gerd Janssen, Michel W. F. Nielen, Francesco Simone Ruggeri, *Wageningen University & Research*

(IR-06.5) **Infrared nanospectroscopy of local electric-field dependent effects probed with atomic-force-microscopy in contact mode**  
**Maria Eleonora Temperini**, Raffaella Polito, Antonia Intze, Michele Ortolani, Valeria Giliberti, Tommaso Venanzi, *Italian Institute of Technology, Sapienza University Of Rome*

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**23PAT01: Looking 50 Years into the Future of PAT**, Southern Pacific E  
Chair: Marissa Dobulis, *Dow Chemical*  
Co-Chair: Zoe Whalley, *University of Birmingham*

(PAT-01.1) **50 Years (and More) of PAT in Nuclear Materials Processing**  
**Robert Lascola**, *Savannah River National Laboratory*

(PAT-01.2) **Application of Structured Approaches to Implementation of Advanced Preprocessing Techniques**  
**Magdalene Chong**, Alison Nordon, *University Of Strathclyde*

(PAT-01.3) **Towards Standardisation of Data Acquisition Software for PAT Applications**  
**Brad Swarbrick**, Rajani Davuluri, Joonsup Lee, KAX Group Pty Ltd, Stephen Hammond, *Steve Hammond Consulting*

(PAT-01.4) **Innovations in Online Analyzers: An End-User Perspective**  
**James Tate**, *Ibird Consultants*

(PAT-01.5) **The use of simulation to optimize fiber optic probe performance for on-line applications**  
**Stephen Hammond**, *Steve Hammond Consulting*

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**23PMA05: Measurement of Proteins and Modifications towards Precision Medicine,**  
Southern Pacific D  
Chair: John Marshall, *YYZ Pharmatech*  
Co-Chair: John Wasyluk, *Bristol Myers Squibb*

(PMA-05.1) **Development and Implementation of Clinical Proteomics for Bedside Applications: Precision Oncology and Cancer Detection**  
Emanuel Petricoin, *George Mason University*

(PMA-05.2) **Use of longitudinal serum samples for early detection and risk assessment of cancer**  
Karin Rodland, *Oregon Health & Science University*, Tao Liu, Vladislav Petyuk, *Pacific Northwest National Laboratory*, Craig Shriver, *Murtha Cancer Center*

(PMA-05.3) **Giving Gold Wings with Bright and Stable Mass Spectrometry Tags**  
Nathaniel Dominique, Isabel Jensen, David Jenkins, Gurkiran, *Knoxville, Chandler Kotseos*, William Boggess, Jon Camden, *University of Notre Dame*, Kaur University of Tennessee

(PMA-05.4) **COVID19 versus ICU Respiratory Distress Controls or Normal Human Plasma by Liquid Chromatography Nano Electrospray Ionization and Tandem Mass Spectrometry**  
Jaimie Dufresne, John Marshall, *YYZ Pharmatech*

(PMA-05.5) **The Tryptic Peptides and Proteins of Fetal Versus Adult Serum from MS/MS Spectra**  
Jaimie Dufresne, John Marshall, *YYZ Pharmatech*

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**23RAM14: Industrial Raman**, Cascade 1  
Chair: Ian Lewis, *Endress+Hauser Optical Analysis*

(RAM-14.1) **Process Analytical Utility of Raman Spectroscopy in Therapeutic T-Cell Manufacturing**  
Shreyas Rangan, Katherine N. MacDonald, Smilla Colombini, Miles Huynh, Hans Georg Schulze, Martha Z. Vardaki, Michael W. Blades, Megan K. Levings, Robin F.B. Turner, James M. Piret, *University Of British Columbia*

(RAM-14.2) **Automation and sampling technologies enabling new frontiers in Raman spectroscopy as a PAT for bioprocessing**  
Karen Esmonde-White, Maryann Cuellar, Sean Gilliam, Justin Moretto, Ian Lewis, *Endress+Hauser*

(RAM-14.3) **Quantitative Analysis Of Common Components In A Chemical Mechanical Polishing Slurry Using Raman Spectroscopy**  
Michelle Sestak, Timothy Holt, *HORIBA Scientific*

(RAM-14.4) **Automated Quantitative Raman-based Analysis of (Microplastic) Particles and Fibers down to 1 µm**  
Natalia Ivleva, Oliver Jacob, Alejandro Ramírez-Piñero, Martin Elsner, *Technical University of Munich*

(RAM-14.5) **In situ Raman-electrochemistry for Routinely Characterizing Electronic Properties of Doped SWCNTs**  
Joanne Yam, Adam Hopkins, *Metrohm*

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**23RAM16: Nano Raman 2**, Cascade 3  
Chair: Andrew Whitely, *HORIBA*  
Co-Chair: Abdrey Krayev, *HORIBA*

(RAM-16.1) **High Resolution Ambient Tip-Enhanced Optical Microscopy and Spectroscopy**  
Patrick El-Khoury, *PNNL*

(RAM-16.2) **Unconventional Moiré Electrons and Phonons in the Magic Material Probed by Tip-Enhanced and Gate-Dependent Raman Spectroscopy**  
Andreij Gadelha, Douglas Ohlberg, Cassiano Rabelo, Eliel Neto, Thiago Vasconcelos, Joao Campos, Jessica Lemos, Vinicius Ornelas, Daniel Miranda, Rafael Nadas, Fabiano Santana, Kenji Watanabe, Takashi Taniguchi, Benoit Troeye, Michael Lamparski, Vincent Meunier, Viet-Hung Nguyen, Dawid Paszko, Jean-Christophe Charlier, Leonardo Campos, Luiz Cancado, Gilberdo Medeiros-Ribeiro, Ado Jorio, *Federal University of Minas Gerais*

(RAM-16.3) **Investigation of Transition Metal Dicalcogenides Flakes with TERS and Wide-field Raman Microscopy with Stochastic Optical Reconstruction.**

Joachim Jelken, Cedric Lambin, **Francois Lagugne**, *Western Ontario University*

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**23SPR04: Plasmonics and Catalysis**, Cascade 4

Chair: Malama Chisanga, *University of Montreal*

(SPR-04.1) **Promoting Unique Molecular Processes with Plasmonics**

**Matthew Sheldon**, *Texas A&M University*

(SPR-04.2) **Plasmonic Magnesium Nanoparticles for SERS and Catalysis**

**Andrey Ten**, Vladimir Lomonosov, Christina Boukouvala, Jean-Francois Masson, Emilie Ringe, *HORIBA Scientific*

(SPR-04.3) **Investigating the Relationship of Electron Transfer and Heating of Nanomaterials with a Homemade Photothermal Heterodyne Imaging System**

**Yechan Moon**, Zachary Schultz, Susan Olesik, *The Ohio State University*

## TECHNICAL PROGRAM – THURSDAY, OCTOBER 12, 2023

**Awards and Plenary Lectures | 10:45AM – 12:00PM | Sierra 5**

**Plenary Sessions: SAS and Applied Spectroscopy William F. Meggers Award; Johannes Pedarnig**

(PLEN-L4.1) **LIBS and LA-SD-OES: Laser Ablation and Electric Sparks for Chemical Element Analysis**

**Johannes Pedarnig**, Nikos Giannakaris, Stefan Grünberger, *Johannes Kepler University Linz*

**Plenary Sessions: Spectroscopy's Emerging Leader in Molecular Spectroscopy; Dmitry Kuroski**

(PLEN-L4.2) **Structural Characterization of Biological Systems at Macro and Nanoscale Using Vibrational Spectroscopy**

**Dmitry Kuroski**, *Texas A&M University*

## TECHNICAL PROGRAM – THURSDAY, OCTOBER 12, 2023

**Oral Symposia | 1:30PM – 3:10PM**

**23AWD08: SAS and Applied Spectroscopy William F. Meggers Award Symposium**

**Honoring Johannes Pedarnig**, Cascade 3  
Chair: Johannes Pedarnig, *Johannes Kepler University Linz*

(AWD-08.1) **Investigation of LIBS-RF Plasma for Analytical Spectroscopy**

**Igor Gornushkin**, Cristina Méndez-lópez, Nerea Bordel, *Department of Physics, University Of Oviedo, BAM*

(AWD-08.2) -Withdrawn

(AWD-08.3) **Remote detection of Li isotopes**

**Vassilia Zorba**, Kevin Touchet, Jose Chirinos, Changmin Kim, Zach Alvidrez, Xianglei Mao, *Lawrence Berkeley National Lab & Uc Berkeley*

(AWD-08.4) **On The Significance Of Laser Ablation Efficiency For LIBS Signal Enhancement.**

**Alessandro De Giacomo**, *University of Bari*

(AWD-08.5) **LIBS and LIMS in the context of planetary/space research**

**Jose M. Vadillo**, Javier Moros, Javier Lasema, *University of Bari, Universidad de Malaga*

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**23AWD09: Spectroscopy's Emerging Leader in Molecular Spectroscopy Award**

**Symposium Honoring Dmitry Kuroski**, Sierra 5

Chair: Dmitry Kuroski, *Texas A&M University*

(AWD-09.1) **Measuring Chemical Composition, Optical and Thermal Properties at the Nanoscale with AFM Probes**

**Andrea Centrone**, *Nist*

(AWD-09.2) **Nano-Chemical Infrared Imaging and Spectroscopy from Supramolecular Protein Aggregates to Single Polymer Chains**

**Francesco Simone Ruggeri**, *Wagenigen University*

(AWD-09.3) **Monitoring Chemistry on Plasmonic Nanoparticles**

**Zachary Schultz**, *South Dakota Mines*

(AWD-09.4) **Plasmon-enhanced Raman Spectroscopy Assessed by a Holistic Quantum Mechanical Approach**

**Stephan Kupfer**, Kevin Fiederling, Stefanie Gräfe, *Friedrich Schiller University Jena*

(AWD-09.5) **Multimodal Spectral Nano-Imaging of Plasmonic Nanoparticles**

**Patrick El-Khoury**, *PNNL*

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**23FORENS05: Early Career Research in Forensic Science**, Southern Pacific A/G

Chair: Alexis Weber, *University at Albany, SUNY*

(FORENS-05.1) **Chemical Anthropology: The Forensic Chemist's Perspective on Bones**

**Kristen Livingston**, *University Of Central Florida*

(FORENS-05.2) **Multimodal Raman Spectroscopy for Comprehensive Forensic Analysis**

**Matt Gabel**, Sudhir Dahal, Thermo Fisher Scientific

(FORENS-05.3) **Near Infrared for rapid screening for oil type used in fried snacks manufacturing**

**Alessandra Victorio**, Luis Rodriguez-saona, Siyu Yao, *The Ohio State University*

(FORENS-05.4) **High Ionic Strength-Resistant Colorimetric Sensor for Lead Ion Quantification in Tap Water**

**Hanwei Wang**, Seo Won Cho, Craig Butler, Haoran Wei, *University of Wisconsin–Madison*

(FORENS-05.5) **Hyperspectral Threat Anomaly Detection (Hyper ThreAD)**

**Technique for Potential Explosive Threats**  
**Eric Languirand**, Matthew Collins, *DEVCOM CBC*

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**23IR11: IR Frequency Combs**, Sierra 3

Chair: Pedro Martin Mateos, *Universidad Carlos III de Madrid*

(IR-11.1) **Frequency combs for precision hyperspectral imaging**

**Pedro Martín Mateos**, *Universidad Carlos III de Madrid*

(IR-11.2) **Paradigm Changes in Time**

**Resolved Infrared Spectroelectrochemistry**

**Scott Rosendahl**, Ian Burgess, *University Of Saskatchewan, Canadian Light Source Inc.*

(IR-11.3) **Frequency Combs for Spectroscopy and 3D Imaging**

**Nathalie Picque**, *MPI Of Quantum Optics*

(IR-11.4) **High-resolution Quantum Cascade Laser Dual-comb Spectroscopy and**

**Hyperspectral Imaging in the Mid-infrared**  
**Gerard Wysocki**, *Princeton University*

(IR-11.5) **Ultraviolet Dual-Comb Absorption Spectroscopy of Neutral and Ionized Fe in a Laser-Produced Plasma**

**John McCauley**, Mark Phillips, Yu Zhang, Jason Jones, Sivanandan Harilal, Reagan Weeks, *Air Force Research Laboratory, University Of Arizona, Pacific Northwest National laboratory*

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**23IR13: Applications of Optical- and AFM-Photothermal IR Spectroscopy**, Sierra 2

Chair: Minghe Li, *Boehringer Ingelheim*

Co-Chair: Curtis Marcott, *Light Light Solutions*

(IR-13.1) **Correlative Fluorescent and Infrared Imaging and Spectroscopic Analysis of Human Primary Skin Fibroblasts**

**Kathleen Gough**, Sabine Mai, Matheus Fabiao de Lima, Benoit Girouard, Sheyenne Gamage, D , Rohith Reddy, Chalapathi-charan Gajjala, Darryl Dyck, *Lumiere Microscopy, Winnipeg MB, University of Manitoba, Univ. Of Houston,*



(IR-13.2) -Withdrawn

(IR-13.3) **Challenges and constraints of multimodal-multiscale vibrational spectroscopy imaging in biomedical: A breast microcalcifications case study**  
Margaux Petay, Alexandre Dazzi, Dominique Bazin

Ariane Deniset-besseau, Maguy Cherfan,  
*Institut de Chimie Physique, CNRS, Université Paris-Saclay, Université Paris-Saclay, Hopital NOVO, GHT Nord Ouest Val D'oise*

(IR-13.4) **Advancing bottom-illuminated photothermal nanoscale chemical imaging - in air and liquid - by introducing cost-effective, flat silicon carriers**

Ufuk Yilmaz, Bernhard Lendl, Georg Ramer,  
*Technische Universität Wien*

(IR-13.5) **Bond Selective Fluorescence Imaging with Single Molecule Sensitivity**  
Dongkwan Lee, Haomin Wang, Lu Wei,

Kourtney Dalzell, Leah Thomas, Thomas Ledergerber, Courtney Vander Pyl, Tatiana Trejos, Luis Arroyo, Jhanis Gonzalez, Chunyi Liu, Miyeun Yoo, Richard Russo, *West Virginia University, Excimer Laser Ablation-Based Tandem Approach to the Analysis of Solid Samples*

(LIBS-03.4) **Advances in Tandem LA – LIBS Technology and Data Analysis**

Jhanis Gonzalez, Charles Sission, Chunyi Liu, Steve Shuttleworth, Miyeun Yoo, Richard Russo, *Applied Spectra Inc, Excimer Laser Ablation-Based Tandem Approach to the Analysis of Solid Samples, Advances in Tandem LA – LIBS Technology and Data Analysis*

(LIBS-03.5) **Performance of  $\mu$ XRF and LIBS for the forensic analysis of small and irregular glass fragments**

Ruthmara Corzo, Nist Oriana Ovide, Tatiana Trejos, *West Virginia University*

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**23PAT06: PAT in Petroleum and Refinery Industries**, Southern Pacific E  
Chair: Toni Miao

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**23LIBS03: LIBS for Forensics and Security**, Southern Pacific B/C  
Chair: Tatiana Trejos, *West Virginia University*  
Co-Chair: Ruthmara Corzo, *Nist*

(LIBS-03.1) **A Two-Step Method for the Identification and Highly Specific Analysis of Organic Gunshot Residue Using Raman and Laser-Induced Breakdown Spectroscopies**

Igor Lednev, Shelby Khandasammy, Lenka Halámková, Matthieu Baudelet, *University at Albany, SUNY, University Of Central Florida, Texas Tech University*

(LIBS-03.2) **Development of a method for the forensic discrimination of solder by LIBS-LA-ICPMS**

Claude Dalpe, Nigel Hearn, Royal Canadian Mounted Police, Katie Moghadam, Diane Beauchemin, *Queen's University, Department of Chemistry*

(LIBS-03.3) **Advancement of LIBS Mobile Technology for the Detection of Firearm Discharge Residue from Various Substrates and Assessment at Mock Crime Scenes**

(PAT-06.1) **Detailed PIONA of Mogas built by GC and predicted using Multivariate IR**  
Bryan Bowie, Aditya Shetkar, Payman Pirzadeh, *Exxonmobil*

(PAT-06.2) **The Use Of Static Optics FTIR For Controlling Petrochemical And Refinery Operations With Mid Infrared**  
Victoria Grigson, Jonathon Speed, Adam Wilson, Kiran Haroon, Carolina Cruz, *Keit Industrial Analytics*

(PAT-06.3) **Portable FT-NIR spectral sensing for instant and global insights**  
Bob Schumanns, Mostafa Medhat, *Si-Ware System*

(PAT-06.4) **Site-Independent Determination of Total Petroleum Hydrocarbons in Soil by Handheld NIR Spectroscopy: Locally Weighted Regression**

Marina De Gea Neves, Toni Miao, Natasha Sihota, Cory McDaniel, Heinz Siesler, *University Duisbr-essen, Department of Physical Chemistry, Chevron Technical Center*

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**23PMA09: Analysis of Proteins, Antibodies, Biologicals and Nucleic Acids**, Southern Pacific D

Chair: Jaimie Dufresne, *YYZ Pharmatech*

Co-Chair: John Wasylyk, *Bristol Myers Squibb*

**(PMA-09.1) A Multiomics Assessment of CAR-T Potency and Toxicity in Hematological Malignancies**

**Devanand Pinto**, *Dalhousie University*

**(PMA-09.2) Enzyme Linked Mass Spectrometric Assay (ELiMSA) for Sensitive Detection of DNA from SARS-CoV2, HIV and pUC19**

John Marshall, **Ming Miao**, *YYZ Pharmatech*

**(PMA-09.3) Plate-based Infrared Spectroscopy for Rapid Peptide Quantitation: A Potential Drug Discovery Workflow**

**Raffael Bennett**, Donovan A. Adpressa, Alexey A. Makarov, Merck, Nathaniel Hendrick, Kaitlyn Corazzata, Aaron Beeler, Douglas Fraser, *Department of Chemistry, Boston University, Tornado Spectral Systems*

**23RAM08: Raman Imaging**, Cascade 1  
Chair: Katsumasa Fujita, *Osaka University*

**(RAM-08.1) Raman-fingerprint-activated cell sorting**

**Kotaro Hiramatsu**, *The University of Tokyo*

**(RAM-08.2) In search of chemoresistance markers of acute lymphoblastic leukemia: Raman-based in vitro evolution of drug-induced metabolic changes**

**Katarzyna Majzner**, Patrycja Dawiec, Adriana Adamczyk, Anna M. Nowakowska, Justyna Jakubowska, Marta Ząbczyńska, Agata Pastorczak, Kinga Ostrowska, Wojciech Młynarski, Malgorzata Baranska, *Jagiellonian University In Krakow*

**(RAM-08.3) The Development and Implementation of Spectroscopic Coherent Raman Imaging as a Discovery Tool for Biology**

**Marcus Cicerone**, *Georgia Institute Of Technology*

**(RAM-08.4) Stimulated Raman Photothermal Microscopy towards Ultrasensitive Chemical Imaging**

**Yifan Zhu**, Xiaowei Ge, Hongli Ni, Jiaze Yin, Haonan Lin, Le Wang, Yuying Tan, Chinmayee Prabhu Dessai, Ji-Xin Cheng, *Boston Univeristy*

**(RAM-08.5) Multimodal imaging analysis using Stimulated Raman Scattering Microscopy and Secondary Ion Mass spectroscopy to study drug penetration into skin**

**Vasundhara Tyagi**, Jean-Luc Vorng, Alex Dexter, Panagiota Zarnpi, Natalie Belsey, Dimitrios Tsikritsis, Begona Delgado-Charro, Richard Guy, *National Physical Laboratory*

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**23RAM17: Bioanalytical Applications of Raman Spectroscopy**, Cascade 4

Chair: William Tipping, *The University Of Strathclyde*

Co-Chair: Gregory Wallace, *The University Of Strathclyde*

(RAM-17.1) **Molecular Insights into the Binding of Linear Polyethyleneimines and Single-Stranded DNA Using Raman Spectroscopy: A Quantitative Approach**  
Rusul Mustafa, David Punihaole, *University of Vermont*

(RAM-17.2) **On the Potential of Stable Isotope Raman Microspectroscopy for Analysis of Microbial Degradation of Microplastics**  
Natalia Ivleva, Kara Müller, Martin Elsner, *Technical University of Munich, Chair of Analytical Chemistry and Water Chemistry, University of Münster*

(RAM-17.3) **Ensuring Optimal Detection Outcomes in Handheld Raman Spectroscopy**  
Luisa T.M. Profeta, Brian L. Bures, John T. Wiesemann, Christopher Langford, Michael D. Hargreaves, *Rigaku Analytical Devices*

(RAM-17.4) **A study on relationship between development of neuronal cells and susceptibility to bisphenol A (BPA) using Raman spectroscopy**  
Kosuke Hashimoto, Shogo Sato, Hidetoshi Sato, *Kwansei Gakuin University*

(RAM-17.5) **Reaching stars: unique characteristics of gold nanostars for sensing and targeting applications**

Anastasiia Tukova, Alfonso Garcia-Bennett, Alison Rodger, Yuling Wang, *Macquarie University*

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**23SPECIAL01: Skilled: Scientific Discoveries and Professional Lessons After Academia**, Southern Pacific F  
Chair: Kristy Mckeating, *Google*  
Co-Chair: Sam Hinman, *PhenomeX*

(SPEC-01.1) **Rapid Discovery of Functional Human Memory B Cell-Derived Antibodies for SARS-CoV-2 Using the Beacon® Optofluidic System**  
Sam Hinman, *PhenomeX*

(SPEC-01.2) **Publish and/or Flourish: A National Lab Perspective**  
FREDERIC POITEVIN, *SLAC National Accelerator Laboratory*

(SPEC-01.3) **Apparently Healthy: Biosensors for Wellness Applications**  
Kristy Mckeating, *Google*

(SPEC-01.4) **Careers beyond the bench: Publishing, Product Management and Pivots**  
Marshall Brennan, *Cell Press*

## TECHNICAL PROGRAM – THURSDAY, OCTOBER 12, 2023

### FACSS Innovation Award Finalists Plenary Session 10:45AM – 12:00PM | Sierra 5

#### FACSS Innovation Award Finalists Plenary Session

*Polytechnic Institute, Federal Institute for Materials Research and Testing (BAM)*

**Real-time Controlling a Single DNA in Hotspot for Programmable Surface-enhanced Raman Spectroscopy Scanning in Solution**  
Jinqing Huang, *The Hong Kong University Of Science And Technology*

**Acoustic Ion Manipulation: A Novel Approach to Enhance Ion-based Spectroscopies**  
Jacob Shelley, Yi You, Julia Danischewski, Jens Riedel, *University of Utah, Rensselaer*

**Unveiling Superior Spectroscopic Precision: A Shoebox-Sized, Low-Cost Spatial Heterodyne Spectrometer with 1-pm Resolution**  
Yi You, Xunyu Li, Steven Ray, , Jens Riedel, *SUNY Buffalo Dept of Chemistry, Federal Institute For Materials Research And Testing (bam)*

**New Opportunities for Mass Spectrometry in Nanocrystal Surface Chemistry**  
Mengliang Zhang, Kevin Cavey, P. Gregory Van Patten, *Middle Tennessee State University*

# **TECHNICAL PROGRAM – FRIDAY, OCTOBER 13, 2023**

## **FACSS SciFri Sessions and Closing Sessions**

**8:30AM - 10:00AM | Sierra 5**

**Should Anyone Care about Scientific Instruments (Besides Us)?**

**Roger Turner**, *Science History Institute*

# TECHNICAL PROGRAM- MONDAY POSTERS

Poster Sessions | 10:10AM – 10:45AM & 3:10PM- 3:50PM | Nugget Foyer

**(Mon-P1) Direct Analysis Of Trace Elements in Seawater Using ICP-MS with Versatile Reaction Modes**

Aaron Hineman, Liyan Xing, Tamas Ugrai, Chady Stephan, *PerkinElmer*

**(Mon-P2) The Analysis of Major and Trace Elements in Plant-Based Foods Using the NexION ICP-MS**

Aaron Hineman, Liyan Xing, Tamas Ugrai, Chady Stephan, *PerkinElmer*

**(Mon-P3) Gold nanoparticles influence on accumulation and translocation of essential elements in hydroponic common bean sprouts (*Phaseolus vulgaris* L.)**

Aline Pereira de Oliveira, Juliana Naozuka, Cassiana Nomura, *University of Sao Paulo*

**(Mon-P4) -Withdrawn**

**(Mon-P5) Propagating highly-correlated error structures through multivariate classification models to optimize class-differentiation thresholds**

Helder V. Carneiro, Caelin Celani, Karl S. Booksh, *University Of Delaware*

**(Mon-P6) Multivariate Classification of Geospatial Origin of Ash Analyzed by Inductively Coupled Plasma Mass Spectrometry**

Maria Delgado-Cornelio, Collin White, James A. Jordan, Michael E. Ketterer, Helder V. Carneiro, Caelin Celani, Barry Lavine, Karl S. Booksh, *University Of Delaware*

**(Mon-P7) Making the Process of Multivariate Analysis Accessible to the Data Science Novice: A Workflow for Getting Answers From Fluorescence A-TEEMs**

Karen Gall, Eunah Lee, Jeffrey Julien, Linda Kidder, Brad Swarbrick, Rajani Davuluri, Joonsup Lee, *Horiba Scientific*

**(Mon-P8) Multivariate Analysis of Granule Size Distributions: A Tool for Process Understanding in Continuous Granulation Systems**

Samuel Henson, Jacob Guess, Md. Nahid Hasan, James Drennen, Carl Anderson, *Duquesne University*

**(Mon-P9) Automated Pipelines for Deployment of Web-based Tools in Chemometrics, Machine Learning & Research Data Management**

Julian Hniopek, Jonas Eichhorn, Rodrigo Escobar, Nazar Stefaniuk, Thomas Bocklitz, *Leibniz Institute of Photonic Technology Jena*

**(Mon-P10) Effects of Crystalline Micro-Structures on the Application of Multivariate Curve Resolution to Hyperspectral Raman Images**

Elizabeth Licht, Rachel McCormick, Joseph Smith, Karl S. Booksh, *University Of Delaware Graduate Student*

**(Mon-P11) Integration of Immersive Virtual Reality with Machine Learning for Calibration Model Selection and Classification**

Jordan Peper, John Kalivas, Rajiv Khadka, *Idaho State University*



**(Mon-P12) Application Of A Spectral Window Angle Mapper For Variable Selection To Improve Iterative Optimization Technology Algorithm Prediction Robustness**

Adam Rish, Natasha Velez-Silva, Samuel Henson, Md. Nahid Hasan, James Drennen, Carl Anderson, *Duquesne University: Graduate School Of Pharmaceutical Sciences*

(Mon-P13) -Withdrawn

**(Mon-P14) Exploration of Acoustic-Based Ion Optics for the Control of Gaseous Ions**

Julia Danischewski, Yi You, Jens Riedel, Jacob Shelley, *Rensselaer Polytechnic Institute*

**(Mon-P15) Analysis of Industrial Gasses, Sulfur Hexafluoride (SF<sub>6</sub>) and Novec™ 4710, Using Mass Spectrometry, Gas Chromatography, and Raman Spectroscopy**

Dawson Dodd, Theresa Evans-Nguyen, *University Of South Florida*

(Mon-P16) -Withdrawn

**(Mon-P17) Design and Optimization of a new microwave microreactor for mass spectrometry**

Buddhika Kumara, Steven Ray, *The State University Of New York at Buffalo*

**(Mon-P18) Monitoring long-term chemical exposome by characterizing the hair metabolome using a high-resolution mass spectrometry-based suspect screening approach**

Pao-Chi Liao, *National Cheng Kung University*

(Mon-P19) -Withdrawn

(Mon-P20) -Withdrawn

**(Mon-P21) Understanding Harmful Algal Blooms in Chautauqua Lake, New York through Toxin Detection and Genetic Analysis**

Abigail Ross, Vincent Moriarty, Manuel Castro-Berman, Jonathan Dordick, Jacob Shelley, *Rensselaer Polytechnic Institute*

**(Mon-P22) Investigation of potential anthropogenic pollution of rare metals in urban river water and sewage treatment effluent**

Akane Yaida, Akitoshi Okino, Kazuhiko Nakano, Akihito Itoh, *First Tokyo Institute Of Technology*

**(Mon-P23) Quantitative screening of Tuberculosis targeting isoniazid tablets using handheld Raman spectrometer. Ed Bethea, Melissa Growney, Jonelle Carson, Matthew Eady, David Jenkins, *FHI360***

(Mon-P24) **International supply chain implementation logistics of multiple handheld spectrometers for rapid screening of public health commodities**  
Matthew Eady, Christopher Harmon, Chayanee Changpim, Mohammed Jinnah, Jonelle Carson, Melissa Gowney, Noah Peters, David Jenkins, *Fhi 360*

(Mon-P26) **A Top-Down Spectroscopic Approach to Correlating Coating Thickness Distributions with the Dissolution Profiles of Enterically Coated Drug Pellets**  
Daniel Willett, Huzeyfe Yilmaz, Wenjing Xi, Zongming Gao, Jason Rodriguez, *US Food & Drug Administration*

(Mon-P28) **Using Ultra-High Resolution to Overcome Isobaric Interferences with the Liquid Sampling-Atmospheric Pressure Glow Discharge / Orbitrap Coupling**  
Joseph Goodwin, Benjamin Manard, Brian Ticknor, Paula Cable-Dunlap, R. Kenneth Marcus, *Goodwin*

(Mon-P29) **Development of a Spectral Reaction Library for 78 Elements with a Variety of Reaction Gases**  
Aaron Hineman, Ewa Pruszkowski, Karl Andreas Jensen, Valeriia Morozova, *PerkinElmer*

(Mon-P30) **Speciation of Selenium and Chromium in Drinking Waters using an Inert HPLC and DRC-ICP-MS**  
Aaron Hineman, *PerkinElmer*

(Mon-P31) **Microplastic Particle Quantification in Seawater Using Single-particle ICP-TOFMS with Online Microdroplet Calibration**  
Stasia Harycki, Alexander Gundlach-Graham, *Iowa State University*

(Mon-P32) **Determination of silicon in biological samples by ICP-MS: Stabilization of volatile silicon species during evaporative removal of hydrofluoric acid from digests**  
Zikri Arslan, *Arslan*

(Mon-P33) **Improving the Lithium Battery Supply Chain: from Raw Materials Testing to Recycling**  
Aaron Hineman, Chady Stephan, *PerkinElmer*

(Mon-P34) **Influence of optical configuration on FT-IR imaged breast Tissue Microarrays classification**  
Danuta Liberda-Matyja, Tomasz Wrobel, *Solaris National Synchrotron Radiation Centre, Jagiellonian University*

(Mon-P35) **Machine Learning for Classification of Particles from Noisy spICP-TOFMS Data**  
Raven Buckman, Hark Karkee, Alexander Gundlach-Graham, *Iowa State University*

(Mon-P35) **Rapid ICP-MS Analysis of Dried Blood Spots via Direct Microextraction from Solid Substrates**  
Cameron Stouffer, R. Kenneth Marcus, *Clemson University*

(Mon-P38) **Just A Drop: A Simplified Small-Droplet Device And Modified Sampling Substrate for LMJ-SSP-MS**  
Daniel Reddy, Lishen Zhang, Thomas Covey, Richard Oleschuk, *Queen's University*

(Mon-P40) **Recent Advances in Continuous Fast Data Acquisition < 100  $\mu$ s for Single-Particle ICP-TOFMS**  
Lyndsey Hendriks, Fredrik Oestlund, Martin Rittner, *TOFWERK*

## TECHNICAL PROGRAM- TUESDAY POSTERS

Poster Sessions | 10:10AM – 10:45AM & 3:10PM- 3:50PM | Nugget Foyer

(Tues-P1) **Optimization of cell recovery for label-free dielectrophoretic cell sorting in microfluidic systems**  
 Syleah Manns, Ella Fitzgerald, Dean Thomas, KATHERINE DEGEN, Ridi Barua, Alexandra Hyler, *George Mason University, Virginia Tech, CytoRecovery*,

(Tues-P2) **[FeFe] and [NiFe] Hydrogenase Stability at Low Temperatures in Cryosolvents: An Alternate Approach for Capturing Fleeting Intermediates**  
Alexander Jackson, James A. Birrell, Olaf Rüdiger, Sagie Katz, Kushal Sengupta, Nina L. Breuer, Ingo Zebger, Simon J. George, Serena DeBeer, Stephen P. Cramer, *University Of California, Davis, School of Life Sciences, University of Essex, Inorganic Spectroscopy, Max Planck Institutue for Chemical Energy Conversion, Institute of Chemistry, Technische Universität Berlin, Carl Sagan Center for Research, SETI Institute*

(Tues-P3) **Analyzing Stomach Cancer Tissue using Convolutional Neural Networks (CNN) and Autofluorescence**  
Jin Il Jang, Hyung Min Kim, *Kookmin University*

(Tues-P4) **Determining the Effects of Glycocalyx Modification on Human Mesenchymal Stem Cells' Electrophysiology**  
Sydney Joseph, Rominna Valentine, Lexi Crowell, Stephany Alonso, Tayloria N.G. Adams, *Wake Forest University, University of California, Irvine*

(Tues-P5) **(O-PTIR Spectral Imaging of Human Bone Biopsies Embedded in Thick Blocks at Sub-Micron Resolution**  
Sofia Mehmood, Isha Dev, Yana Bronfman, Edward DiCarlo, Nancy Pleshko, William Querido, *Temple University, Hospital for Special Surgery*

(Tues-P6) **Design of Multi Wavelength and Output Laser system for Biomedical Applications**

Youngmin Moon, Junyoung Seo,  
Hwangryol Ryu, Kisung You, Jonghyun  
Woo, Chang-Su Na, *Research Institute of  
Industrial Science And Technology,  
Dongshin University*

**(Tues-P7) Analytical Methods for  
Implantable Medical Devices:  
Bioprosthetic Heart Valves and Hip  
Implants**

Chady Stephan, Ken Neubauer, Ewa  
Pruszkowski, Bin Yuan, Kamal Yadav,  
*PerkinElmer*,

**(Tues-P8) Optimization of Approach for  
Differentiation of Saline and Hydrated  
Joint Tissues During Vis-NIR**

**Arthroscopic Fiber Optic Assessment**  
Amanda Spurri, William Querido,  
Mohammed Shahriar Arefin, Chetan Patil,  
Nancy Pleshko, *Temple University, Indian  
Institute Of Technology–Bhilai*

**(Tues-P9) A SERS-based substrate for a  
rapid and efficient detection of mutations  
in acute myeloid leukemia**

Alexandra Teixeira, Maria Sousa-Silva,  
Alexandre Chícharo, Ahmed Mahmoud,  
Sara Abalde-Cela, Lorena Diéguez, *Inl -  
International Iberian Nanotechnology  
Laboratory (inl)*

**(Tues-P10) Towards imaging millisecond  
neural computations with an electro-  
optical two-photon microscope**

Harishankar Jayakumar, Deano Farinella,  
Chris Warkentin, Samuel Stanek, Jacob  
Gable, Zachary Newman, Sakal Singla,  
Biswanath Chakraborty, Aaron Kerlin,  
*University of Minnesota, Indian Institute of  
Technology Jammu*

**(Tues-P11) Study on the Global Oncology  
Challenges Using Biotechnology**

Xianfang YUE, *University of Science and  
Technology Beijing*

**(Tues-P12) Analytical Method  
Development for Quantification of Quartz  
Using Raman Spectroscopy**

Elizabeth Ashley, Vasileia Vogiazzi, Chen  
Wang, Pramod Kulkarni,  
*CDC/NIOSH/HELD/CBMB*

**(Tues-P13) A SERS-based Galactose  
Sensor using Molecular Reporter-  
Immobilized Ag Shell-Au Satellite  
Hetero-Nanostructure**

Hyejin Chang, Eun Hae Heo

**(Tues-P14) Measuring Glass Transition  
Kinetics of Polymers with Low-Frequency  
Raman**

Robert Chimenti, James Carriere, Danielle  
D'Ascoli, Jamison Engelhardt, Alyssa  
Sepcic, Kayla Bensley, Alexandra Lehman-  
Chong, Joseph F. Stanzione, III, Samuel  
Lofland, *Rowan University, Coherent*

**(Tues-P15) Optimization of Nano-  
materials for Surfaced Enhancement  
Raman Spectroscopy Lateral Flow Assays**

Alexander Cikanek, Lyndsay Kissell,  
Daewoo Han, Andrew Steckl, Pietro  
Strobbia, *University of Rochester, University  
of Cincinnati*

**(Tues-P16) Lego™ Blocks as Evaluation  
Samples For Raman Spectrometers**

Richard Crocombe, Brooke Kammrath,  
Pauline Leary, *Crocombe Spectroscopic  
Consulting, SAS & Coblenz Society,  
CBRNE Subject Matter Expert*

**(Tues-P17) Screening and Differentiation  
of Virus-like-particles Using Vibrational  
Spectroscopy**

Ankit Dodla, Magdalena Giergiel, Aaron  
McLean, Linda Earnest, Melissa Barrow,  
Julie McAuley, Dale Godfrey, Damian  
Purcell, Joseph Torresi, Bayden Wood,  
*Monash University, University of Melbourne*

*at the Peter Doherty Institute for Infection and Immunity*

**(Tues-P18) Non-Invasive Screening of Otitis Media with In vivo Raman Spectroscopy**

Sean Fitzgerald, Alexander Ho, Guillermo Monroy, Jay Werkhaven, Kevin Mason, Alistair Harrison, Stephen Boppart, Anita Mahadevan-Jansen, *Vanderbilt University, University of Illinois Urbana-Champaign, Nationwide Children's Hospital*

**(Tues-P19) Characterization of multi-photon polymerized microstructures without photoinitiator by using in situ Raman and Brillouin spectroscopy and biocompatibility analysis**

Atsushi Nakayama, Yasuaki Kumamoto, Menglu Li, Teng Li, Meiling Zheng, Katsumasa Fujita, *Osaka University, Chinese Academy of Science*

**(Tues-P20) Raman Spectroscopy Characterization of Antibody-ligand Association at Supported Phospholipid Bilayers**

Julia Clista Galecki, Grant Myres, Jay Kitt, Joel Harris, *University Of Utah*

**(Tues-Pg21) Monitoring of Environmental Pollutants using Quantitative Surface Enhanced Raman Spectroscopy**

Il Han, Wei Yu, Melissa Gelwicks, Micheal Allen, *B&W Tek, Metrohm*

**(Tues-P22) Phase transitions in low dimensional materials characterized by Raman spectroscopy**

Shayne Harrel, Adam Wise, Antoine Varagnat, *Andor Technology*

**(Tues-P23) The Role of Race/Ethnicity, Sex, and Age in Surface-Enhanced Raman Spectroscopy- and Infrared**

**Spectroscopy-Based Analysis of Artificial Colorants on Hair**

Aidan Holman, Dmitry Kurouski, *Texas A&M University*

**(Tues-P24) Sensitive Detection of Exosomes as Cancer Biomarkers using SERS Immunoassay**

Sila Jin, Woojeong Lim, Eungyeong Park, Ahhyun Woo, Igor Lednev, Jongmin Park, Young Mee Jung, *Kangwon National University, Korea, University at Albany, SUNY*

**(Tues-P25) Enhancing Plasmonic Activity of Graphene through Femtosecond Laser-Assisted Selective Metallization.**

Sarika Joshi, Gaurav Pratap Singh, Ankit Dodla, Donald McNaughton, Bayden R. Wood, Sumit Saxena, Shobha Shukla, *IITB-Monash Research Academy, Indian Institute of Technology Bombay, Monash University*

**(Tues-P26) Time-Resolved Confocal Raman Microscopy of Post-Melting Crystallization in Linear Polyethylenimine**

Miharu Koh, Jay Kitt, Carol Korzeniewski, Joel Harris, Shelley Minter, *University Of Utah, Texas Tech University*

**(Tues-P27) Lyophilizing SERS Sensors for point-of-care (POC) Diagnostics**

Lutfun Naher, Steven Quarin, Pietro Strobbia, *University Of Cincinnati*

**(Tues-P28) Nanomaterials Platform for Surface-Enhanced Raman Spectroscopic Chemical Fingerprinting of Cancer-Associated Volatile Organic Compounds**

Hannah O'Toole, Ambarish Kulkarni, Marie Heffern, Randy Carney, *University Of California, Davis*

**(Tues-P29) Fillings of Single-Walled Carbon Nanotubes**



Dale L Perry, Nataliya Kalashnyk, Eric Faulques, Victor G Ivanov, Charlotte Slade, Jean-Luc Duvail, Stéphane Cordier, Ann Sanchez, Jeremy Sloan, *Lawrence Berkeley National Laboratory, University of California, Berkeley, CA, Univ. Lille, CNRS, Centrale Lille, Univ. Polytechnique Hauts-de-France, UMR 8520 -IEMN – Institut d'Electronique, de Mic, University of Nantes, CNRS, Institut des Matériaux Jean Rouxel, IMN, F-44000 Nantes, France, Sofia University, Faculty of Physics, 5 James Bourchier Boulevard, 1164 Sofia, Bulgaria, Department of Physics, University of Warwick, Gibbet Hill Road, Coventry CV4 7AL, United Kingdom, UMR Institut des Sciences Chimiques de Rennes URI-CNRS 6226, Université de Rennes 1, Campus de Beaulieu, CS 74205, F-350*

**(Tues-P31) Confocal Raman Microscopy Investigations of the Two-Step Functionalization of Porous Chromatographic Silica**  
Maran Sardoni, Joel Harris, Jay Kitt, *University Of Utah*

**(Tues-P32) SERS-based Kinetic Monitoring of the Pt-catalyzed Reduction of the Three Nitrothiophenol Isomers on Gold Nanorods**  
Daniel Schäfer, Jesil Jose, Roland Grzeschik, Sebastian Schlücker, *University Duisburg-Essen*

**(Tues-P33) Design of Aptamer-based Reagentless SERS Sensors for Environmental Analysis**  
Manisha Sheokand, Lyndsay N. Kissell, Pietro Strobba, *University Of Cincinnati*

**(Tues-P35) Optimizing Label-Free Exosome Analysis with Surface-Enhanced Raman Scattering (SERS) and Machine Learning for Non-Invasive Cancer Diagnostics**

Der Vang, Maria S. Kelly, Manisha Sheokand, Manju Sharma, Leyla Esfandiari, Ruxandra I. Dima, Pietro Strobba, *University Of Cincinnati*,

**(Tues-P36) Non-Negative Matrix Factorization with Raman Hyperspectral Imaging for Immobilized Biocatalyst Analysis**  
Hong Wei, Joseph Smith, *Merck*

**(Tues-P37) Visual Time-Temperature Indicators of Biospecimen Exposure to Thawed Conditions**  
Jorvani Cruz Villarreal, Emil Ljungberg, Aaron Gabriel Uy, Chad Borges, *Arizona State University*

**(Tues-P39) Synchrotron-infrared microspectroscopy of live Leishmania major infected macrophages and isolated promastigotes and amastigotes**  
Thulya Chakkumpulakkal Puthan Veettil, Rebekah Duffin, Supti Roy, Jitraporn Vongsvivut, Mark Tobin, Miguela Martin, John Adegoke, Philip Andrews, Bayden Wood, *Monash University, Australian Synchrotron*

**(Tues-P40) Smart Polymer Analysis using Raman Two-Dimensional Correlation Spectroscopy**  
Julian Hniopek, Josefine Meurer, Robin Kampes, Stefan Zechel, Martin Hager, Michael Schmitt, Juergen Popp, *Leibniz Institute of Photonic Technology Jena, Friedrich Schiller University Jena, Institute of Organic and Macromolecular Chemistry*,

**(Tues-P42) Molecular Compositional Study of Lipid Droplets During De Novo**

**Lipogenesis in Hyperglycaemic Live  
Hepatic Cells Using Confocal Raman  
Micro-spectroscopy**

Pradjna Novedya Paramitha, Bibin Bintang  
Andriana, Kosuke Hashimoto, Hidetoshi  
Sato, *Kwansei Gakuin University*,

**(Tues-P43) Photostability and Excited-  
State Features of Vulpinic Acid, a Natural  
Ultraviolet-Screening Compound**

Derek Moore, Tanzil Mahmud, Christopher  
Jeffrey, Matthew Tucker, *University Of  
Nevada, Reno*

**(Tues-P45) The CytoR1™: Optimization  
of a Commercial Dielectrophoretic Label-  
Free Cell Sorting Platform**

KATHERINE DEGEN, Alexandra Hyler,  
Dean Thomas, Kyle Brown, Ridi Barua,  
*CytoRecovery*

## **TECHNICAL PROGRAM- WEDNESDAY POSTERS**

**Poster Sessions | 10:10AM – 10:45AM & 3:10PM- 3:50PM | Nugget Foyer**

**(Wed-P1) Investigating Recycled Battery  
Materials using ICP-MS and TG-IR  
Spectroscopic Methods**

Aniket, Kieran Evans, Chady Stephan,  
*PerkinElmer*

**(Wed-P2) -Withdrawn**

**(Wed-P3) Investigating the bacterial  
protein quality control system with  
AFM-IR nanospectroscopy**

Wouter Duverger, Grigoria Tsaka, Katerina  
Konstantoulea, Ladan Khodaparast, Laleh  
Khodaparast, Nikolaos Louros, Joost  
Schymkowitz, Frederic Rousseau, *Catholic*

*University Leuven / Flemish Institute of  
Biotechnology*

**(Wed-P4) Chemical Characterization of  
Single Seeds with Fourier Transform  
Near Infrared Spectroscopy**

Warren Edmunds, Justin Linehan, Ryan  
Smith, *PerkinElmer*

**(Wed-P5) An Optimized Purification  
Protocol for Enzymatically Synthesized S-  
Adenosyl-L-Methionine (Sam) for  
Applications in Solution State Infrared  
Spectroscopic Studies**

ISAIAH ODEYEMI, Teri Douglass,  
Nosakhare Igie, James Hargrove, Grace  
Hamilton, Brianna Bradley, Cathy Lee,  
Brenden Le, Maitra Unjia, Dylan Wicherts,  
Zackery Fernyhough, Anjali Pillai,

Shailendra Koirala, Laure Hagge, Raymond Trieval, Robert Fick, Allison Stelling, *UTD*

**(Wed-P6) Inhibition of vibrational energy flow within an aromatic scaffold via heavy atom effect**

Majid Hassani, *University Of Nevada Reno*

**(Wed-P7) Total Value Chain Testing Solutions for Biodiesel and Bioethanol Production – from Feedstock to Final Blend**

Nicholas Lancaster, Chady Stephan, Aaron Hineman, *PerkinElmer*

**(Wed-P8) Structural Elucidation of Methylpyridine Derivatives Using Complimentary Analytical Techniques Coupled with Computational Modelling.**

Joshua Johnson, Ms Michael Bishop, David Archer, Brett Marsh, *Corteva Agriscience*, Ziyang Fan, University of California, Berkley, Hannah Zimmerman-Federle, *Indiana University - Purdue University, Indianapolis*

**(Wed-P9) Vibrational energy flow in complex ligand scaffolds revealed via 2D IR spectroscopy**

Christopher Mallon, Mohammad Zafar Abbas, Matthew Tucker, Ana de Bettencourt-Dias, *University Of Nevada, Reno*

**(Wed-P10) Sophisticated ATR correction**

Thomas Mayerhoefer, Juergen Popp, *Leibniz Institute Of Photonic Technology*, William Costa, *Fiveash Data Management, Inc.*

**(Wed-P11) The Effect of Agglomeration of Colloidal Particles on Near-Infrared Light Scattering Properties: Studied by Molecular Dynamics Simulation and Electromagnetic Wave Theory**

Hyeonwoo Na, Hiroyuki Fujii, Kazumichi Kobayashi, Masao Watanabe, *Hokkaido University*

**(Wed-P12) Light scattering properties for a coagulation process in soy milk**

Koyata Nishikawa, *Hokkaido University*

**(Wed-P13) Investigating the Stability of Biodegradable, Bio-Based, and Compostable Materials with Infrared Spectroscopy and Microscopy**

Lauren Ostopowicz, Victoria Benitez, Liang Zhao, Gilbert Vial, *Shimadzu Scientific Instruments*

**(Wed-P14) -Withdrawn**

**(Wed-P15) ID Testing of Raw Materials for Cell Therapy Products.**

Kristia Rivera, John Vergara, Mark Wang, Ravi Kalyanaraman, *Bristol-Myers Squibb (BMS)*

**(Wed-P16) -Withdrawn**

**(Wed-P17) Protein-Membrane Fiber Interactions in Hemodialyzers: A Multimodal Infrared Spectroscopy and Imaging Approach**

Suruthikha Vijay, William Querido, Azita HassanMazandarani, Rouzbeh Tehrani, Nancy Pleshko, *Temple University*

**(Wed-P18) Evaluation of the Quality and Safety of Hand Sanitizers Marketed in Saudi Arabia**

Ibrahim Alothaim, *Saudi Food and Drug Authority*

**(Wed-P19) Advancing Wheat Crop Nutrient Profiling Using Hyperspectral Sensing**

Anmol Kaur Gill, Darren T. Drewry, *The Ohio State University*

**(Wed-P20) Overview of Additive Manufacturing and 3-D Printing Utilizing Numerous Analytical Techniques**

Thomas Dillon, Chady Stephan, *Perkinelmer*

**(Wed-P22) -Withdrawn**

**(Wed-P23) Development of a Microwave-Enhanced Glow Discharge Atomic Emission Spectrophotometer**

Mitchell Stry, Steven Ray, *Department of Chemistry, Federal University of Piauí - UFPI*

**(Wed-P24) Real-time upstream process monitoring by Time-gated Raman spectroscopy**

Jacopo Zini, Amuthachelvi Daniel, *Janssen Pharmaceuticals*, Mari Tenhunen, *Timegate Instruments Ltd.*

**(Wed-P25) Timegate Raman for continuous in-line monitoring of extracellular vesicles purification.**

Jacopo Zini, Heikki Saari, *Finnish Red Cross Blood Service, Helsinki, Finland*, Saara Laitinen, Amuthachelvi Daniel, Mari Mari Tenhunen, *Timegate Instruments Ltd.*

**(Wed-P26) Electronic structure of lipid thin films using attenuated total reflectance spectroscopy in the far-ultraviolet region**

Yoshiki Hanjo, Yusuke Morisawa, *Kindai University*

**(Wed-P27) Investigating the Solution Structure of Hydrate Melt (HM) using NearInfrared Spectroscopy**

Shoichi Higashi, Yusuke Morisawa, *Kindai University*

**(Wed-P28) Development and Applications of Full-Vacuum FT-IR with Fully Automatic Switching Mechanism of Optical Elements for Seamless Analysis in Wide Wavenumber Range from Far-infrared to Near-infrared**

Kohei Tamura, Ken-ichi Akao, Yukihiro Ozaki, *JASCO Corporation*

**(Wed-P29) -Withdrawn**

**(Wed-P30) Optical and Structural Characterization of Plasmonic Nanocrescents as a Tunable Platform for Vibrational Circular Dichroism Spectroscopy**

Flore Elliott, *Westminster University*, Aria Ballance, Jennifer Shumaker-Parr, *University Of Utah*

(Wed-P31) **Effects of Crime Scene Contaminants on Surface-Enhanced Raman Analysis of Hair**  
Isaac Juarez, Dmitry Kurouski, *Texas A&M*

(Wed-P32) **Quantifying the ultrafast and steady-state molecular reduction potential of a plasmonic photocatalyst**  
Chris Warkentin, Renee Frontiera, *University Of Minnesota*

(Wed-P33) -Withdrawn

(Wed-P34) **Quantitative evaluation of IR and corresponding VCD spectra** Thomas Mayerhoefer, Singh, Jer-Shing Huang, Christoph Krafft, Juergen Popp, *Leibniz Institute Of Photonic Technology*

(Wed-P35) **Cavity Ring-Down Spectroscopy: High Sensitivity in Littoral Environments**  
Eric Languirand, Ian Pardoe, DEVCOM *CBC*

(Wed-P36) **Understanding Kink Formation In Cellulose Nanocrystals** Sung Park, Yun Jing, Jia Hui Lim, Edgar Rauch, Yu Ogawa

(Wed-P37) **Widefield Super-Resolution IR Imaging with Fluorescence Enhanced Photothermal Infrared Spectroscopy**  
Mustafa Kansiz, Jay Anderson, *Photothermal Spectroscopy Corp.*

(Wed-P38) **On-site quality screening of pisco distillates based on spectroscopy techniques**

Yalan Wu, Didem Aykas, Ahmed Menevseoglu, Siyu Yao, Luis Rodriguez-saona, *The Ohio State University*

(Wed-P39) **Two-Pulse and Three-Pulse UV-Vis-mid IR Transient Absorption Spectroscopies to Explore Photophysical Dynamics of Energy Harvesting “Molecular Speedometers”**

Dalath Kasun Mendis, Xiao Li, Igor Rubtsov, *Tulane University*, Jesús Valdiviezo, Peng Zhang, David Beratan, *Duke University*, Susannah Banziger, *Purdue University*, Tong Ren, *aGhent University*

(Wed-P40) **Investigating local environment effects on intramolecular proton transfer dynamics in anthrarufin films**  
Yingshi Feng, Christopher Jeffrey, Matthew Tucker, *University of Nevada, Reno*

(Wed-P41) **Standoff Infrared Detection of Thin-Layer Deposits Using Synthetic Reference Signatures from the Optical Constants**  
Olivia M. Primera-Pedrozo, Charmayne Lonergan, Jeremy Erickson, Sarah Burton, Bruce Bernacki, Molly Rose Kelly-Gorham, Michael Wilhelm, Brenda Forland, Kendall Hughey, Tanya Myers, Timothy Johnson

(Wed-P42) **Flipping Out (Or In) About Vitamin E: What Nonlinear Optical Spectroscopy Can Teach Us About the Movement of Vitamin E Through Membranes**  
Joshua Taylor, John Conboy, *University of Utah*



**(Wed-P43) Integrating AI-based Software  
RAMANMETRIX and Raman  
Spectroscopy for Real-time Analysis of  
Complex Bioprocesses**

Olivia Treuheit, Joerg Weber, Biophotonics  
Diagnostics GmbH, Oleg Ryabchykov,  
Darina Storozhuk, Leibniz Institute of  
Photonic Technology (IPHT), Oliver Valet,  
MIBIC GmbH & Co KG

**(Wed-P44) Precise Testing of Surface  
Modification/Functionalization Processes  
for Biotech Devices**

Sung Park, Derek Nowak, Padraic O'Reilly,  
Molecular Vista

**TECHNICAL PROGRAM- THURSDAY POSTERS**  
**Poster Sessions | 10:10AM – 10:45AM & 3:10PM- 3:50PM | Nugget Foyer**

**(Thurs-P1) On the Behavior of  
Microplastics Subjected to AC Insulator-  
based Dielectrophoresis**

Shulin Bu, Domin Koh, Alexandra Ros,  
*Arizona State University*

**(Thurs-P2) Dielectrophoresis as a  
detection tool for Rickettsial diseases**

Negar Farhang Doost, Soumya K  
Srivastava, *Department Of Chemical And  
Biomedical Engineering, West Virginia  
University*

**(Thurs-P3) Self-focusing DLP-based 3D  
Printing Enables On-chip Integration Of  
Soft Functional Materials In  
Electrokinetic Microfluidic Devices**

Guillermo Ramirez, Diego Cabello,  
Gongchen Sun, *University Of Texas At San  
Antonio*

**(Thurs-P4) 3DEP Characterization of  
Human Mesenchymal Stem Cells and the  
Development of DEP-based Cell Sorting  
Strategies**

Zuri Rashad, Anthony Tsai, Kiara Lacy,  
Sune Terbush, Lexi Crowell, Stephany  
Alonso, Tayloria N.G. Adams, *University of  
California, Irvine*

(Thurs-P5) -Withdrawn

**(Thurs-P6) Human Mesenchymal Stem  
Cell Sorting with Dielectrophoretic-  
based Microfluidic Devices**

Sune Terbush, Tayloria N.G. Adams,  
*University of California Irvine*

**(Thurs-P7) Dielectric characterization of  
ductal adenocarcinoma using murine  
PyMT+/- model**

Raphael Oladokun, Sai Deepika Reddy  
Yaram, Timothy Eubank, Soumya K  
Srivastava, *West Virginia University*

**(Thurs-P8) Investigation of Zinc Soap  
Formation and Damage Mechanisms in  
Oil Paintings**

Klavdija Bukovec, Stephanie Zaleski,  
*California State University East Bay*

**(Thurs-P12) GC–MS and GC–IR of  
Regioisomeric 4-N-Methoxy- and  
Dimethoxybenzyl Derivatives of 3-  
Chlorophenylpiperazine**

Randall Clark, Mohammad Almalghrabi,  
Younis Abiedalla, Auburn University

**(Thurs-P13) The Application of Particle-  
Correlated Raman Spectroscopic  
Analysis of Soils to Mock-Casework  
Scenarios**

Samantha Gong, Brooke Kammrath,  
University of New Haven, Marisia Fikiet,  
Peter De Forest, *Forensic Consultants*

(Thurs-P14) -Withdrawn

**(Thurs-P15) Enhancing Forensic Science:  
Urine Stain Analysis with Raman  
Spectroscopy and Chemometrics for  
Race Identification**

Bhavik Vyas, Igor Lednev, University at  
Albany, Lenka Halamkova, Texas Tech  
University

**(Thurs-P16) Identifying the effects of  
Bluestar Forensic Spray on the ability to  
identify bloodstains using Raman  
spectroscopy**

Alexis Weber, Igor Lednev, *University at  
Albany*

**(Thurs-P17) Single Particle Interaction  
With Short Focus and Filament Laser  
Produced Plasmas**

Thiago Arnaud, Digital Surf, Kyle Latty,  
Kyle C. Hartig, *University Of Florida*

**(Thurs-P18) Laboratory time-resolved  
LIBS to support the SuperCam analyses  
on Mars.**

Bruno Bousquet, University Of Bordeaux,  
Elise Clavé, *DLR, Sylvestre Maurice, IRAP*

**(Thurs-P19) Heavy Metal Quantitation  
Comparison of Hand-Held Laser Induced  
Breakdown Spectroscopy to Other  
Analytical Instrumentation**

Jay Clausen, Sam Beal, *US Army Corps of  
Engineers, Engineer Research And  
Development Center*, Michael Bishop,  
*Corteva Agriscience*, Patrick Sims, *Naval  
Information Warfare Center Pacific*

**(Thurs-P20) Feasibility of laser-induced  
breakdown spectrometry for  
determination of neodymium in magnet  
alloys**

Aline de Carvalho Elias, Maciel Santos Luz,  
Ivanise Gaubeur, Juliana Naozuka, Fábio  
Rocha, Cassiana Nomura, *University Of Sao  
Paulo*

**(Thurs-P21) Distribution Of Rare-Earth  
Elements In Metamorphic Rocks : New  
Contributions From Micro Laser Induced  
Breakdown Spectroscopy Imaging**

Cecile Fabre, Alexandre Tarantola, Behzad  
Monfaredi, Lucas Marulier, Vincent Motto-  
Ros *Georessources*

**(Thurs-P22) Identification of  
Fluoroquinolone-Resistant  
Mycobacterium Tuberculosis through  
Random Forest-Support Vector Machine  
Combined with Intensity Ratio Analysis  
using Laser-Induced Breakdown  
Spectroscopy**

Hohyun Keum, Gookseon Jeon, Soogeun  
Kim, Kyunghwan Oh, Heejoo Lee, Janghee  
Choi, *Korea Institute of Industrial  
Technology*

**(Thurs-P24) Hybrid Raman spectroscopy and laser-induced breakdown spectroscopy system applied to food safety**

Sungho Shin, Iyll-Joon Doh, Kennedy Okeyo, Euiwon Bae, J. Paul Robinson, Bartek Rajwa, *Purdue University*

**(Thurs-P25) High-resolution high-speed LIBS imaging**

Elena Vasileva

**(Thurs-P26) Excimer Laser Ablation-Based Tandem Approach to the Analysis of Solid Samples**

Jhanis Gonzalez, Charles Sisson, Excimer Laser Ablation-Based Tandem Approach to the Analysis of Solid Samples Chunyi Liu, Steve Shuttleworth, Miyeun Yoo, *Applied Spectra Inc*, Richard Russo, *LBNL/ASI*, *Applied Spectra Inc*

**(Thurs-P27) Optimization of Cannabinoid Extraction Conditions Including Solvent Choices Using Microwave and Ultrasonication Methods**

Joshua Animasaun, Ngee Chong, Beng Ooi, *Middle Tennessee State University*

**(Thurs-P28) Cationic Isotachophoresis of Engineered Gold Nanoparticles For Enhanced Lateral Flow Assay**

Devon McCornack, Wen-Ji Dong, *Washington State University*

**(Thurs-P29) Scandium Stabilized Lipid Bilayer Coatings**

Christopher Harrison, Juliette Gonzales, *San Diego State University*

**(Thurs-P30) Increasing DEP-based separation to generate multiple A single-cell transcriptomic study of DEP-sorted mouse neural stem cell fractions**

Alan Jiang, Jazmine Moore, Nicole Lav, Lisa Flanagan, *University Of California, Irvine*

**(Thurs-P32) Determination of Chloride Ions in Water via Fluorescence Quenching of Rose Bengal**

Sulayman Oladepo, *King Fahd University of Petroleum and Minerals*

(Thurs-P33) -Withdrawn

(Thurs-P34) -Withdrawn

**(Thurs-P35) Lithium-Ion Battery Recycling with Field-Portable Handheld LIBS**

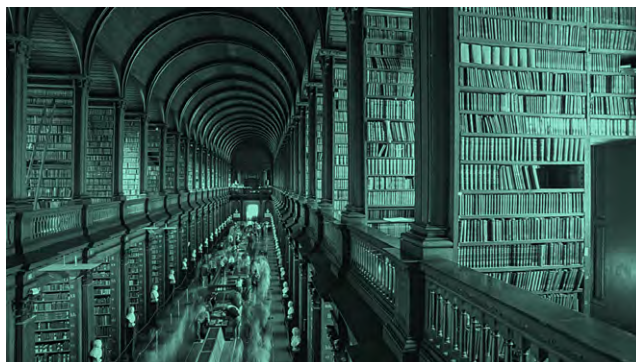
Brendan Connors, *Sciaps, Inc.*

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