

FACSS PRESENTS

SCIX 2024

51 St
ANNUAL MEETING



OCTOBER 20-25, 2024
RALEIGH CONVENTION CENTER
RALEIGH, NC

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*Please 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 SCI X 2024

On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) and the 2024 SciX organizational team, it is my pleasure to welcome you to Raleigh, North Carolina for the SciX 2024 Conference. Last year we reached our 50th anniversary milestone and celebrated our past meetings. This year we continue our journey pursuing the latest technological achievements and challenges facing analytical chemistry, measurement and data sciences. The digital world is advancing rapidly and the theme to this year's meeting addresses this head on. Those familiar with the SciX meeting know it brings an international community together to present and discuss their latest research, network and socialize in relaxed environments, see longtime friends, and create new friendships. If you're new to SciX, you will experience a very welcoming community where you can see and meet with world renowned scientists, discuss topics ranging from the latest discoveries to how to balance life, and pursue the science that we all have a deep passion to pursue. We truly believe SciX is the "Right Size, Right Science, Right Conference", where people come together and foster new ideas.

The cornerstone of the meeting revolves around the technical program which has been organized by our **Program Chair, Jake Shelley**, from Rensselaer Polytechnic Institute. Jake has selected "**Sci eX Machina: Analytical Instrumentation in the Age of Artificial Intelligence**" as the very relevant topic for our current time. The Sunday keynote lecture will be presented by Joseph Viviano, an emerging leader in the field of Artificial Intelligence. The theme extends into the rest of the technical program, where presentations exploring AI and machine learning are spread across the 125 oral sessions within the 17 different sections of the meeting. In addition to the 600+ invited and contributed oral presentations, there will be 8 plenary lectures showcasing award winners and 200+ posters from Sunday to Thursday. The final "SciFri" session on Friday morning (with breakfast!) features **Prof. Gary Hieftje** from Indiana University discussing the history and impact of computers on chemical instrumentation. **Dr. Caelin Celani**, from the University of Delaware, will follow that presentation with a discussion of the current-state and future prospects for how AI and machine learning will revolutionize chemical analysis. Speaking of Prof. Hieftje, there will be three sessions on Wednesday and Thursday honoring his illustrious 50+ career that includes former students, post-docs, colleagues, and collaborators. Two of those sessions will be in the "shootout" style pioneered by Prof. Hieftje; you won't want to miss those!

A tremendous "thank you" goes out to the large number of Section and Session Chairs! An enormous amount of their time and effort has gone into organization, planning, invitations, fund-raising, etc. to make this conference a success. This meeting and gathering would not be what it is without the tireless efforts of these volunteers. Thank you all!

SciX is also where we get to recognize numerous outstanding scientists for excellence in their fields and present them with awards for their work. The **Awards Chair** (who is also next year's Program Chair), **Brooke Kammrath**, from the University of New Haven, has done a tremendous job organizing the awards plenaries and symposia.

In addition to the world-class technical program, SciX has a very active Exhibition, organized by our **Exhibits Chair, Scott Rudder**, from OptoSigma. Integrated into the exhibits this year will be a **Career Fair with Professional Development Seminars**. This year for the first time, entry into the exhibits and career fair will be **FREE**.

FACSS and SciX believe we never stop learning and our short courses offer a wide range of topics. **Ellen Miseo, Short Course Chair**, has arranged a wonderful slate of courses that will entice students and seasoned scientists alike to continue their intellectual pursuits.

Diversity, Equity, and Inclusion (DEI) is an idea where EVERYONE can benefit and make synergistic progress when we include the ideas, opinions, and cultures from ALL our peers. This year for the first time, we have Dr. Alexis Weber as our DEI Chair. Alexis has taken on this role with an ambition and gusto as only she can. In addition to establishing goals and reaching out to HBCU's, she has arranged for the first "Celebrating Women in Spectroscopy" networking breakfast on Tuesday morning.

In order to get the word out and grow our meeting, we have a talented **Marketing Chair, Tina Gong**, who will be stepping down after this year. **THANK YOU, TINA!** for all your efforts over the years. Your contributions have been very much appreciated. The incoming **Marketing Chair, Abigail Bauer**, has been shadowing Tina this year and is ready to carry the torch forward. **Mike Sullivan, Local Chair**, provided great local support and outreach.

Karen Esmonde-White, Governing Board Chair for FACSS, has been a very welcoming and easy-going leader thru this year to get us where we are today. In addition, conference issues, she runs the Federation which consists of 14 scientific organizations. Karen also chairs the FACSS Executive Committee which includes the Past Governing Board Chair **Mike Carrabba**, Governing Board Chair Elect **Mark Hayes**, Treasurer **Ian Lewis**, Secretary **Gary Brewer** and Marketing Chair **Tina Gong**. While their efforts may be more behind the scenes, their extraordinary dedication provides the continued leadership for continuity and growth of FACSS year to year. Everyone I have mentioned are volunteers who get involved for the love of moving the conference into the next 50 years. Are you one of the next leaders of FACSS/SciX?

We also have an association management team at Talley that keeps us on task and who you will be seeing at registration and around the conference. Many Thanks to **Stephanie Moyer, Lindsey Boadi, and Andrea Taylor** at Talley, we couldn't have done it without you.

Finally, I want to say that SciX is truly a networking scientific conference and we have provided many networking opportunities for you thru the week. These are great opportunities to ask that question of a speaker, meet with companies on the exhibition floor, discuss new collaborations or job opportunities, or just socialize with old/new friends. There will be coffee breaks and lunches during the week, an exhibit opening on Monday and happy hour on Tuesday, an SAS Wine and Cheese on Tuesday, a Coblenz event on Wednesday night (see booth for details!), and of course the Gala on Thursday. This year's gala theme will be Spirit Week, homecoming, and tailgating. We encourage everyone to dress up (costume prizes) in their best game face, homecoming queen/king, cheerleader, or where your imagination takes you. There will be plenty of food, drinks, games, music and dancing to wrap of the conference with a festive atmosphere.

Sincerely,



SciX 2024 General Chair
Greg Klunder
Lawrence Livermore National Laboratory

SciX 2024 Committee



SciX 2024 Program Chair
Jake Shelley
Rensselaer Polytechnic Institute



SciX 2024 Awards Chair
Brooke Kammrath
Henry C. Lee Institute of Forensic Science



SciX 2024 Exhibits Chair
Scott Rudder
OptoSigma



SciX 2024 Short Course Chair
Ellen Miseo
Miseo Consulting



SciX 2024 DEI Chair
Alexis Weber
University of Albany, SUNY



FACSS/SciX Marketing Chair
Tina Gong
Revvity



FACSS/SciX Incoming Marketing Chair
Abigail Bauer
Oxford Instruments Andor



SciX 2024 Local Chair
Mike Sullivan
SensIR Inc.

FACSS AND SciX CONFERENCE ORGANIZATION

FACSS Member Organizations

American Chemical Society Division of Analytical Chemistry
AES Electrophoresis Society
American Society for Mass Spectrometry
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

2024 FACSS Executive Committee



Governing Board Chair: Karen Esmonde-White
Endress+Hauser

Governing Board Chair-Elect: Mark Hayes, *Arizona State University*

Past Governing Board Chair: Mike Carrabba, *Droplet Measurement Technologies*

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

Treasurer: Ian Lewis, *Endress+Hauser*

Marketing Chair: Tina Gong, *Revvity*

SciX 2024 Section Chairs

Hunter Andrews
Caelin Celani
Xiaoyun Chen
Malama Chisanga
Chris Chouinard
Mary Kate Donais
Michael George
Duncan Graham
Peter Harrington
Katherine Hollywood
Alexandra Hyler
Brooke Kammrath
Rob Lascola

Bernhard Lendl
Ian Lewis
Kristen Livingston
Benjamin Manard
Curt Marcott
Jean-Francois Masson
Pavel Matousek
Yusuke Morisawa
David Muddiman
Gabe Nagy
Fay Nicolson
Yukihiro Ozaki
Juergen Popp

Derrick Quarles
Georg Ramer
Emilie Ringe
Mike Roper
Jim Rydzak
Bhavya Sharma
Jacob Shelley
Sian Sloan-Dennison
Soumya Srivastava
John Wasyluk
Alexis Weber
Andrew Zipkin

GENERAL INFORMATION

LOCATION of all plenaries, symposia, short courses, workshops, and exhibits is the Raleigh Convention Center and Marriott Raleigh City Center. A facility map can be found in the mobile app.

CONFERENCE REGISTRATION / INFORMATION DESK

is in the Exhibit Hall Foyer on the 100 level and hours are as follows:

Sunday	3:00 pm – 7:30 pm
Monday	7:00 am – 6:00 pm
Tuesday	7:30 am – 5:00 pm
Wednesday	7:30 am – 5:00 pm
Thursday	7:30 pm – 4:30 pm

INTERNET ACCESS is available in all meeting areas. Select the Raleigh Convention Center network. There is not a password.

PRESENTERS should check the author index 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.

ORAL SYMPOSIA are scheduled Monday through Thursday.

Monday	10:30am – 12:10pm; 1:30 – 3:10pm; 3:50 – 5:30pm
Tuesday	10:30am – 12:10pm; 1:30 – 3:10pm; 3:50-5:30pm
Wednesday	10:30am – 12:10pm; 1:30 – 3:10pm; 3:50-5:30pm
Thursday	10:30am – 12:10pm; 1:30 – 3:10pm

POSTER SESSIONS

The location of the poster sessions changes depending on the day, so please be sure to check the program on where the poster session will take place that day.

Posters must remain up all day on your designated day – early removal is not permitted. On the day of your poster presentation, you should be present for both poster sessions. Please set your poster up no later than 9:15am on the day of your poster session. Please remove your poster by 4:00pm on the day of your poster session. Any posters that have not been picked up from the poster board area by the end of the day will be discarded.

Sunday, Ballroom B

7:15 – 9:15pm

Welcome Mixer and Student Poster Event, Sponsored by FACSS, SAS, Coblenz, and Procter & Gamble

Monday, Ballroom B

9:30 – 10:30am and 3:10 – 3:50pm
Coffee & Poster Session

Tuesday, Exhibit Hall B

9:30 – 10:30am and 3:10 – 3:50pm
Coffee/Refreshments & Poster Session

Wednesday, Exhibit Hall B

9:30 – 10:30am and 3:10 – 3:50pm
Coffee/Refreshments & Poster Session

Thursday, Ballroom Foyer

9:30 – 10:30am and 3:10 – 3:30pm
Coffee/Refreshments & Poster Session

SHORT COURSES / WORKSHOPS offer a variety of introductory and fundamental topics. Onsite registration is available at the registration desk – space permitting. Deeply discounted rates available for students. See page 21 for all course offerings.

EXHIBITS information is available on page 10.

Hours are:

Monday Opening Reception	5:30 – 7:30pm
Tuesday Hall Hours	9:30am – 5:00pm
What's Hot Presentations	12:00 – 1:30pm
Wednesday Hall Hours	9:30am – 4:00pm
What's Hot Presentations	12:00 – 1:30pm

COMPLIMENTARY LUNCH is offered in the exhibit hall on Tuesday and Wednesday from 12:00 – 12:30pm only for registered conferees. A **TICKET IS REQUIRED** and can only be obtained when you pick up your badge.

COMPANION REGISTRATION includes the Sunday Evening Welcome Mixer, Monday Exhibit Hall Opening Reception, and Thursday night Gala Event. Cost is \$175 and companions may be added at registration.

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

Welcome Mixer and Student Poster Event,

Sponsored by FACSS, SAS, Coblenz, and Procter & Gamble

Sunday, 7:15pm, Ballroom B

Exhibit Opening and Reception

Monday, 5:30pm, Exhibit Hall B

Exhibitor Happy Hour

Tuesday, 5:30pm, See App for location

SCIX 2024 Gala Event

Thursday, 7:00pm, Ballroom B&C

MOBILE APP includes the most current program information, updated as changes happen. Accept all prompts for updates!



EVENTS OF INTEREST TO STUDENTS, JOB BOARD, CODE OF CONDUCT AND GALA

Events of Interest to Students

Sunday • 7:15 – 9:15 pm	Welcome Mixer and Student Poster Event, Sponsored by FACSS, SAS, Coblenz, and Procter & Gamble <i>Ballroom B</i>
	Student Award presentations by SAS, FACSS, and Coblenz
Monday through Friday	FACSS Student Poster Awards will be announced daily before each Plenary Session <i>Ballroom A</i>
Monday • 12:10 – 1:30pm	Coblenz Speed Mentoring, (seating is limited) <i>Ballroom C</i>
Tuesday • 7:00am	Networking Breakfast Honoring Women in Spectroscopy, Sponsored by FACSS, SAS, Coblenz, and Spectroscopy Magazine (SOLD OUT) <i>Room 304</i>
Monday through Thursday	Job Board, Registration Area <i>Exhibit Hall Lobby</i>
Tuesday & Wednesday • 9:30am – 4:00pm	Career Fair <i>Exhibit Hall B</i>

Job Board

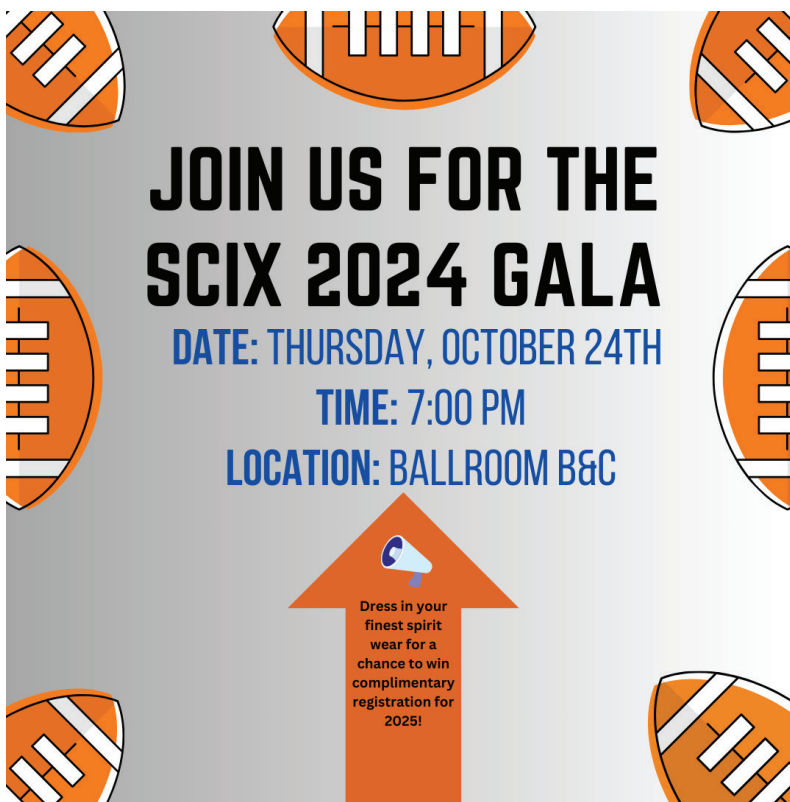
There is a job board located in the Career Fair in Exhibit Hall

EMPLOYERS: Bring a hard copy of job opportunities to display on a poster board.

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

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

SciX 2024 Gala



**JOIN US FOR THE
SCIX 2024 GALA**

DATE: THURSDAY, OCTOBER 24TH

TIME: 7:00 PM

LOCATION: BALLROOM B&C

Dress in your finest spirit wear for a chance to win complimentary registration for 2025!

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 and/or expelled from the conference without a refund at the discretion of the conference organizers.



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Special

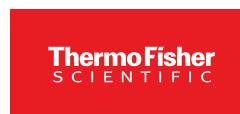


Analyst

Royal Society of Chemistry - Journal of Analytical

Atomic Spectrometry

Atomic



Thermo Scientific

Atomic

FRIENDS OF SCI-X

Applied Spectra Inc — *Atomic*
Barry M Wise/Eigenvector — *Chemometrics*
Burgener Research Inc. — *Atomic*
Drs. Ian and Mary Lewis
Elemental Scientific Lasers — *Atomic*
Farida Fadly — *Atomic*
Glass Expansion — *Atomic*
Harrington Center for Intelligent
Instrumentation — *Chemometrics*
LECO Corporation — *Atomic*
MassTech — *Mass Spectrometry*

Mettler Toledo — *Process Analytical Technology*
Nu Instruments — *Atomic*
Nu Instruments - AMETEK — *Atomic*
PerkinElmer — *Atomic*
Photothermal Spectroscopy Corp — *IR*
Roger Easton — *Art and Archeology*
Royal Society of Chemistry – Analyst — *Raman*
SciAps Inc — *Art and Archeology*
Sociedad Española de Espectroscopia Aplicada (SEA) —
Atomic
Teledyne Princeton Instruments — *Atomic*
YYZ Pharmatech — *Pharmaceutical Analysis*

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NECSEL IP, Inc.

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Spectroscopy Magazine

MEDIA PARTNERS

American Pharmaceutical Review
The Analytical Scientist
Applied Spectroscopy
AuthentiCHEM

BioPharma Asia
ICP Winter Conference
Photothermal Spectroscopy Corp.
Pittcon
Separations

SOCIETY AND COMMITTEE MEETINGS

FACSS / SciX

Sunday, October 20

1:00 – 3:00pm

SciX 2025: Budget/General Planning/Program | *Room 304*

3:00 – 5:30pm

FACSS Long Range Planning | *Room 304*

Monday, October 21

12:00 – 1:30pm

SciX 2026 General Planning | *Room 304*

Tuesday, October 22

12:00 – 1:30pm

FACSS Budget Committee and Finance Committee | *Room 304*

Wednesday, October 23

7:00 – 8:30am

Executive Committee Meeting (for the Executive Committee only) | *Room 304*

Thursday, October 24

12:00 – 2:00pm

Governing Board Meeting (for Governing Board Members only) | *Room 304*

AES ELECTROPHORESIS SOCIETY

Monday, October 21

12:10 – 1:30pm

AES Monday General Body Meeting (AES Members Only) | *Room 306C*

COBLENTZ

Monday, October 21

7:00 – 8:00am

Coblentz Member Meeting and Breakfast | *Room 304*

12:10 – 1:30pm

Coblentz Speed Mentoring | *Ballroom C*

Registration is free; lunches will be provided with priority given to those who have pre-registered prior to the conference.

Wednesday, October 23

7:00 – 10:00pm

Members Only Coblentz Reception

Stop by the Coblentz booth for details and tickets!

SOCIETY FOR APPLIED SPECTROSCOPY/ COBLENTZ

Tuesday, October 22

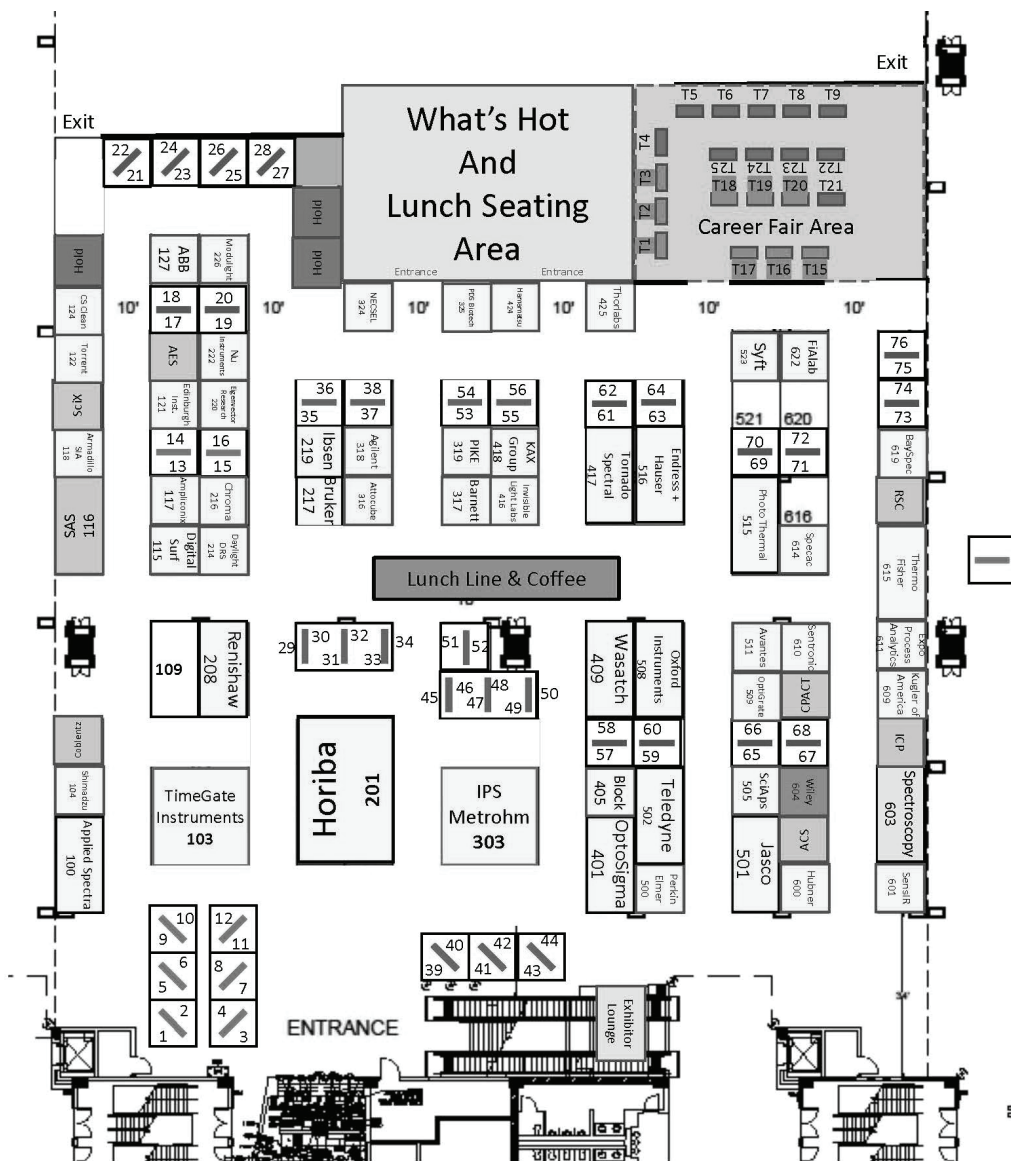
12:00 – 5:00pm

Headshots in Exhibit Hall | *Exhibit Hall B*

SciX EXHIBITS KEY

ABB Inc.....127
 ACS Division of Analytical Chemistry.....602
 AES Electrophoresis Society.....123
 Agilent.....318
 Ampliconx Oy.....117
 Applied Spectra Inc.....100
 Armadillo SIA.....118
 Arizona State University - School of Molecular.....T15
 attocube systems.....316
 Avantes.....511
 Barnett Technical Services.....317
 Block Engineering.....405
 Bruker.....217
 Chroma Technology.....216
 Coblenz Society.....106
 CPACT.....608
 CPACT.....T2
 CS Clean Solutions INC.....124
 Digital Surf.....115
 DRS Daylight Solutions.....214
 Edinburgh Instruments.....121
 Eigenvector Research.....220
 Endress+Hauser.....516
 Expo Process Analytics.....611
 FIALab Instruments.....622
 Hamamatsu Corporation.....424
 HORIBA.....201
 HORIBA.....T18
 HUBNER Photonics Inc.....600
 Ibsen Photonics.....219
 ICP Information Newsletter.....621
 Invisible-Light Labs GmbH.....416
 IPS/Metrohm.....303
 IPS/Metrohm.....T20
 Jasco Inc.....501
 KAX Group.....418
 Kugler of America, LTD.....609
 Modulight Corp.....226
 Nessel IP.....324
 Next Success.....T19
 Nu Instruments.....222
 Oak Ridge National Laboratory.....T16
 OptiGrate Corp.....509
 OptoSigma.....401
 Oxford Instruments.....508
 PerkinElmer.....500
 Photon Systems, Inc.....521
 PhotoThermal Spectroscopy Corp.....515
 PIKE Technologies.....319
 Protein Dynamic Solutions, Inc.....325
 Renishaw.....208
 Rensselaer Polytechnic Institute.....T17
 Royal Society of Chemistry.....617
 SciAps.....505
 SciX.....625

SensIR.....601
 Sentronic US Corp.....610
 Shimadzu.....104
 Society for Applied Spectroscopy.....114
 Specac.....614
 Spectroscopy.....603
 Syft Techno.....523
 Teledyne Princeton Instruments.....502
 Thermo Fisher Scientific.....615
 Thorlabs Inc.....425
 Timegate Instruments Ltd.....103
 Tornado Spectral Systems.....417
 Torrent Photonics.....122
 Wasatch Photonics.....409
 Wasatch Potonics.....T21
 Wiley Science Solutions.....604
 Wise Investigator LLC.....T1



FACSS AWARDS

FACSS TOMAS 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.



Henry T. Manelski

Henry T. Manelski is a Ph.D. student at Purdue University in the Department of Earth, Atmospheric, and Planetary Sciences (EAPS). After completing a Summer Undergraduate Research Fellowship (SURF) at JPL/Caltech working with data from the Curiosity rover, Henry earned a B.S. in Applied Mathematics from Columbia University in 2022.



Heidi V. Kastenholz

Heidi V. Kastenholz is a Ph.D. candidate in Chemistry at Duke University, advised by Dr. Warren S. Warren. She received her B.S. from Butler University in Indianapolis, IN.

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.



Mahsa Zarei

Mahsa Zarei is a Ph.D. candidate in Professor Edward Grant's group at the University of British Columbia.

FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS CALL FOR 2025 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 2025 at scixconference.org. To be considered for either award, students must submit an abstract for oral presentation at SciX (submission opens later winter/early spring 2025), then submit the following as a single PDF file:

- The application form (check in early 2025 for next year's application form)
- Two letters of nomination, including one by the student's mentor
- A copy of the candidate's résumé
- A copy of the candidate's graduate transcript
- Copies of reprints and/or preprints of research accomplished



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

FACSS AWARDS

FACSS INNOVATION AWARD

The FACSS Innovation Award is given to the most innovative and outstanding new research advancements debuted orally at the SciX Conference. All program areas are included. Only research findings presented for the first time in the public domain qualify for entry. Work based on submitted papers not yet published electronically or in print at the time of abstract submission also qualifies. All attendees are eligible for the award irrespective of educational level or professional vocation. 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.

2024 FACSS Innovation Award Symposium
Thursday, October 24 3:30- 5:30pm | Ballroom A



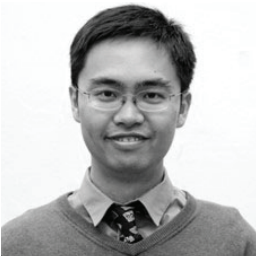
Robert Chimenti

“Entropically Induced Negative Absolute Temperature During Epoxy-Amine Polymerization”



Will Jones

“Calibration by Proxy”



Xiaoji Xu

“Development of Atomic Force Microscopy-Based Two-dimensional Infrared Nano-spectroscopy”



Yi You

“Advanced Repetition-Rate Modulation and Computational Strategies for Background-Free LIBS Using Non-Gated Spectrometers”

FACSS CHARLES MANN AWARD

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



Nick Stone

Prof Nick Stone worked as a Consultant Medical Physicist for almost 20 years in the NHS



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

SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

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.

Benjamin Manard

Benjamin T. Manard is a Senior R&D Staff Scientist and the Group Leader of the Chemical & Isotopic Mass Spectrometry Group at Oak Ridge National Laboratory (ORNL).

SAS APPLIED SPECTROSCOPY WILLIAM F. MEGGERS AWARD



This award is given by the Society of Applied Spectroscopy to the author(s) of an outstanding paper appearing in Applied Spectroscopy.

It is being awarded to:

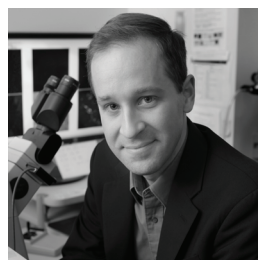
Ioan Notingher; Nathan Woodhouse; Jan Majer; Peter Marshall; Steve Hood for their paper "Quantification of Drugs in Brain and Liver Mimetic Tissue Models Using Raman Spectroscopy."

Ioan Notingher

Ioan Notingher is a Professor in the School of Physics and Astronomy, University of Nottingham and leads the Biophotonics Group

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.

Conor L. Evans

Dr. Conor L. Evans is an Associate Professor at the Harvard Medical School, an Affiliated Faculty member of the Harvard University Biophysics Program and leads his lab at the Wellman Center for Photomedicine at Massachusetts General Hospital.

WILLIAM G. FATELEY STUDENT AWARD



In 2010, the family and former group members of William G. Fateley, in conjunction with The Coblentz Society and The Society for Applied Spectroscopy, announced the formation of a Student Award to honor the career and life of William G. Fateley. The award consists of a cash prize to the selected student and a plaque. Winners are recognized at the annual SciX conference presented by FACSS.

Thulya Chakkumpulakkal Puthan Veetil

Thulya is hailing from a small state in India called Kerala. She has graduated in analytical chemistry from a prestigious joint Ph.D. programme between Monash University, Australia and University of Bath, United Kingdom (UK) under the guidance of Prof. Bayden R. Wood and Dr. Paul De Bank in March 2024.



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

COBLENTZ SOCIETY 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.



Riley Alpuché



Piyush Raj



Mireia Sainz-Menchón



Arnaud Laramee



Polly Lynch

COBLENTZ TRAVEL GRANT AWARDS

The Coblentz Society is committed to fostering the professional development of scientists practicing in the field of vibrational spectroscopy. To further this aim, the Society has grants designed to assist students and early-career professionals. Travel grants are available to assist in defraying the cost of travel to one of the conferences where the Coblentz Society is an active participant. Travel grants are intended to assist early-career professionals.

Dependent care grants are designed to assist parents, especially when both parents are involved in the scientific community, by defraying child or other dependent care costs to allow parents to attend conferences. Childcare grants are available to both students and early-career professionals. For more information, please visit the Coblentz Society website.

2024 Travel Grant Winners:

Yeran Bai (University of Arizona)
Alexis Weber (SupreMEtric LLC)
Magdalene Chong (University of Strathclyde)
Tabitha Jones (University of Cambridge)
Megha Mehta (University of Exeter)
Tanveer Shaik (Friedrich-Schiller-Universität Jena (University of Jena) Germany)

2024 Dependent Care Grant Winners:

Yeran Bai (University of Arizona)
Arun and Deepti Sharma (Dept. of Food Engineering, Natl. Inst. of Food Technology Entrepreneurship and Management (NIFTEM)), Haryana, India



For full bios, scan here to visit
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.

Jason Dwyer

Jason R. Dwyer is a Professor of Chemistry at the University of Rhode Island focusing on bioanalytical chemistry, nanofabrication, and technology development for the life sciences.

AES BLUE FINGERS STUDENT AWARD

The AES Student Award recognizes the most outstanding student paper submitted for the AES Annual Conference by a graduate student at the time of application



Alaleh Vaghef Koodehi
Rochester Institute of Technology



Raphael Oladokun
West Virginia University

AES LIFETIME ACHIEVEMENT AWARD



The AES Lifetime Achievement Award is given for exceptional career contributions to the fields of Electrophoresis, Electrokinetics, and related areas. One award is presented every year at the AES Annual Meeting. The recipient of the award will receive a plaque, a certificate of lifetime membership in the society, and one complementary registration to the annual meeting where the award will be presented.

Victor Ugaz

Victor Ugaz is a Professor and former Interim Department Head at the Artie McFerrin Department of Chemical Engineering at Texas A&M University.

ADDITIONAL AWARDS

ACS ANALYTICAL DIVISION AWARD IN SPECTROCHEMICAL ANALYSIS



The American Chemical Society award is given in recognition of advancing the fields of spectrochemical analysis and optical spectrometry.

Ji-Xin Cheng

Ji-Xin Cheng is currently the Inaugural Theodore Moustakas Chair Professor in Photonics and Optoelectronics at Boston University.



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

ADDITIONAL AWARDS

CHALMERS AND DENT STUDENT TRAVEL AWARD



The Chalmers and Dent Student Travel Award has been established to recognize and support an outstanding PhD student through financial support to present their research to an international audience at the annual SciX meeting.

Alberto Lux

Alberto Lux graduated with honours in 2022 at Politecnico di Milano in Materials Engineering and Nanotechnology. During his thesis he analysed graphene nanoparticles with IR, UV and most of all Raman Spectroscopy, sparking his interest in vibrational spectroscopy

RSC 2023 ANALYTICAL SCIENCE OPEN PRIZE: THEOPHILUS REDWOOD PRIZE



The Theophilus Redwood Prize is awarded by the Royal Society of Chemistry for outstanding contributions to the chemical sciences in the area of analytical chemistry.

Frank Vanhaecke

Frank Vanhaecke received a PhD from Ghent University (UGent) in 1992. He carried out postdoctoral research at UGent and at the Johannes Gutenberg University of Mainz, Germany. Currently, he is Senior Full Professor in Analytical Chemistry at UGent, where he also leads the 'Atomic & Mass Spectrometry – A&MS' research group that is specialized in the determination, speciation and isotopic analysis of (ultra)trace elements via ICP-mass spectrometry (ICP-MS).

SPECTROSCOPY MAGAZINE EMERGING LEADER IN MOLECULAR SPECTROSCOPY



The Emerging Leader in Molecular Spectroscopy 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.

Joseph Smith

Dr. Joseph P. Smith is currently a Director at Merck within the Data Rich Experimentation organization in the Process Research & Development department. At Merck, Dr. Smith leads a research group devoted to inventing, developing, and deploying data rich tools to enable process-focused efforts across small molecules, biologics, and vaccines. Dr. Smith earned his B.S. in Chemistry from the Pennsylvania State University in 2012, where his research focused on synthesis, purification, and characterization of magnetic nanoparticles. Dr. Smith then earned his Ph.D. in Analytical Chemistry from the University of Delaware in 2017, where his research focused on developing novel analytical tools leveraging spectroscopy, hyperspectral imaging, and multivariate analysis to analyze geological and planetary materials.

ANACHEM AWARD



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

Facundo M. Fernandez

Prof. Facundo M. Fernández is the Regents' Professor and Vasser-Woolley Chair in Bioanalytical Chemistry in the School of Chemistry and Biochemistry at the Georgia Institute of Technology.



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

SCHEDULE AT-A-GLANCE

SUNDAY, OCTOBER 20

8:30 AM – 4:30 PM	Short Courses (Full Day)	Various Locations
1:00 PM – 4:30 PM	Short Courses (Afternoon)	Various Locations
3:00 PM – 7:30 PM	Registration	Exhibit Hall Lobby
5:15 PM – 6:00 PM	Networking Opportunities at Scientific Conferences: A Guide for Emerging Scientists	Ballroom A
6:00 PM – 7:15 PM	KEYNOTE PRESENTATION: Can an AI Understand a Scientist?, Joseph Viviano	Ballroom A
7:00 PM – 9:00 PM	Welcome Mixer and Student Poster Event, Sponsored by FACSS, SAS, Coblenz, and Procter & Gamble	Ballroom B

MONDAY, OCTOBER 21

7:00 AM – 6:00 PM	Registration	Exhibit Hall Lobby
8:15 AM – 8:30 AM	Award Presentations	Ballroom A
8:30 AM – 9:00 AM	RSC 2023 Analytical Science Open Prize: Frank Vanhaecke	Ballroom A
9:00 AM – 9:30 AM	AES Mid-Career Award: Jason Dwyer	Ballroom A
8:30 AM – 12:00 PM	Short Courses (Morning)	Various Locations
8:30 AM – 4:30 PM	Short Courses (Full Day)	Various Locations
9:30 AM – 10:30 AM	Coffee & Posters	Ballroom B
10:30 AM – 12:10 PM	PARALLEL SESSIONS	
	24AES01: AES Early Career	306C
	24AWD02: AES Mid-Career Award Session	301B
	24PMA01: Analytical Characterization of BioTherapeutics	306B
	24RAM01: Emerging Raman	302B
	24PAT01: Future of PAT	302C
	24ATOM01: Glow Discharge	305A
	24MASS01: Ionization and Imaging in Mass Spectrometry	306A
	24CHEM01: Recent Advances in Chemometrics	305B
	24BIM01: Spectroscopy and the Role it Plays in the Successful Development and Manufacture of Novel Biopharmaceuticals	302A
	24CTPEARLY02: Women in Analytical Science	303
	24IR01: Two-Dimensional Correlation Spectroscopy-I	301A
12:10 PM – 1:30 PM	Lunch (on own)	
12:15 – 1:30 PM	Lunch and Learn on O-PTIR Technology: Sponsored by Photothermal Spectroscopy Corp (Registration Required)	Ballroom A
1:00 PM – 4:30 PM	Short Courses (Afternoon)	Various Locations
1:30 PM – 3:10 PM	PARALLEL SESSIONS	
	24AES02: AES Lifetime Achievement Award	306C
	24CHEM02: Chemometrics: Something Borrowed, Something New	305B
	24PMA02: Chirality in Pharma	306B
	24ATOM02: Data Analysis for Atomic Spectroscopy	305A
	24BIM02: Machine and Deep Learning for Biomedical Diagnostics	302A
	24MASS02: Novel MS Methods for Clinical, Forensic, and Toxicological Applications	306A
	24RAM12: Raman Spectroscopy for Security and Forensics Purposes	302C
	24AWD01: RSC 2023 Analytical Science Open Prize: Theophilus Redwood Prize Award Session	301B
	24RAM02: SERS 1	302B
	24CTPEARLY01: Showcasing Career Paths in the Spectroscopic Sciences (Organized by SAS Early Career)	303
	24IR02: Two-Dimensional Correlation Spectroscopy-II	301A
3:10 PM – 3:50 PM	Coffee & Posters	Ballroom B
3:50 PM – 5:30 PM	PARALLEL SESSIONS	
	24AES03: AES Emerging Leaders	306C
	24ATOM03: Analytical Geochemistry	305A

SCHEDULE AT-A-GLANCE

	24CTPEARLY04: Commercialization of Analytical Technologies	303
	24CHEM04: Data Driven Materials Discovery: Expanding Beyond Traditional Chemometrics	305B
	24IR12: Focus on Artificial Intelligence in Infrared Spectroscopy	301B
	24PMA03: Innovations in Vibrational Spectroscopy for Pharmaceutical Development	306B
	24SPSJ01: Low-Frequency Vibrational Spectroscopy	302A
	24MASS03: New Approaches to Biomolecular Sequence and Structure Characterization	306A
	24PAT02: PAT Pharma/Biotech	302C
	24RAM03: SERS 2	302B
	24IR06: Unlocking Molecular Landscapes: Exploring Complex Systems with Excitation-Emission Matrix Spectroscopy	301A
5:30 PM – 7:30 PM	Opening Exhibit Hall Reception	<i>Exhibit Hall B</i>

TUESDAY, OCTOBER 22

7:00 AM – 8:30 AM	Women's Breakfast (Registration Required)	304
7:30 AM – 5:00 PM	Registration	<i>Exhibit Hall Lobby</i>
8:15 AM – 8:30 AM	Award Presentations	<i>Ballroom A</i>
8:30 AM – 9:00 AM	FACSS Charles Mann Award: Nick Stone	<i>Ballroom A</i>
9:00 AM – 9:30 AM	Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award: Joseph Smith	<i>Ballroom A</i>
8:30 AM – 12:00 PM	Short Courses (Morning)	<i>Various Locations</i>
8:30 AM – 4:30 PM	Short Courses (Full Day)	<i>Various Locations</i>
9:30 AM – 10:30 AM	Coffee & Posters	<i>Exhibit Hall B</i>
10:30 AM – 12:10 PM	PARALLEL SESSIONS	
	24RAM13 Applications of Micro Raman Spectroscopy	302C
	24MASS06 Breaking Boundaries in Mass Spectrometry: To Infinity and Beyond	306A
	24CHEM03 Chemical Data Science in the 21st Century: Where We Might Be Going	305B
	24AES04 Electrokinetic Fundamentals	306C
	24FORENS02 Food Forensics	303
	24ATOM04 Laser Based Applications I	305A
	24IR04 Materials Science Applications of Optical Photothermal IR Spectroscopy	301A
	24BIM03 Optical Technologies and Companion Diagnostics in Healthcare Management	302A
	24RAM04 SERS 4	302B
	24PMA04 Solving Industrial Problems with Vibrational Spectroscopy	306B
	24AWD08: FACSS Charles Mann Award	301B
12:10 PM – 1:30 PM	Lunch & Exhibits	<i>Exhibit Hall B</i>
1:00 PM – 4:30 PM	Short Courses (Afternoon)	<i>Various Locations</i>
1:30 PM – 3:10 PM	PARALLEL SESSIONS	
	24MASS04 Advances in Mass Spectrometry-Based Glycomics	306A
	24PMA05 Analysis of Biologicals in Blood 1	306B
	24CHEM06 Applications of AI and Chemometrics in Forensic Chemistry	305B
	24AES05 Innovations in Device Fabrication & Applications	306C
	24RAM05 IRDG	302B
	24ATOM05 Laser Based Applications II	305A
	24SPSJ02 NIR Spectroscopy Multidimensional Approaches	302A
	24IR05 Novel Laser Based Chemical Sensing	301A
	24PAT03 Novel PA Technologies & Applications	302C
	24CTPEARLY03 Rising Talents in Enhanced Raman Spectroscopy	303
	24AWD07 Spectroscopy Magazine Emerging Leader in Molecular Spectroscopy Award Session	301B
3:10 PM – 3:50 PM	Refreshments & Posters	<i>Exhibit Hall B</i>
3:50 PM – 5:30 PM	PARALLEL SESSIONS	

SCHEDULE AT-A-GLANCE

	24BIM05 AI-Driven Multimodal Chemical Imaging for Biomedical Diagnostics	302A
	24ATOM06 Atomic Based Imaging	305A
	24CHEM05 Chemometrics in Food & Agriculture	305B
	24AES06 Electrokinetic Bioanalysis	306C
	24RAM06 Food	302B
	24PMA06 Generative AI and Machine Learning Advancing Pharmaceutical Development with Vibrational Spectroscopy	306B
	24RAM14 Industrial Raman	302C
	24IR03 Life Science Applications of Photothermal IR Spectroscopy	301A
	24FORENS01 Nuclear Forensics	303
	24SPR02 Young Investigators in Plasmonics	306A
5:30 PM – 7:30 PM	Exhibitor-Hosted Happy Hour	See App for Location
7:00 PM – 8:00 PM	SAS Award Presentations	Ballroom A
8:00 PM – 9:30 PM	SAS Members Awards Reception	Ballroom B
WEDNESDAY, OCTOBER 23		
7:30 AM – 5:00 PM	Registration	Exhibit Hall Lobby
8:15 AM – 8:30 AM	Award Presentations	Ballroom A
8:30 AM – 9:00 AM	ACS Analytical Division Award in Spectrochemical Analysis: Ji-Xin Cheng	Ballroom A
9:00 AM – 9:30 AM	NESAS Lester W. Strock Award: Benjamin Manard	Ballroom A
8:30 AM – 12:00 PM	Short Courses (Morning)	Various Locations
8:30 AM – 4:30 PM	Short Courses (Full Day)	Various Locations
9:30 AM – 10:30 AM	Coffee & Posters	Exhibit Hall B
10:30 AM – 12:10 PM	PARALLEL SESSIONS	
	24AWD03 ACS Analytical Division Award in Spectrochemical Analysis Award Session	301B
	24IR07 Advances in Nanoscale Spectroscopy from Mid-Ir to Beyond	301A
	24AES07 Commercialization & Industry Applications	306C
	24FORENS03 Forensics Analysis in the Lab and at the Crime Scene	303
	24PMA07 Frontiers in Drug Sensing and Nanoendoscopic Theragnostic	306B
	24PAT04 In Situ Spectroscopy for industrial R&D	302C
	24ATOM09 Non-Traditional Plasmas	305A
	24ATOM12 Novel Approaches to and Applications of LIBS	302B
	24MASS05 Novel Instrumentation, Analysis Tools, and Chemistry in Mass Spectrometry	306A
	24BIM04 Optical Point-of-Use Technologies for Automated Biomedical and Life-Sciences Analysis	302A
	24SPECIAL04 Spectrochimica Acta Part B award	305B
12:10 PM – 1:30 PM	Lunch & Exhibits	Exhibit Hall B
1:30 PM – 3:10 PM	PARALLEL SESSIONS	
	24CHEM07 Answering Age Old Questions with Data: Chemometrics in Art Conservation	305B
	24SPR05 Applications of AI in plasmonics	306A
	24AES08 Future 50: AES Innovations	306C
	24PMA08 Measuring Quality in Complex Raw Materials Used in Biotech and Biopharma: Spectroscopic Methods Of Analysis	306B
	24AWD05 NESAS Lester W. Strock Award Session	301B
	24FORENS04 Pharmaceutical Micro and Macro Forensics 1	303
	24RAM08 Raman Imaging/Microscopy/SRS/CARS	302B
	24RAM15 Raman in Regenerative Medicine	302C
	24ATOM08 sp- and sc-ICP-MS	305A
	24SPSJ03 Ultraviolet Resonance Raman Spectroscopy	302A
	24IR08 Vibrational Nano-Imaging of Molecular Structure, Coupling, and Dynamics	301A
3:10 PM – 3:50 PM	Refreshments & Posters	Exhibit Hall B

SCHEDULE AT-A-GLANCE

3:50 PM – 5:30 PM PARALLEL SESSIONS		
24PAT05 AI in PAT		302C
24SPECIAL03 All in the Family: A Peaceful Gathering of Hieftje Descendants		305B
24BIM06 Biomedical Spectroscopy and Imaging (CLIRSPEC)		302A
24PMA09 Making Spectroscopy Deployable On-Line Innovations and Trends in BioPharm PAT		306B
24IR09 NanoIR in Biosciences		301A
24SPR01 Plasmonic sensors		306A
24IR14 Recent Advances in Near-Infrared Spectroscopic Sensing		301A
24ART01 Student Research in Archaeological Chemistry		306C
24RAM09 Spatially Offset Raman Spectroscopy (SORS)		302B
24ATOM07 Time-of-Flight Spectrometry		305A

THURSDAY, OCTOBER 24

7:30 AM – 4:30 PM	Registration	Exhibit Hall Lobby
8:15 AM – 8:30 AM	Award Presentations	Ballroom A
8:30 AM – 9:00 AM	SAS and Applied Spectroscopy William F. Meggers Award: Ioan Notingher	Ballroom A
9:00 AM – 9:30 AM	Coblentz Society Clara Craver Award: Conor Evans	Ballroom A
8:30 AM – 12:00 PM	Career Development Courses	Various Locations
8:30 AM – 4:30 PM	Career Development Courses	Various Locations
9:30 AM – 10:30 AM	Coffee & Posters	Ballroom Foyer
10:30 AM – 12:10 PM PARALLEL SESSIONS		
24IR10 Advances in QCL-IR Spectroscopy		301A
24AWD04 Applied Spectroscopy William F. Meggers Award Award Session		301B
24RAM16 Early Career Raman		302C
24ART02 LA-ICP-MS Applications in Art and Archaeology		306C
24RAM10 Low Frequency Raman		302B
24ATOM10 Multi-Collector ICP-MS		305A
24BIM07 Nanotheranostics: Diagnosis and Treatment of Disease Using Nanomaterials		302A
24SPR03 New Plasmonic Materials and Architectures		306A
24FORENS06 Pharmaceutical Micro and Macro Forensics 2		303
24SPECIAL01 Shootout at Hieftje's Atomic Spectroscopy Corral		305B
24PMA10 Analysis of Biologicals in Blood 2		306B
12:10 PM – 1:30 PM	Lunch (on own)	
1:30 PM – 3:10 PM PARALLEL SESSIONS		
24IR11 Advanced Application of Vibrational Spectroscopy		301A
24AWD06 Coblentz Society Clara Craver Award Session		301B
24FORENS05 Early Career Research in Forensic Sciences		303
24ATOM11 Elemental Analysis		305A
24RAM11 Enhanced Raman Analysis Via Hybridization and Multivariate Approaches		302B
24ART03 Imaging Technologies for Cultural Heritage		306C
24PAT06 PAT in Petroleum and Refinery Industries		302C
24SPR04 Photothermal Plasmonics		306A
24PMA11 Real Time and Offline Analysis for Bioprocessing 4.0		306B
24SPECIAL02 Shootout at Hieftje's Molecular Spectroscopy Corral		305B
24SPSJ04 Spectroscopy in Far Ultraviolet Region		302A
3:10 PM – 3:30 PM	Coffee & Posters	Ballroom Foyer
3:30 PM – 5:30 PM	Innovation Award Session	Ballroom A
7:00 PM – 11:30 PM	SciX Gala	Ballroom B&C

FRIDAY, OCTOBER 25

8:45 AM – 10:00 AM	SciFri Talks & SciX 2025 Preview	304
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SHORT COURSES / WORKSHOPS

Workshops are available for a separate registration fee. Visit the registration desk to sign up. Space is limited and some courses may sell out. All short courses/workshops will be taking place in the Raleigh Convention Center. Please reference the App for room locations and all available short courses as this may have changed since print.

SUNDAY, OCTOBER 20

8:30 AM – 4:30 PM Room 202	1:00 PM – 4:30 PM Room 203
Spectral Interpretation of Vibrational Spectra (Day1)	Introduction to Infrared, Raman and Near Infrared Spectroscopy

MONDAY, OCTOBER 21

8:30 AM – 12:00 PM Room 204	8:30 AM – 4:30 PM Room 205
Searching Infrared and Raman Spectra	How to select, configure, and optimize Raman spectrometer for your application: from theory to practice
8:30 AM – 12:00 PM Room 203	1:00 PM – 4:30 PM Room 204
Sample Selection Design of Experiments (DOE) for Multivariate Calibration	Problems with FT-IR Spectra and How to Avoid
8:30 AM – 4:30 PM Room 202	
Spectral Interpretation of Vibrational Spectra (Day 2)	

TUESDAY, OCTOBER 22

8:30 AM – 12:00 PM Room 202	8:30 AM – 4:30 PM Room 205
Fundamentals of Scientific Cameras	Introduction to Quantitative Spectroscopy for Near Infrared and Raman Instrumentation
8:30 AM – 12:00 PM Room 203	1:00 PM – 4:30 PM Room 202
Beyond the Beer-Lambert Approximation: Towards Evaluating Infrared Spectra Based on Wave Optics and Dispersion Theory	Optimizing Microspectroscopy with Microscopy
8:30 AM – 12:00 PM Room 204	1:00 PM – 4:30 PM Room 203
Technologies and applications for miniature optical spectrometers and spectroscopic sensors	Laser Fundamentals for Spectroscopy

THURSDAY, OCTOBER 24

8:30 AM – 12:00 PM Room 202	8:30 AM – 12:00 PM Room 204
Job Search Roadmap	ABC to PMP: A Project Management Crash Course
8:30 AM – 12:00 PM Room 203	1:00 PM – 4:30 PM Room 202
Expert to Entrepreneur	Optimizing Microspectroscopy with Microscopy

TECHNICAL PROGRAM - SUNDAY, OCTOBER 20, 2024

Welcome & Keynote Lecture | 6:00 PM – 7:15 PM | *Ballroom A*

PROFDEV: Networking Opportunities at Scientific Conferences: A Guide for Emerging Scientists | *Ballroom A*

5:15 PM **Networking Opportunities at Scientific Conferences: A Guide for Emerging Scientists**

Alexis Weber¹ *SupreMEtric*

24KEYNOTE: Can an AI Understand a Scientist? | *Ballroom A*

6:00 PM **Joseph D. Viviano, Mila - Quebec Artificial Intelligence Institute**

TECHNICAL PROGRAM- MONDAY, OCTOBER 21, 2024

Award & Plenary Lectures | 8:15 AM – 9:30 AM | *Ballroom A*

8:15 AM **Award Presentation**

8:30 AM **RSC 2023 Analytical Science Open Prize: Theophilus Redwood Prize: ICP-MS: Jack of All Trades in the Life Sciences?**

Frank Vanhaecke¹ *Ghent University*

9:00 AM **AES Electrophoresis Mid-Career Award: Carbohydrate Analysis at the Single-Molecule Limit Using Chemically-Tuned Nanopores**

Jason R. Dwyer¹ *University of Rhode Island*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Monday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom B*

(Mon-P1) **Cellular Biophysical Changes Induced due to Simulated Microgravity Environment**

Alexa L. Bostic¹, Sai Deepika Reddy Yaram¹,
Soumya Srivastava¹ *West Virginia University*

(Mon-P2) **Monte Carlo Simulations of DNA Electrophoresis Via Entropic Trapping Transport through Polydisperse Nanoscale Pores**

Sourav Bandyopadhyay¹, Victor Ugaz¹ *Texas A&M University*

(Mon-P3) **Understanding Polymer-Specific Partition Coefficients for Enhanced Entropic Trapping in Nanoporous Media**

Sourav Bandyopadhyay¹, Victor Ugaz¹ *Texas A&M University*

(Mon-P4) **Investigating Manufacturing Techniques and Raw Materials for Dielectrophoresis-Based Microfluidic Sorting Devices on the CytoRITM Platform**

Kyle M. Brown¹, Kyle S. Kinskie², Dean E. Thomas², Alexandra R. Hyler², Josie Duncan³, Jaka Cemazar⁴, Jeff Schultz⁵, Simeon Brown⁵, Farhad M. Shiri⁶, Steven Soper⁷, Rafael V. Davalos⁸ ¹*Cytorecovery*, ²*CytoRecovery, Inc.*, ³*Georgia Institute of Technology*, ⁴*Combination Product Development and Gene Therapies*, ⁵*Phase AM*, ⁶*Kansas University*, ⁷*Center of BioModular Multi-Scale Systems for Precision Medicine at University of Kansas*, ⁸*Georgia Tech*

(Mon-P5) **Micro- and Nanoplastic Reference Material Characterization and Application to Dielectrophoretic Properties in Body Fluids**

Shulin Bu¹, Alexandra Ros¹ *Arizona State University*

(Mon-P6) **Zeta Potential as a Biosensor for Human Red Blood Cells in ECMO Bypass Circuits**

Brandon K. Eberl¹, Erin Henslee² ¹*Wake Forest University School of Medicine*, ²*Wake Forest University*

(Mon-P7) **Long-Axis 3D-Printed Brace for Increased Normally-Closed Valve State Biasing**

Joshua G. Howell¹, Joanne Y. Seow¹, Christopher J. Easley¹ *Auburn University*

(Mon-P8) **An Investigation of Materials Used in Microfluidic Fabrication of CytoChips™ for Dielectrophoresis-Based Cell Sorting**

Kyle S. Kinskie¹, Dean Thomas², Kyle Brown², Josie Duncan³, Jaka Cemazar⁴, Jeff Schultz⁵, Simeon Brown⁵, Farhad Shiri⁶, Steven Soper⁶, Rafael Davalos³, Alexandra R. Hyler¹ ¹*CytoRecovery, Inc.*, ²*CytoRecovery Inc.*, ³*Georgia Institute of Technology*, ⁴*Combination Product Development and Gene Therapies*, ⁵*Phase AM*, ⁶*Center of BioModular Multi-Scale Systems for Precision Medicine at University of Kansas*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Monday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom B*

(Mon-P9) **Modelling of parametric optimization for micro/nanofiber based dielectrophoresis trapping**
Tonoy K. Mondal¹, Stuart J. Williams¹ ¹*University of Louisville*

(Mon-P10) **Unveiling The Dielectric Signatures Of Candida Auris**
Negar Farhang Doost¹, Tagbo Niepa², Soumya K Srivastava³ ¹*Chemical and Biomedical Engineering Department, West Virginia University*, ²*Departments of Chemical Engineering and Biomedical Engineering, Carnegie Mellon University*, ³*West Virginia University*

(Mon-P11) **A Surface Venting Strategy That Enables More Complexity In High Resolution 3d-Printed Microchannel Designs**
Hieu M. Pham¹, Christopher J. Easley¹, Joanne Y. Seow¹ ¹*Auburn University*

(Mon-P12) **Dielectrophoretic Characterization of Breast Cancer Immune Cells Using PBMCs from MMTV-PyMT Models**
Raphael O. Oladokun¹, Timothy Eubank¹, Soumya K Srivastava¹ ¹*West Virginia University*

(Mon-P13) **Streaming Mode Dielectrophoresis to Characterize Micro and Nanoscale Particles**
A K M Fazlul Karim Raseel¹, Eron Ristich¹, Sean L. Seyler¹, Mark A. Hayes¹ ¹*Arizona State University*

(Mon-P14) **Characterizing HL-60 Cells Infected with Anaplasma spp.: A Dielectrophoresis Approach**
Sai Deepika Reddy Yaram¹, Soumya K Srivastava¹ ¹*West Virginia University*

(Mon-P15) **Polyjet 3d Printed Microchip Electrophoresis Devices With Electrochemical Detection For Neurotransmitters Analysis**
MAJOR A. SELEMANI¹ ¹*Saint Louis University*

(Mon-P16) **Ac Electrokinetic Cross-Stream Migration Of Particles In A Straight Rectangular Microchannel**
Seyed Mojtaba Tabarhoseini¹, Peter Koniers¹, Aidan Patterson¹, Mahmud Raihan¹, Xiangchun Xuan¹ ¹*Clemson University*

(Mon-P17) **Ac Electrokinetic Focusing Of Nanoparticles In A Ratchet Microchannel**
Aidan Patterson¹, Peter Koniers¹, Seyed Mojtaba Tabarhoseini¹, Xiangchun Xuan¹ ¹*Clemson University*

(Mon-P18) **PDMS Permeability Affects Cell Recovery and Viability in DEP-Based Cell Sorting Microfluidics**
Dean E. Thomas¹, Kyle S. Kinskie¹, Kyle M. Brown², Josie Duncan³, Jaka Cemazar⁴, Jeff Schultz⁵, Simeon Brown⁵, Farhad M. Shiri⁶,

Steven Soper⁷, Rafael V. Davalos⁸, Alexandra R. Hyler¹ ¹*CytoRecovery, Inc.*, ²*Cytorecovery*, ³*Georgia Institute of Technology*, ⁴*Combination Product Development and Gene Therapies*, ⁵*Phase AM*, ⁶*Kansas University*, ⁷*Center of BioModular Multi-Scale Systems for Precision Medicine at University of Kansas*, ⁸*Georgia Tech*

(Mon-P19) **Dielectrophoretic slide: A Novel Dielectric Microparticle Analysis Platform**
Aaditya Venkatesha Babu Bangaru¹, Holton Shults¹, Axel Gumira¹, Stuart J. Williams¹ ¹*University of Louisville*

(Mon-P20) **Assessment Of The Effect Of Cell Shape On Their Nonlinear Electrophoretic Mobility**
Viswateja Kasarabada¹, Olivia Ernst¹, Alaleh Vaghef-Koodehi¹, Blanca H. Lapizco-Encinas¹ ¹*Rochester Institute of Technology*

(Mon-P21) **Continuous Separation Of Live And Dead Cells With Nonlinear Electrophoresis.**
Viswateja Kasarabada¹, Gabriela Martinez-Martinez¹, Nuzhet Nihaar Ahamed¹, Alaleh Vaghef-Koodehi¹, Blanca H. Lapizco-Encinas¹ ¹*Rochester Institute of Technology*

(Mon-P22) **Simulating Separation of Healthy Vero Cells from those Infected with Rickettsia montanensis Using COMSOL Multiphysics**
Kayla E. Wagner¹, Soumya K Srivastava¹, Negar Farhang Doost², Sai Deepika Reddy Yaram¹ ¹*West Virginia University*, ²*Chemical and Biomedical Engineering Department, West Virginia University*

(Mon-P23) **A Numerical Study On Electroosmosis Of Shear-Thinning Fluids In A Rectangular Microchannel**
WAI YUEN LEUNG¹, Joseph A. Bantor², Xiangchun Xuan² ¹*CLEMSON UNIVERSITY*, ²*Clemson University*

(Mon-P24) **Electroosmotic Fluid Flow And Electrophoretic Particle Motion In Shear-Thinning Polymer Solutions**
Joseph A. Bantor¹, Wai Yuen Leung¹, Xiangchun Xuan¹ ¹*Clemson University*

(Mon-P25) **Effects Of Fluid Rheology On Insulator-Based Dielectrophoretic Focusing Of Particles In A Multi-Constriction Microchannel**
Sanskruti Raut¹, Joseph A. Bantor¹, Xiangchun Xuan¹ ¹*Clemson University*

(Mon-P26) **Fluid Shear Thinning Effects On Electrokinetic Flow Instabilities**
Yu-Hsiang Lee¹, Nicole Miller¹, Jason Reggero², Seyed Mojtaba Tabarhoseini¹, Xiangchun Xuan¹ ¹*Clemson University*, ²*SC Governor's School for Science and Mathematics*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Monday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom B*

(Mon-P27) Optimizing Xurography Technique to Produce Economical Microfluidic Devices

Anushka Pathak¹, Soumya K. Srivastava¹, Sai Deepika Reddy Yaram¹, Negar Farhang Doost² ¹West Virginia University, ²Chemical and Biomedical Engineering Department, West Virginia University

(Mon-P28) Detection of Plant-Based Adulterants in Turmeric Using Fourier Transform Infrared (Ftir) and Chemometrics

Adejoke M. Areo¹, Peter B. Harrington² ¹Ohio University, ²OHIO University

(Mon-P29) Real-time Monitoring of Monoclonal Antibodies Manufacturing Process Using Chemometrics Methods

Samira Beyramysoltan¹, Sushrut Marathe², Giulia Marchese³, Nathaniel Berendson⁴, Elahesh Ardalani², Theodore Vu⁴ ¹PerkinElmer, ²GSK, Colleagueville, Upper Providence, United States, ³GSK, Stevenage SG1 2NY, United Kingdom, ⁴GSK, Upper Merion, Conshohocken, United States

(Mon-P30) Rapid Quantification of Diesel Particulate Matter by a Variety of Optical Techniques

David Parks¹, Arthur L. Miller¹, Seth L. Finley¹ ¹NIOSH

(Mon-P31) Raman Spectroscopy and Chemometrics for the Quantification of Sulfuric Acid in an Ammonia Scrubber System Across Temperature Gradients

Daniel E. Felton¹, Luke R. Sadergaski², Jennifer N. Neu¹, Avery L. Wood¹, Roger J. Kapsimalis¹ ¹Oak Ridge National Lab, ²Oak Ridge National Laboratory

(Mon-P32) Material-sparing Approach in Monitoring Blending Processes: Implementing Iterative Optimization Technology

Md. Nahid Hasan¹, Samuel R. Henson¹, James K. Drennen¹, Carl A. Anderson¹ ¹Duquesne University

(Mon-P33) Data-Augmentation using Semi-Empirical Quantum Chemistry – A Better Way to Pre-Train Deep Raman Models?

Julian Hniopek¹, Jawad Kamran¹, Thomas Bocklitz² ¹Department of Photonic Data Science, Leibniz Institute of Photonic Technology, Jena, Germany, ²Photonic Data Science department, Leibniz Institute of Photonic Technology, Jena, Germany

(Mon-P34) Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) Method Development with Variable Selection for the Detection and Quantification of Commercial Captan and Malathion Pesticides

Kudirat Abidemi Obisesan Olawuni¹, Peter de Boves Harrington² ¹University of Barcelona, ²Ohio University

(Mon-P35) Assessment of Conformal Prediction and Standard Normal Distribution for Autonomous One-Class Classification

Hyrum J. Redd¹, John Kalivas¹ ¹Idaho State University

(Mon-P36) Combining Photoluminescence, Raman Spectroscopy, and Multivariate Analysis for the Quantification of Uranium(VI) in Nitric Acid

Luke R. Sadergaski¹, Daniel E. Felton², Jennifer N. Neu², Avery L. Wood², Andrew Miskowicz², Roger J. Kapsimalis² ¹Oak Ridge National Laboratory, ²Oak Ridge National Lab

(Mon-P37) Adapting PRISM for Spectral Local Modeling and Model Updating with Future Application in Virtual Reality

Nakiah M. Shanafelt¹, John H. Kalivas² ¹Idaho State University / Student, ²Idaho State University

(Mon-P38) Leveraging Compact NIR Spectrometers for Determination of Protein and Moisture Content in Oats

Stephanie Butron¹, Yalan Wu², Silvia de Lamo Castellvi³, John Gilmore¹, Luis Rodriguez-Saona³ ¹Hamamatsu Corporation, ²The Ohio State University, ³The Ohio State University

(Mon-P39) Modernized Machine Learning Approach To Illuminate Enzyme Immobilization For Biocatalysis

HONG WEI¹, Joseph P. Smith¹ ¹Merck

(Mon-P40) Quantitation of Isoniazid in Tablets for Tuberculosis Treatment by Raman Spectroscopy with Chemometric Analysis Method Validation

Ed Bethea¹, Matthew Eady¹, Mary Beth Sowers¹, Christopher L. Harmon¹, David Jenkins¹ ¹FHI360

(Mon-P41) Quantifying Nitric Acid and Temperature via Design of Experiments, Chemometrics, and Raman Spectroscopy

David V. Russell¹, Luke R. Sadergaski², Jeffrey Einkauf², Laetitia Delmau², Jonathan Burns¹ ¹University of Alabama at Birmingham, ²Oak Ridge National Laboratory

(Mon-P42) Automated Raman Spectroscopy Of Urine For Disease Screening

Ryan Senger¹, Amr Sayed-Issa¹, John Robertson² ¹Virginia Tech, ²Ramatrix Technologies, Inc.

(Mon-P44) The Morphology Of Teeth Using Optical Coherence Tomography And Principal Component Analysis.

Jorge Castro-Ramos¹, Roba Izzeddin-Abou², Héctor Nahum Chavarria-Lizárraga³, Freddy Narea-Jiménez⁴, David Iturbe-Castillo³ ¹Instituto Nacional de Astrofísica Óptica y Electrónica, ²Universidad de Carabobo, ³INAOE, ⁴BUAP

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Monday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom B*

(Mon-P45) **Environmental Monitoring with Semi-Selective Receptors and Surface Plasmon Resonance Imaging**
Simon Jobst¹, Patrick Recum², Peter Hausler¹, Elisabeth Moser¹, Laurin Hastreiter², Ángela Écija-Arenas², Rudolf Bierl¹, Thomas Hirsch² ¹Regensburg University of Applied Sciences, ²University of Regensburg

(Mon-P47) **Tunable 3D Nanoconfinement via PDMS Diaphragm Collapse in Bead-Array Microfluidic Platforms for Enhancing Biomolecular Binding Kinetics**
Abdullah-Bin Siddique¹, Jui-Hong Weng², Deng-Kai Yang², Chia-Fu Chou², Nathan S. Swami¹ ¹University of Virginia, ²Institute of Physics, Academia Sinica, Taiwan

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

24AES01: AES Early Career | 306C

Chair: Gongchen Sun, University of Texas at San Antonio
Co-Chair: Robert Williamson, North Carolina State University

10:30 AM (AES-01.1) **On The Use Of Nonlinear Electrophoresis For Altering Migration Order In Electrokinetic Separations**

Alaleh Vaghef-Koodehi¹, Blanca H. Lapizco-Encinas¹ ¹Rochester Institute of Technology

10:50 AM (AES-01.2) **Microfluidic Isotachopheresis For Accelerating And Streamlining Crispr-Based Molecular Assays**

Ashwin Ramachandran¹ ¹Princeton University

11:10 AM (AES-01.3) **Nanopore Array Platforms Towards Biomimetic Ionic Circuits**

Ethan Cao¹, Zuzanna S. Siwy¹ ¹University of California, Irvine

11:30 AM (AES-01.4) **Next Generation multimodal technologies for pure fractionation followed by ultrasensitive detection of Extracellular vesicles (EVs), Lipoprotein (LLPs), and Ribonucleoprotein protein (RNPs) from biofluids**

Himani Sharma¹ ¹Avery Digital Data Inc.

24ATOM01: Glow Discharge | 305A

Chair: Gerardo Gamez, Texas Tech University

10:30 AM (ATOM-01.1) **Looking At The Fundamentals Of Glow Discharge Emission Spectroscopy: What 'Complete' Emission Spectra Can Say**

Zdenek Weiss¹ ¹FZU - Inst. of Physics of the Czech Academy of Sciences

10:50 AM (ATOM-01.2) **Compositional Depth Profiling with Glow Discharge Optical Emission Spectrometry using True Plasma Power Pulsed Radio Frequency (RF)**

Rebecca Quardokus¹, Sara Alexander¹, Jessica Russell¹, Kevin Brushwyler¹ ¹LECO Corporation

11:10 AM (ATOM-01.3) **Glow Discharge Optical Emission Spectrometry Elemental Mapping For Studying Nanoparticle Interaction and Uptake in Cells**

Rajendra Joshi¹, Harshit Agrawaal¹, Gerardo Gamez¹ ¹Texas Tech University

11:30 AM (ATOM-01.4) **The Glow Bubbler: A Novel Sensor For In Situ Material Quantification Of Liquids**

Alex W. Bataller¹ ¹North Carolina State University

11:50 AM (ATOM-01.5) **Improvement Of Manufacturing Processes Of Li-Ion Batteries By Glow-Discharge Optical Emission Spectroscopy**

Carlos Abad¹, Beatrice Battistella², Alexander Winkelmann², Volker Hoffmann³, Zengchao You², Silke Richter², Sebastian Recknagel⁴

¹Bundesanstalt für Materialforschung und -prüfung (BAM), ²Bundesanstalt für Materialforschung und -prüfung (BAM), ³Leibniz Institute for Solid State and Materials Research Dresden, ⁴Bundesanstalt für Materialforschung und -prüfung (BAM),

24AWD02: AES Mid-Career Award Session | 301B

Chair: Jason Dwyer, University of Rhode Island

10:30 AM (AWD-02.1) **Infrared Spectroscopy Of Bio Organisms And Structures – From Macro To Nano And Back Again**

Kathleen M. Gough¹ ¹University of Manitoba

10:50 AM (AWD-02.2) **The Theater of Nanopore Sensing: The Fond Memories in Past, Present, and Future Episodes of Sensing**

Nuwan D. Bandara¹, Buddini Karawdeniya¹, Shankar Dutt¹, Jugal Saharia², Patrick Kluth¹, Jason R. Dwyer³, MinJun Kim⁴, Kevin Freedman⁵, Antonio Tricoli⁶ ¹Australian National University, ²University of Houston Clear Lake, ³University of Rhode Island, ⁴Southern Methodist University, ⁵University of California, Riverside, ⁶University of Sydney

Nathan Fuenffinger¹, Jennifer Pai Wang¹, Louis Obando¹ ¹Merck & Co., Inc.

11:10 AM (AWD-02.3) **Small Channels And Big Challenges: Using Nanopore Sequencing, Mass Spectrometry, And Deep-Learning Algorithms To Revise The Molecular Model Of An Ovarian Cancer Biomarker**

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

Rebecca Whelan¹, Chien-Wei Wang¹, Simon Weaver², Nicha Boonpatrawong³, Naviya Schuster-Little¹, Manish Patankar³ ¹University of Kansas, Department of Chemistry, ²University of Notre Dame, Department of Chemistry and Biochemistry, ³University of Wisconsin, Department of Obstetrics and Gynecology

11:30 AM (AWD-02.4) **Developments In Translational Glycosaminoglycan Analysis Using Solid-State Nanopores**

Adam R. Hall¹ ¹Wake Forest University Health Sciences

11:50 AM (AWD-02.5) **Predicting retention time of microparticles in electrokinetic separations**

Alaleh Vaghef-Koodehi¹, Blanca H. Lapizco-Encinas¹ ¹Rochester Institute of Technology

24BIM01: Spectroscopy and The Role it Plays in the Successful Development and Manufacture of Novel Biopharmaceuticals | 302A

Chair: Andrew Whitley, HORIBA Scientific

10:30 AM (BIM-01.1) **Towards Label Free Approaches for Designing Novel Analytical Tools in the Pharmaceutical Industry**

Prabuddha Mukherjee¹ ¹Sartorius Stedim North America, Inc.

10:50 AM (BIM-01.2) **Post-Packaging Identification of Live Attenuated Virus Vaccines Using Simultaneous Absorbance, Transmission, and Fluorescence Excitation-Emission Matrix Spectroscopy and Chemometrics**

Nathan Fuenffinger¹, Jennifer Pai Wang¹, Louis Obando¹ ¹Merck & Co., Inc.

11:10 AM (BIM-01.3) **Advancing Cell Culture Media Screening with A-TEEM Technology**

Rita C. Barral¹, Marina Hincapie¹, John Bobiak², Esra Kiran², Lia Tescione² ¹Sanofi, Process Analytical Technology – Mammalian Platform, Framingham, Massachusetts, USA, ²Sanofi, Manufacturing, Science & Technologies – Mammalian Platform, Framingham, Massachusetts, USA

11:30 AM (BIM-01.4) **Rapid Raman Plate Reader for High Throughput Screening in Pharmaceutical Industry**

Chris George¹, Aashish Tuladhar¹, Eunah Lee¹ ¹HORIBA Instruments Inc

11:50 AM (BIM-01.5) **Applications of Process Analytical Technology (PAT) to Vaccine Drug Substance and Drug Product Process Development and Clinical Manufacturing**

Nicole Ralbovsky¹ ¹Merck

24CHEM01: Recent Advances in Chemometrics | 305B

Chair: Peter Harrington, Ohio University

10:30 AM (CHEM-01.1) **Artificial Intelligence, Machine Learning, and Chemometrics**

Peter B. Harrington¹ ¹OHIO University

10:50 AM (CHEM-01.2) **Synergizing Machine Learning with Human Cognition in Immersive Virtual Reality for Unsupervised Data Exploration**

John Kalivas¹, Jordan Peper¹ ¹Idaho State University

11:10 AM (CHEM-01.3) **Chemical Imaging Enabled by Multi-Agent Consensus Equilibrium (MACE) Methods**

Garth J. Simpson¹ ¹Purdue University

11:30 AM (CHEM-01.4) **Multi-Spectral Techniques with Machine Learning for Lithium Isotope Measurement**

Madison Moran¹, Ashwin Rao², Christina Dugan³, Anil Patnaik³ ¹Air Force Institute of Technology, ²AFRL, ³AFIT

11:50 AM (CHEM-01.5) **Dimension Expansion via Generative Adversarial Linear Discriminant Analysis**

Yechan Hwang¹, Garth J. Simpson¹ ¹Purdue University

24CTPEARLY02: Women in Analytical Science | 303

Chair: Andrea Locke, Vanderbilt University

10:30 AM (CTPEARLY-02.1) **A career path aimed at translating light-based tools to improve global women's health**

Christine M. O'Brien¹ ¹Washington University in St. Louis

10:50 AM (CTPEARLY-02.2) **From DNA to Diamonds: A Career in Analytical Instrumentation**

Karen E. Gall¹ ¹HORIBA Instruments Inc.

11:10 AM (CTPEARLY-02.3) **First-Generation College Student to a National Laboratory: The Third Option**

Kelsey L. Williams¹ ¹Los Alamos National Laboratory

11:30 AM (CTPEARLY-02.4) **Embracing a Moving Career Target**

Mackenzie Speer¹ ¹Metrohm

11:50 AM (CTPEARLY-02.5) **Panel Discussion**

24IR01: Two-Dimensional Correlation Spectroscopy-I | 301A

Chair: Young Jung, Kangwon National University

Co-Chair: Isao Noda, University of Delaware

10:30 AM (IR-01.1) **Application of Correlation Filter for 2D-COS Analysis of Biodegradable Polyester Solution Crystallization Process**

Isao Noda, Yeonju Park¹, Young Mee Jung² ¹Kangwon National University, ²Kangwon National University

Next year: October 5-10, 2025 • Northern Kentucky Convention Center

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

10:50 AM (IR-01.2) Characterization of Binary and Ternary Adsorption at Solid Surfaces

Dennis Hore¹, Harpreet Kaur¹ ¹*University of Victoria*

11:10 AM (IR-01.3) An Alternative Structure for Polyhydroxybutyrate-hexanoate Based on Raman Spectroscopy and Two Dimensional Correlation Spectroscopy

Fran Adar¹, Isao Noda ¹*Horiba Scientific*

11:30 AM (IR-01.4) Extraction of descriptive features from entire two-dimensional correlation map using convolutional autoencoder and use them for discriminant analysis

Seongsoo Jeong¹, Hociil Chung¹ ¹*Hanyang University*

11:50 AM (IR-01.5) 2D Hetero-Correlation Analysis of Blood Fluorescence Spectra During ex vivo aging

Sila Jin¹, Alexis Weber², Yeonju Park³, Young Mee Jung⁴, Igor K. Lednev⁵ ¹*Kangwon Radiation Convergence Research Support Center*, ²*SupreMEtric*, ³*Kangwon National University*, ⁴*Kangwon National University*, ⁵*University at Albany, SUNY*

24MASS01: Ionization and Imaging in Mass Spectrometry 306A

Chair: David Muddiman, North Carolina State University
Co-Chair: Alena Joignant, North Carolina State University

10:30 AM (MASS-01.1) The Current State of Infrared Matrix Assisted Laser Desorption Electrospray Ionization at NC State

Alena N. Joignant¹, Kevan T. Knizner¹, Mary F. Wang¹, Tana V. Palomino¹, David C. Muddiman¹ ¹*North Carolina State University*

10:50 AM (MASS-01.2) Evaluation of Similarities and Differences between Fresh Frozen and Formalin Fixed, Paraffin Embedded Tissue for Spatial Metabolomics

Erin H. Seeley¹, Danielle L. Stolley², Erik N.K. Cressman² ¹*University of Texas at Austin*, ²*MD Anderson Cancer Center*

11:10 AM (MASS-01.3) Driving Towards Democratization of Spatial Biology with Multimodal Imaging and Machine Learning

Olga Ovchinnikova¹ ¹*Thermo Fisher Scientific*

11:30 AM (MASS-01.4) Refining the landscape of high dimensional molecular phenomics – strategies for enantiomer separations with high resolving power ion mobility-mass spectrometry

Benjamin K. Blakley¹, Jody C. May¹, John A. McLean¹ ¹*Vanderbilt University*

11:50 AM (MASS-01.5) Quantitative Mass Spectrometry Imaging of Liposomal Doxorubicin Delivery and Bilayer Fate in Three-Dimensional Tumor Models

Arbil Lopez¹, Joseph Holbrook¹, Gabrielle Kemper¹, Jessica Lukowski², William Andrews¹, Amanda Hummon¹ ¹*The Ohio State University*, ²*The Ohio State University*

24PAT01: Future of PAT | 302C

Chair: Marissa Dobulis
Co-Chair: Zoe Whalley, University of Birmingham

10:30 AM (PAT-01.1) What's Next in PAT for Nuclear Materials Processing

Robert Lascola¹, John T. Kelly¹, Chelsea M. Goetzman², William Gilbraith² ¹*SRNL, DOE*, ²*Savannah River National Laboratory*

10:50 AM (PAT-01.2) Application of calibration free approaches for rapid polymorph discrimination by Raman spectroscopy

Magdalene Chong¹, Martin Ward¹, Catriona McFarlan¹, Andrew Parrott¹, Iain Oswald¹, Alison Nordon¹ ¹*University of Strathclyde*

11:10 AM (PAT-01.3) Challenges in Developing Sensors for Microgravity Applications in Space

Dom Hebrault¹ ¹*Veranova*

11:30 AM (PAT-01.4) Raman Spectroscopy as a PAT Tool for Process Gas

Colin W. Couper¹, Mark Kemper², Shaun J. Fraser³ ¹*Bruker*, ²*Bruker Corp*, ³*Bruker Corporation*

11:50 AM (PAT-01.5) Innovative Moisture Analysis: Overcoming Industrial Calibration Challenges

Adam J. Hopkins¹ ¹*Metrohm USA*

24PMA01: Analytical Characterization of BioTherapeutics 306B

Chair: Rina Dukor, BioTools

10:30 AM (PMA-01.1) Understanding and protecting dry proteins

Gary J. Pielak¹, Oskar Hutcheson², Caroline Davis², Grace Nieu Kirk², Rashmika Revankar² ¹*UNC-Chapel Hill*, ²*UNC-CH*

10:50 AM (PMA-01.2) Structural Differences in mAbs upon Conjugation of Different Payloads (ADCs) Through the Eyes of Multiple Techniques

Sophia Seaman¹, Sophia Levitskaya-Seaman² ¹*MacroGenics*, ²*MacroGenics*

11:10 AM (PMA-01.3) Current State, Challenges, and Future Opportunities in Studying Structural Information for Viral Protein Stability Throughout the Lifecycle

Yun-Chu Chen¹ ¹*Purdue University*

11:30 AM (PMA-01.4) Toward determining amyloid fibril structures using experimental constraints from Raman microscopy

Madeline Harper (Hatch)¹, David Punihaole¹ ¹*University of Vermont*

11:50 AM (PMA-01.5) Rapid HPTLS Determination of Low Level Surfactants in Protein Formulations

Gregory K. Webster¹, Bryan Hassell² ¹*AbbVie*, ²*Nirrin Technologies, Inc.*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

24RAM01: Emerging Raman | 302B

Co-Chair: Pavel Matousek, STFC Rutherford Appleton Laboratory
Co-Chair: Bhavya Sharma, University of Tennessee, Knoxville

10:30 AM (RAM-01.1) **Single-molecule spectroscopic probing of N-heterocyclic carbenes on a two-dimensional metal**
Linfei Li¹, Nan Jiang¹ ¹*University of Illinois Chicago*

10:50 AM (RAM-01.2) **Waveguide-Enhanced Raman Spectroscopy for Field Detection of Threat Vapors**
Phillip G. Wilcox¹, Todd Stievater², Nathan Tyndall², Kevin Hung³, Erik Roesse¹, Ashish Tripathi¹, Jason Guicheteau¹, Erik D. Emmons¹ ¹*U.S. Army DEVCOM Chemical Biological Center*, ²*U.S. Naval Research Laboratory*, ³*Science and Technology Corporation*

11:10 AM (RAM-01.3) **Development of a Raman plate reader and the application for observation of drug-induced cellular responses in 3D spheroids**
Kazuki Bando¹, Katsumasa Fujita¹ ¹*Osaka University*

11:30 AM (RAM-01.4) **Shifted Excitation Raman Difference Spectroscopy – A potential tool for a sustainable recycling industry**

Martin Maiwald¹, Kay Sowoidnich¹, Katharina Rudisch², Karsten Pufahl², Valentin Regir³, Bernd Sumpfl¹ ¹*Ferdinand-Braun-Institut*, ²*Technische Universität Berlin*, ³*LLA Instruments GmbH*

11:50 AM (RAM-01.5) **Frontiers of Standoff Deep Ultraviolet Resonance Raman Spectroscopy**
Sergei V. Bykov¹, Sanford A. Asher¹ ¹*University of Pittsburgh*

12:15 PM- 1:30 PM **Lunch and Learn on O-PTIR Technology:**
Sponsored by Photothermal Spectroscopy Corp, *Ballroom A*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

24AES02: AES Lifetime Achievement Award | 306C

Chair: Blanca Lapizco-Encinas, Rochester Institute of Technology
Co-Chair: Sourav Bandyopadhyay

1:30 PM (AES-02.1) **The power of small: From microscale phenomena to macroscale impact**

Victor M. Ugaz¹ ¹*Texas A&M University*

2:10 PM (AES-02.2) **Microfluidic enrichment of live circulating pancreatic cancer cells from drug-treated adherent cultures**

Nathan S. Swami¹ ¹*University of Virginia*

2:30 PM (AES-02.3) **Microfluidic integration for detection of biomarkers of infectious disease**

Robert J. Meagher¹, Gihoon Choi¹, Betty Mangadu¹, Rohan Krishna¹, Nic Stromme¹ ¹*Sandia National Laboratories*

2:50 PM (AES-02.4) **Physisorbed Drag-Tags for Electrophoretic Separations of DNA and RNA**

James W. Schneider¹ ¹*Carnegie Mellon University*

24ATOM02: Data Analysis for Atomic Spectroscopy | 305A

Chair: Hunter Andrews, Oak Ridge National Laboratory

1:30 PM (ATOM-02.1) **Novel applied data science approaches in optical sensing for nuclear safeguards**

Ashwin Rao¹, Jonah B. Taylor¹, Justin I. Borrero Negrón², Janos Braun³, Paige Anderson², Kyle C. Hartig² ¹*Air Force Research Laboratory*, ²*University of Florida*, ³*New Mexico State University*

1:50 PM (ATOM-02.2) **Advanced Data Analysis Approaches for Atomic Spectroscopy – Elemental Image Analysis and ICP-TOF-MS Screening**

Hunter B. Andrews¹, Benjamin T. Manard¹, Sawyer B. Irvine¹, C. Derrick Quarles Jr.², Joseph Petrus³, Bence Paul³, Lyndsey Hendriks⁴ ¹*Oak Ridge National Laboratory*, ²*Elemental Scientific, Inc.*, ³*Elemental Scientific Lasers*, ⁴*TOFWERK AG*

2:10 PM (ATOM-02.3) **Establishing LIBS data libraries and their efficient transfer between systems**

Pavel Porizka¹, Jakub Vrabec¹, Jakub Buday¹, Jozef Kaiser¹ ¹*CEITEC Brno University of Technology*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

2:30 PM (ATOM-02.4) **Machine learning-based strategies for predicting plasma robustness and matrix effect severity in the analysis of nutrient elements in foods by inductively coupled plasma optical emission spectrometry**

Jake A. Carter¹ *US FDA CFSAN*

2:50 PM (ATOM-02.5) **Real-time monitoring of high-speed laser cleaning process by deep learning**

Soojin Choi¹, Jiyeon Choi², Jiwhan Noh² *KOREA INSTITUTE OF MACHINERY & MATERIALS*,
²*Korea Institute of Machinery and Materials*

Julian Hniopek³, Thomas W. Bocklitz⁴ *Photonic Data Science department, Leibniz Institute of Photonic Technology, Jena, Germany*, ²*Institute of Physical Chemistry & Abbe Center of Photonics (ACP) Friedrich Schiller University Jena, Germany*, ³*Department of Photonic Data Science, Leibniz Institute of Photonic Technology, Jena, Germany*, ⁴*Leibniz Institute of Photonics Technology*

1:50 PM (BIM-02.2) **Tandem Raman Microscopy (TRAM) and data fusion significantly improves morpho-chemical analysis**

Anna M. Nowakowska¹, Krzysztof Brzozowski¹, Anna Pieczara², Wiktoria Korona³, Barbara Orzechowska¹, Jakub Firlej¹, Adrianna Wislocka-Orlowska¹, Malgorzata Baranska⁴ *Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387, Krakow, Poland*, ²*Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics (JCET), Bobrzynskiego 14, 30-348 Krakow, Poland*; *Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, Lojasiewicza 11, Krakow, Poland*, ³*Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387, Krakow, Poland*; *Jagiellonian University in Kraków, Doctoral School of Exact and Natural Sciences, Lojasiewicza 11, Krakow, Poland*, ⁴*Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387, Krakow, Poland*; *Jagiellonian University, Jagiellonian Centre for Experimental Therapeutics (JCET), Bobrzynskiego 14, 30-348 Krakow, Poland*

2:10 PM (BIM-02.3) **Model transfer in Raman spectroscopy: towards better clinical applications**

Shuxia Guo¹, Thomas W. Bocklitz² *Leibniz Institute of Photonic Technology (Leibniz-IPHT)*,
²*Leibniz Institute of Photonics Technology*

2:30 PM (BIM-02.4) **Raman hyperspectroscopy of saliva and machine learning for Sjögren's disease diagnostics**

Bhavik Vyas¹, Ana Khatiaashvili², Neil Gildener-Leapman², Melinda Larsen¹, Lisa Galati², Khoa Ngo², Igor K. Lednev³ *University at Albany*,
²*Albany Medical College*, ³*University at Albany, SUNY*

2:50 PM (BIM-02.5) **Automated Framework for High-Throughput Raman Spectra Analysis in Cellular Differentiation Monitoring**

Piyush Raj¹, Menglu Li², Yukiko Ueyama-Toba², Hiroiyuki Mizuguchi², Katsumasa Fujita², Ishan Barman¹ *Johns Hopkins University*, ²*Osaka University*

24AWD01: RSC 2023 Analytical Science Open Prize: Theophilus Redwood Prize Award Session 301B

Chair: Frank Vanhaecke, Ghent University

1:30 PM (AWD-01.1) **50 ways to size your nanomaterials via single-event ICP-MS**

Antonio Bazo¹, Eduardo Bolea-Fernández¹, Ana M. Rua-Ibarz¹, Maite Aramendia¹, Martin Resano¹ *Universidad de Zaragoza*

1:50 PM (AWD-01.2) **Evaluation of the analytical performance of femtosecond laser ablation ICP-TOFMS for the direct analysis of challenging samples**

Jorge Pisonero¹, Cristian Soto-Gancedo¹, Ana Méndez-Vicente¹, Alex Calon², Ines García³, Jaime Orejas¹, Nerea Bordel¹ *University of Oviedo*, ²*Hospital del Mar Medical Research Institute (IMIM)*, ³*Khis Group*

2:10 PM (AWD-01.3) **A Novel Standards-Addition Isotope Dilution Method for Inductively-Coupled Plasma Mass Spectrometry Isotope Ratio Measurements**

Steven Ray¹, Khue Nguyen¹, Joe Gatewood², John Elling², Sheikh Rahman³ *SUNY Buffalo Dept of Chemistry*, ²*Molten Salt Solutions*,

2:30 PM (AWD01-4) **Nonmetal Detection by Post-ICP Chemical Ionization Mass Spectrometry**

Kaveh Jorabchi¹, Grace Hahm¹, Jordan L. Tanen¹, Samuel White¹, Frenio Redeker¹ *Georgetown University*

24BIM02: Machine and Deep Learning for Biomedical Diagnostics | 302A

Chair: Thomas Bocklitz, Leibniz Institute of Photonics Technology

Co-Chair: Oleg Ryabchykov, Leibniz Institute of Photonic Technology Jena, Albert-Einstein-Str. 9, 07745 Jena, Germany; Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University, Lessingstraße 10, 07743 Jena, Germany

1:30 PM (BIM-02.1) **Investigating preprocessing and feature extraction approaches for improved diagnostics**

Oleg Ryabchykov¹, Pegah Dehbozorgi², Mou Adhikari¹, Nazar Stefaniuk², Darina Storozhuk¹,

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

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24CHEM02: Chemometrics: Something Borrowed, Something New | 305B

Chair: Federico Marini, University of Rome La Sapienza

1:30 PM (CHEM-02.1) Fusion of LIBS and RGB Imaging for Enhanced Marble Analysis: A Chemometric Approach

Ruggero Guerrini¹, Ludovic Duponchel², Vincent Motto-Ros³, Federico Marini⁴ ¹LASIRE, UMR 8516, Université de Lille, ²University of Lille, ³ILM, ⁴Dept. of Chemistry, University of Rome "La Sapienza"

1:50 PM (CHEM-02.2) Shift Invariant Tri-linearity (SIT) and Shift Invariant Soft Tri-linearity (SIST) for fast, flexible blind source separation in hyphenated chromatography

Neal B. Gallagher¹, Paul-Albert Schneide², Rasmus Bro³ ¹Eigenvektor Research Inc, ²BASF SE, ³University of Copenhagen

2:10 PM (CHEM-02.3) When Social Media Empowers Analytical Chemists to Explore Millions of Spectra Derived from a Complex Sample

Ludovic Duponchel¹, Vincent Motto-Ros² ¹University of Lille, ²ILM

2:30 PM (CHEM-02.4) Vibrational spectroscopy combined with multivariate analysis, a new diagnostic tool for Fibromyalgia disorder

Shreya M. Nuguri¹, Luis Rodriguez-Saona², Silvia de Lamo Castellvi², Yalan Wu³, Celeste Matos-Gonzalez³, Kevin Hackshaw⁴ ¹The Ohio state University, ²The Ohio State University, ³The Ohio state university, ⁴University of austin

2:50 PM (CHEM-02.5) Strategies for non-linear modeling for multi-block and multi-way data

Federico Marini¹, Alessandra Biancolillo² ¹Dept. of Chemistry, University of Rome "La Sapienza", ²Department of Physical and Chemical Sciences, University of L'Aquila

24CTPEARLY01: Showcasing Career Paths in the Spectroscopic Sciences (Organized by SAS Early Career) 303

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

Co-Chair: Samuel Mabbott, Texas A&M University

1:30 PM (CTPEARLY-01.1) Navigating the Intricated Early Career journey: Opportunities at the UKRI National Laboratories

Sara Mosca¹ ¹STFC - UKRI

1:50 PM (CTPEARLY-01.2) Transitioning from the Lab to Process Control: Leveraging Skills Gained in Graduate School

Cyril Soliman¹ ¹Endress+Hauser

2:10 PM (CTPEARLY-01.3) From PhD to COO: A Discussion of Recent Graduate Transitions

Alexis Weber¹ ¹SupreMEtric

2:30 PM (CTPEARLY-01.4) Nanomaterials to nuclear materials – my transition from PhD to Postdoctoral Researcher at SRNL and a learning lifestyle

Chelsea M. Goetzman¹ ¹Savannah River National Laboratory

2:50 PM (CTPEARLY-01.5) Panel Discussion

24IR02: Two-Dimensional Correlation Spectroscopy-II 301A

Chair: Young Jung, Kangwon National University

Co-Chair: Isao Noda, University of Delaware

1:30 PM (IR-02.1) Applications of 2D correlation spectroscopy in SERS studies

Young Mee Jung¹ ¹Kangwon National University

1:50 PM (IR-02.2) 2D disrelation mapping for characterization of polymer composites

Hideyuki Shinzawa¹ ¹AIST

2:10 PM (IR-02.3) Monitoring of a Polyurethane Synthesis with Lightfiber-Coupled FT-IR/ATR Spectroscopy: Added Value of 2D-COS and MCR-ALS Analyses

Heinz W. Siesler¹, Marina De Gea Neves¹, Miriam Unger² ¹University Duisburg-Essen, ²Photothermal Spectroscopy Corporation

2:30 PM (IR-02.4) Two-trace two-dimensional correlation spectroscopy a valid approach towards therapeutic protein identification and purity assessment: A predictive screening method for product quality attribute for biopharma.

Belinda Pastrana¹ ¹Protein Dynamic Solutions, Inc.

2:50 PM (IR-02.5) Deviations from the Beer-Lambert approximation investigated by 2D-Correlation IR spectroscopy

Thomas G. Mayerhoefer, Juergen Popp¹ ¹Leibniz Institute of Photonic Technology

3:10 PM (IR-02.6) Infrared spectrochemical imaging and Two-Dimensional Correlation spectral analysis of polymer biodegradation

Kathleen M. Gough¹, Fatemeh Jamshidzadehtaleshi², Quintin Litke³, Song Liu³, David Levin³ ¹University of Manitoba, ²Department of Chemistry, University of Manitoba, ³Biosystems Engineering, University of Manitoba

24MASS02: Novel MS Methods for Clinical, Forensic, and Toxicological Applications | 306A

Chair: Christopher Chouinard, Clemson University

1:30 PM (MASS-02.1) Ion source ozonolysis enabled lipid unsaturation analysis in biological samples

Qibin Zhang¹, Ashraf Omar¹, Ryan Smith¹ ¹UNCG

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

1:50 PM (MASS-02.2) **Evaluating microchip capillary electrophoresis-mass spectrometry for the quantification of metabolites from cells and tissues**

Whitney L. Stutts¹, Aurora Cabrera¹, Thomas Webb¹, Scott Lyons¹, Saame Raza Shaikh¹, Jessica Thaxton¹, Erin Redman², J. Will Thompson³, Laura E. Herring¹ ¹University of North Carolina at Chapel Hill, ²908 Devices Inc., ³908 Devices Inc

2:10 PM (MASS-02.3) **Connecting Bioprocess Metabolites to Antibody Quality Attributes using MicroChip CE-HRMS**

Erin Redman¹, Stephanie Klaubert¹, Awab Nehela¹, Sam Stewart¹, Milla Neffling¹, J. Will Thompson² ¹908 Devices Inc., ²908 Devices Inc

2:30 PM (MASS-02.4) **Multimodal Multiplexed Approaches to Assess the Triple-Negative Breast Cancer Microenvironment**

Jaclyn B. Dunne¹, Heather Jensen-Smith², Laura Spruill¹, Taylor S. Hulahan¹, Mark J. Lim³, Gargey Yagnik³, Kenneth J. Rothschild³, Anand S. Mehta¹, Richard R. Drake¹, Graham A. Colditz⁴, Marvella E. Ford¹, Peggi M. Angel¹ ¹Medical University of South Carolina, ²University of Nebraska Medical Center, ³AmberGen, ⁴Washington University St. Louis

2:50 PM (MASS-02.5) **High-Resolution Ion Mobility and Tandem Mass Spectrometry: Novel Insights into NPS Analysis**

Ralph Aderorho¹, Copeland Johnson¹, Christopher D. Chouinard¹ ¹Clemson University

24PMA02: Chirality in Pharma | 306B

Chair: Rina Dukor, BioTools

1:30 PM (PMA-02.1) **Application of Vibrational Circular Dichroism (VCD) in Drug Discovery and Development – Structure Elucidation of Chiral Molecules**

Yanan He¹ ¹GSK

1:50 PM (PMA-02.2) **Fatty Acids and Phospholipids Reverse Supramolecular Chirality of Insulin Fibrils.**

Dmitry Kurouski¹ ¹Texas A&M University

2:10 PM (PMA-02.3) **Absolute Stereochemistry Determination for Small Molecule Inhibitors of EP300/CREBBP Acetyltransferase by Vibrational Circular Dichroism**

Christopher A. LeClair¹, Yuhong Fang¹, Kamaria Butler¹, McKenna Crawford², Deepika Tripu², Yihang Jing², Diamond Gallimore², Stephen Kales¹, Ying Xiong², Anton Simeonov¹, Jordan Meier² ¹National Center for Advancing Translational Sciences, NIH, ²National Cancer Institute, NIH

2:30 PM (PMA-02.4) **Quantum Cascade Laser-Based Rapid Vibrational Circular Dichroism Spectroscopy and Imaging Systems**

Yamuna Phal¹, Viviana Arrunategui Norvick²,

Roya Akrami¹ ¹Colorado School of Mines, ²Colorado School of Mines Phal Group

2:50 PM (PMA-02.5) **Structural characterization of Plant-based Proteins**

Helen K. Gerardi¹ ¹Ingredion

24RAM02: SERS 1 | 302B

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

Co-Chair: Zac Schultz, The Ohio State University

Co-Chair: Roy Goodacre, University of Liverpool

1:30 PM (RAM-02.1) **Tailoring nanoparticle clusters for SERS-enabled temperature measurements during photothermal therapy**

William H. Skinner¹, Natalie Potter², Kamil Sokolowski³, MEGHA MEHTA¹, Sara Mosca⁴, Benjamin Gardner¹, Jeremy Baumberg³, Oren Scherman³, Pavel Matousek⁴, Nicholas Stone¹ ¹University of Exeter, ²Univeristy of Cambridge, ³University of Cambridge, ⁴STFC - UKRI

1:50 PM (RAM-02.2) **Selective Plane Illumination Surface Enhanced Raman Spectral Imaging in Cells**
Abigail E. Smith¹, Zachary D. Schultz¹ ¹The Ohio State University

2:10 PM (RAM-02.3) **Advancing the Design of Reagentless SERS Biosensors**

Pietro Strobbia¹ ¹University of Cincinnati

2:30 PM (RAM-02.4) **Enhancing CoVID-19 Diagnosis: PCR-Comparable Direct Detection of Clinic Specimens Using Surface-Enhanced Raman Spectroscopy and Deep Learning Algorithms**

YanJun Yang¹, Hao Li², Les Jones¹, Jackelyn Murray¹, Hemant Naikare¹, Yung-Yi C. Mosley¹, Teddy Spikes¹, Sebastian Hülck³, Ralph A. Tripp¹, Bin Ai², Yiping Zhao⁴ ¹University of Georgia, ²Chongqing University, ³tec5USA, Inc, ⁴The University of Georgia

2:50 PM (RAM-02.5) **Bimetallic Silver-Gold Nanostars: Development and Application for SERS Sensing**

Supriya Atta¹, Tuan Vo-Dinh¹ ¹Duke University

24RAM12: Raman Spectroscopy for Security and Forensics Purposes | 302C

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

Co-Chair: Lamyaa Almeahmadi, MIT

1:30 PM (RAM-12.1) **Innovative On-Site Raman Techniques for Pathogen Characterization**

Juergen Popp¹ ¹Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics

1:50 PM (RAM-12.2) **Raman spectroscopy and Artificial Intelligence in forensic science: case study - Rapid detection and classifications of pathogens**

Siva Umamathy¹ ¹Indian Institute of science

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2:10 PM (RAM-12.3) **CWA, Narcotic, and Riot Control Agent Library Creation and Validation on Field Portable Standoff Raman Systems**

Katelyn Koll¹, Evan Durnal¹, Sara Paalhar¹, Joshua Lindell¹ ¹*MRIGlobal*

2:30 PM (RAM-12.4) **Probing Antihistamine Drug in Oral Fluid Using Deep Ultraviolet Raman Spectroscopy for Forensic Purposes**

Mohamed O. Amin¹, Fatima Matroodi², Barbara Rossi³, Entesar Alhetlani⁴, Igor K. Lednev⁵ ¹*University at Albany*, ²*Elettra - Sincrotrone*, ³*Elettra-Sincrotrone Trieste*, ⁴*Kuwait University*, ⁵*University at Albany, SUNY*

2:50 PM (RAM-12.5) **In Situ Detection of Gunshot Residue using Raman Spectroscopy**

Igor K. Lednev¹, Alexander Rzhetskii, Shelby R. Khandasammy¹ ¹*University at Albany, SUNY*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 3:50 PM – 5:30 PM | *Various Locations*

24AES03: AES Emerging Leaders | 306C

Chair: Tayloria Adams, University of California, Irvine

Co-Chair: Raphael Oladokun, West Virginia University

3:50 PM (AES-03.1) **Electrochemical Diagnostics to Support Equitable Healthcare**

Ariel Furst¹ ¹*MIT*

4:10 PM (AES-03.2) **Suppression of Non-faradaic Current in DNA Monolayer-based Bowtie Sensors by Engineering the Temporal Response**

A Z M Mainul Islam Mazumder¹, Asanka Gurukandure¹, Christopher J. Easley¹ ¹*Auburn University*

4:30 PM (AES-03.3) **Strategy for enhancing insulator-based electrokinetic device design for tertiary separations**

Alaleh Vaghef-Koodehi¹, Patricia Cyr¹, Blanca H. Lapizco-Encinas¹ ¹*Rochester Institute of Technology*

4:50 PM (AES-03.4) **Spinning Desiccator: A Cost Effective and Generalizable Post Processing Method for Enhanced Optical Quality in 3D Printed Microfluidics**

Gabriel A. Garibaldi¹, Gongchen Sun¹, Guillermo Ramirez², Miguel Garibaldi² ¹*University of Texas at San Antonio*, ²*Univeristy of Texas at San Antonio*

5:10 PM (AES-03.5) **FLEXIBLE NANOLITER DROPLET CONTROL WITH 3D PRINTED PNEUMATIC PULSE TIMERS WITHOUT ELECTRICAL POWER**

Joanne Y. Seow¹, Md Mohibullah¹, Christopher J. Easley¹ ¹*Auburn University*

24ATOM03: Analytical Geochemistry | 305A

Chair: Alicia Cruz-Urbe, University of Maine

3:50 PM (ATOM-03.1) **Extent of matrix effects between Zircon and Baddeleyite in U-Pb geochronology by laser ablation ICP-MS**

Kate Souders¹, Jay M. Thompson¹, Paul Sylvester² ¹*US Geological Survey*, ²*Texas Tech*

University

4:10 PM (ATOM-03.2) **Microscopic Time Machines: Mass Spectral Investigations of Earth's Evolving Atmosphere via Fluid Inclusions**

Justin G. Park¹, Jacob T. Shelley¹, Brent D. Turrin², Morgan F. Schaller¹ ¹*Rensselaer Polytechnic Institute*, ²*Rutgers University*

4:30 PM (ATOM-03.3) **Characterization of downhole fractionation for in situ Rb-Sr dating in natural micas and synthetic reference materials**

Cemil Arkula¹, Alicia M. Cruz-Urbe¹, Joshua Garber² ¹*University of Maine*, ²*The Pennsylvania State University*

4:50 PM (ATOM-03.4) **Use of ICP-MS/MS for accurate in-situ Pb isotopic analysis by laser ablation in the presence of Hg**

Jay M. Thompson¹, Kate Souders¹ ¹*US Geological Survey*

5:10 PM (ATOM-03.5) **Static multi-Daly analysis of small samples yields high precision isotope measurements on the Nu Plasma 3D MC-ICP-MS**

Staci L. Loewy¹, Ye Zhao² ¹*The University of Texas at Austin*, ²*Nu Instruments Ltd, Ametek*

24CHEM04: Data Driven Materials Discovery: Expanding Beyond Traditional Chemometrics | 305B

Chair: Caelin Celani, University of Delaware

3:50 PM (CHEM-04.1) **“Seeing” Chemical Data through Multi-Objective Lenses**

Arthur Lin¹, Christian Jorgensen¹, Rose K. Cersonsky¹ ¹*University of Wisconsin - Madison*

4:10 PM (CHEM-04.2) **Exploration of a Metastable Metal Oxide Synthesis Space through Data-Enabled Approaches**

Rachel D. Davidson¹ ¹*University of Delaware*

4:30 PM (CHEM-04.3) **Understanding the degradation and strain of thin GaSe for quantum technology applications**

Lottie Murray¹, Matthew Doty¹ ¹*University of Delaware*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

Oral Symposia | 3:50 PM – 5:30 PM | *Various Locations*

4:50 PM (CHEM-04.4) **Artificial Intelligence and High-Performance Data Mining for Accelerating Science**

Ankit Agrawal¹ ¹*Northwestern University*

5:10 PM (CHEM-04.5) **Monitoring Simulated Solar Radiation-Induced Weathering of Thiol-capped CdSe/ZnS Semiconductor Quantum Dots using Multivariate Frequency-Domain Photoluminescence Measurements**

Sharon L. Neal¹, Micah J. Murray¹ ¹*University of Delaware*

Lyufei Chen¹, Jeffrey Julien¹ ¹*HORIBA Instruments*

5:10 PM (IR-06.5) **Scalable Continuous Photochemical and Electrochemical Reactions - PAT Challenges and Present Gaps and Future Opportunities: From Picoseconds to Tonnes**

Michael George¹ ¹*University of Nottingham*

24CTPEARLY04: Commercialization of Analytical Technologies | 303

Chair: Alexander Scheeline

3:50 PM (CTPEARLY-04.1) **Translating academic research from the lab to commercial products: a few experiences**

J Michael Ramsey¹ ¹*UNC-Chapel Hill*

4:10 PM (CTPEARLY-04.2) **Rubitection - Translational of optical tool for skin health assessment for chronic wounds and dermatological conditions**

Sanna Gaspard¹ ¹*Rubitection*

4:30 PM (CTPEARLY-04.3) **Commercialization of New Science (VCD & ROA): What Does it Really Take?**

Rina Dukor¹ ¹*BioTools*

4:50 PM (CTPEARLY-04.4) **So you want to build a measurement science startup: Where? What? Who? When? Why?**

Freddy T. Nguyen¹ ¹*Massachusetts Institute of Technology*

5:10 PM (CTPEARLY-04.5) **Panel Discussion**

24IR06: Unlocking Molecular Landscapes: Exploring Complex Systems with Excitation-Emission Matrix Spectroscopy | 301A

Co-Chair: Jeffrey Julien, Horiba Instruments Inc.

Chair: Michael George, U of Nottingham

3:50 PM (IR-06.1) **Monitoring Poly(N-isopropylacrylamide) aggregation using intrinsic emission and Polarized Excitation-Emission Matrix Spectroscopy.**

Alan G. Ryder¹, Matheus A. de Castro¹
¹*Nanoscale Biophotonics Laboratory, University of Galway*

4:10 PM (IR-06.2) **Screening Falsified Biologic Drug Products with A-TEEM Spectroscopy**

Brendon M. Lyons¹, Jeffrey Julien², Lyufei Chen²
¹*Bristol Myers Squibb*, ²*HORIBA Instruments*

4:30 PM (IR-06.3) **Unlocking Molecular Landscapes: Exploring Complex Systems with Excitation Emission Matrix (EEM) Fluorescence Spectroscopy**

Ashley Love¹ ¹*University of Nottingham*

4:50 PM (IR-06.4) **Qualification and quantification analysis of cell media using Absorbance-Transmittance Excitation Emission Matrix (A-TEEM) Fluorescence Spectroscopy**

24IR12: Focus on Artificial Intelligence in Infrared Spectroscopy | 301B

Chair: Axel Mosig, Ruhr-University Bochum

3:50 PM (IR-12.1) **Investigating deep learning-based technologies for vibrational spectroscopic imaging data**

Azadeh Mokari¹, ruihao Luo¹, Christoph Krafft²,
Thomas W. Bocklitz³ ¹*University of Jena*,
²*Leibniz IPHT*, ³*Leibniz Institute of Photonics Technology*

4:10 PM (IR-12.2) **Translational efforts for digital chemical pathology with infrared laser scanning microscopy**

Kevin L. Yeh¹, Kianoush Falahkheirkhah¹,
Yen-Ting Liu¹, Ruo-Jing Ho¹, Ishaan Sharma¹,
Matthew P. Confer¹, Andres C. Orr¹, Mykolas Tamonis¹, Rohit Bhargava¹ ¹*University of Illinois at Urbana-Champaign*

4:30 PM (IR-12.3) **Risk stratification of prostate cancer using infrared spectroscopic imaging**

Peter Gardner¹, Photon S. Institute¹, Photon S. Institute¹ ¹*University of Manchester*

4:50 PM (IR-12.4) **Theory is Dead, Long Live Theory: Trustworthy Artificial Intelligence for Infrared Spectroscopy**

Axel Mosig¹ ¹*Ruhr University Bochum*

5:10 PM (IR-12.5) **Metric-Based Comparison of Threat Anomaly Detection (ThreAD) Parameters to Standard Anomaly Detection Techniques**

Eric R. languirand¹, Matthew Collins¹, Jacob Buchman² ¹*US Army DEVCOM CBC*, ²*Army Educational Outreach Program Fellow*

24MASS03: New approaches to biomolecular sequence and structure characterization | 306A

Chair: Jared Shaw, University of Nebraska-Lincoln

3:50 PM (MASS-03.1) **Linking Native Mass Spectrometry to Structural Biology with Top-Down Proteomics**

Joseph A. Loo¹ ¹*University of California, Los Angeles*

4:10 PM (MASS-03.2) **Combining Trapped Ion Mobility Spectrometry with electron and UV based tandem Mass Spectrometry**

Francisco Fernandez-Lima¹ ¹*Florida International University*

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4:30 PM (MASS-03.3) **Design and Optimization of a new microwave microreactor for mass spectrometry.**

Buddhika T. Kumara¹ *The State University of New York at Buffalo*

4:50 PM (MASS-03.4) **Collisions, Electrons, Enzymes, and Columns with 10 year old Mass Specs Provide Unparalleled, Functionally-Specific Structural Dynamics in the Epigenoproteome and Bad Behavers**

Ian Webb¹, Kymeri Davis¹, Ashlyn Dollar¹, Ankita Gurav¹, Erika Renbarger¹ *Indiana University Indianapolis*

5:10 PM (MASS-03.5) **Complex-Up Characterization of the Ribosome by Infrared Multiphoton Dissociation**

Sachin Tennakoon¹, Bret Perkins², Mashiyat Mubassera¹, Jared Shaw¹ *University of Nebraska-Lincoln*, ²*Northern Arizona University*

24PAT02: PAT Pharma/Biotech | 302C

Chair: Michael Bishop, Corteva

3:50 PM (PAT-02.1) **In-situ Raman in Fermentations of Crop Protection Active Ingredients**

Michael M. Bishop¹, David Archer², David Ferial Gervasio², E. Timothy Davies², Bryon Herbert², Stefanie Casada² *Corteva*, ²*Corteva Agriscience*

4:10 PM (PAT-02.2) **Hyperspectral Imaging in Pharmaceuticals: Enhancing Product Analysis and Overcoming Limitations for inline inspection**

Fabien Chauchard¹ *INDATECH CHAUVIN ARNOUX*

4:30 PM (PAT-02.3) **In-line Raman Spectroscopy for Polymorph Control during Continuous Crystallization**

Sreya Sarkar¹, Andy Stumpf¹, Zhenqi (Pete) Shi², Dawen Kou¹, Peter Yehl¹ *Genentech*, ²*Genentech, Inc.*

4:50 PM (PAT-02.4) **Real-time monitoring of CHO cell metabolites and mAb concentrations using solid-state Raman Spectroscopy**

Janam K. Pandya¹ *Thermo Fisher Scientific*

5:10 PM (PAT-02.5) **In Situ PAT Particle Characterization Probes Compared**

Charles Goss¹, Daniel Green¹ *GSK*

24PMA03: Innovations in Vibrational Spectroscopy for Pharmaceutical Development | 306B

Chair: Zoe Whalley, Bristol Myers Squibb

Co-Chair: Gary McGeorge, Bristol Myers Squibb

3:50 PM (PMA-03.1) **Domain Size and Homogeneity Analysis Using Chemical Imaging**

Patrick Wray¹, Dimuthu Jayawickrama¹, Zoe Whalley¹, Greg Lane¹, Lucy Hawarden¹, Elyse DiMaso¹, Matthew Saunders¹, Gary McGeorge¹ *Bristol Myers Squibb*

4:10 PM (PMA-03.2) **Studying Monoclonal Antibody Aggregation Under Flow Using Fourier Transform Infrared Spectroscopic Imaging**

Celine J. van Haaren¹, Bernadette Byrne¹, Sergei G. Kazarian¹ *Imperial College London*

4:30 PM (PMA-03.3) **Transmission Raman Spectroscopy, Supporting Pharmaceutical Manufacturing to achieve efficiencies and process understanding in continuous drug product manufacturing.**

Julia A. Griffen¹ *Agilent Technologies*

4:50 PM (PMA-03.4) **Diffusion Mapping with Diffractive Optical Elements for Periodically Patterned Photobleaching**

Maura M. Wimsatt¹, Dustin M. Harmon¹, Ziyi Cao¹, Alex Sherman¹, Nita Takanti¹, Kevin Murati¹, Michelle Cousineau¹, YeChan Hwang¹, Lynne S. Taylor¹, Garth J. Simpson¹ *Purdue University*

5:10 PM (PMA-03.5) **Recent advances in deep UV Raman and fluorescence instruments for industrial process analysis and cleaning verification**

Rohit Bhartia¹, Ray D. Reid¹, Kenneth Nguyen¹, Quoc Nguyen², William Hug³ *Photon Systems, Inc.*, ²*Photon Systems, Inc.*, ³*Photon Systems*

24RAM03: SERS 2 | 302B

Co-Chair: Roy Goodacre, University of Liverpool

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

Co-Chair: Zac Schultz, The Ohio State University

3:50 PM (RAM-03.1) **In Vivo Excretable Supramolecular Raman Nanoparticles for Translational Multiplexed Raman Imaging**

Jung-Ho Yu¹ *University of Waterloo*

4:10 PM (RAM-03.2) **Direct Multiplexed Detection of miRNA Biomarkers Using SERS-Based Probes**

Aidan J. Canning¹, Tyler Vasse¹, Hsin-Neng Wang¹, Tuan Vo-Dinh¹ *Duke University*

4:30 PM (RAM-03.3) **High Curvature Surface-enhanced Raman Scattering Sensors for Biomedical Applications**

Malama Chisanga¹, Xingjuan Zhao², Felix Lussier³, Jean-Francois Masson⁴ *University of Montreal*, ²*Shandong Jianzhu University*, ³*McGill University*, ⁴*Universite de Montreal*

4:50 PM (RAM-03.4) **Electrokinetic-Modulated Surface-Enhanced Raman Spectroscopy (EK-SERS) Immunoassay for Viral Detection**

Sonali Srivastava¹, Chuan Xiao¹, Wei Zhou¹, Peter Vikesland² *Virginia Tech*, ²*Professor*

5:10 PM (RAM-03.5) **Blotter Paper, Letter Paper, and Packaging: A Look at Using SERS to Intercept Hidden Narcotics**

Adam J. Hopkins¹, Wei Yu² *Metrohm USA*, ²*Metrohm USA, Inc*

TECHNICAL PROGRAM - MONDAY, OCTOBER 21, 2024

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24SPSJ01: Low-frequency vibrational spectroscopy | 302A

Chair: Yukihiro OZAKI, Kwansei Gakuin University
Co-Chair: Harumi SATO, Kobe University

3:50 PM (SPSJ-01.1) Molecular dynamics of water in the terahertz region

Keiichiro Shiraga¹ *Graduate School of Agriculture, Kyoto University*

4:10 PM (SPSJ-01.2) Low-frequency Raman and far-infrared/terahertz spectroscopy studies of polymers

Harumi SATO¹ *Kobe University*

4:30 PM (SPSJ-01.3) Low-frequency Vibrational Spectroscopy Studies of Minerals, Rocks, and Biogenic Minerals

Yukihiro OZAKI¹, Motohiro TSUBOI¹, Kohei

TAMURA², Ryosuke Kitanaka³, Hiroshi Oka³ *Kwansei Gakuin University*, ²*JASCO Corporation*, ³*School of Biological and Environmental Sciences, Kwansei Gakuin University*

4:50 PM (SPSJ-01.4) Behavior of the state of water drawn from IR/FIR spectra in the 1000–100 cm⁻¹ region and in the 4000–3000 cm⁻¹ region

Daitaro Ishikawa¹, Rin Shinohara¹, Natsumi Shichishima¹, Tomoyuki Fujii¹ *Tohoku university*

5:10 PM (SPSJ-01.5) Glass Transition Mapping of Heterogeneous Polymers using Low-Frequency Confocal Raman Microscopy

Kayla Bensley¹, Robert V. Chimenti¹ *Rowan University*

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Award & Plenary Lectures | 8:15 AM – 9:30 AM | *Ballroom A*

8:15 AM Award Presentation

8:30 AM FACSS Charles Mann Award for Raman Spectroscopy: Raman Nanotheranostics - how can using SESORS add clinical value?

Nicholas Stone¹ *University of Exeter*

9:00 AM Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award: The Intersection of Spectroscopy and Data Science: Developing the Next Generation of Enabling Technologies for Pharmaceuticals and Beyond

Joseph P. Smith¹ *Merck*

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Tuesday Poster Sessions | 9:30 AM – 10:30 AM | *Exhibit Hall B*

(Tue-P1) Applying Cheminformatics to Develop a Structure Searchable Database of Analytical Methods

Antony J. Williams¹, Gregory Janesch², Erik carr², Sakuntala Sivasupramaniam³, Nancy Baker⁴
¹*United States Environmental Protection Agency*,
²*ORAU Student Services Contractor to Center for Computational Toxicology and Exposure*,
³*Senior Environmental Employment Program*,
⁴*ParlezChem Inc*

(Tue-P2) Approaches and Strategies for the Detection and Quantification of Nano and Microplastics by Single Particle Inductively Coupled Plasma Mass Spectrometry

Chady Stephan¹, Aaron Hineman¹, Ruth Merrifield¹, Liyan Xing¹ *PerkinElmer US LLC*

(Tue-P3) Analyzing PFAS in Complex Matrices with Simplicity TM

Jesse S. Leonard¹ *PerkinElmer*

(Tue-P4) Quantitation and identification of microplastics accumulation in human specimens using pyrolysis-gas chromatography mass spectrometry

Rui Liu¹ *University of New Mexico*

(Tue-P5) Study of Age-Induced Isotope Fractionation in Lithium-ion Batteries using Microwave-Induced Cold Nitrogen Plasma Mass Spectrometry

Carlos Abad¹, Dalia Morcillo², Alexander Winckelmann³, Marcus Oelze², Silke Richter³, Jochen Vogl², Sebastian Recknagel⁴, Ulrich Panne³ *Bundesanstalt für Materialforschung und -prüfung (BAM)*, ²*Federal Institute for Materials Research and Testing (BAM)*, ³*Bundesanstalt für Materialforschung und -prüfung (BAM)*, ⁴*Bundesanstalt für Materialforschung und -prüfung (BAM)*,

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

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(Tue-P6) **High Efficiency Sample Introduction System for Superior ICP-MS Performance of Single-Cell, Single-Particle, Nanoparticle, and Low-Volume Analysis**

Randy J. Mercurio¹ *Glass Expansion, Inc.*

(Tue-P7) **Introducing “Full Scan” Glow Discharge Mass Spectrometry of Iron Oxides for Provenience Studies of Ochre Pigments**

Andrew M. Zipkin¹, Gideon Bartov¹ *Eurofins EAG Laboratories*

(Tue-P8) **Elemental Ratios as a Key: Exploring Alzheimer’s Disease through ICP-MS and Machine Learning**

Ali Safi¹, Nouredine Melikechi¹, Kemal Efe Eseller¹, Richard Gaschnig¹, Weiming Xia²
¹*University of Massachusetts Lowell*, ²*Boston University*

(Tue-P9) **Glycosaminoglycan Imaging by IR-MALDESI**

Tana V. Palomino¹, David C. Muddiman¹ *North Carolina State University*

(Tue-P10) **Uncovering the Importance of Diphenylamine in the Fluorescence Analysis of Smokeless Powder and GSR for Forensic Purposes**

Cody Silverman¹, Igor K. Lednev¹ *University at Albany, SUNY*

(Tue-P11) **Achieving Parts-Per-Million Mass Measurement Accuracy of N-linked Glycans**

Adeleke A. Adepoju¹, Tana V. Palomino¹, David C. Muddiman¹ *North Carolina State University*

(Tue-P12) **Analysis of Per and Polyakyl-substances (PFAS) via Laser-Assisted Micro pyrolysis Flowing Atmospheric Pressure After Glow High Resolution Mass spectrometry**

Ejoke Akatugba¹, Daniela Barroso¹, Bibek R. Bhattarai², Songyue Shi³, Gerardo Gamez⁴
¹*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409-1061 US*, ²*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409-1061, US*, ³*Proteomics Core Facility, UT Southwestern Medical Center, Dallas, Texas 75390, US*, ⁴*Texas Tech University*

(Tue-P13) **Optimization of an Ultraviolet Laser for Improved MALDESI Mass Spectrometry Imaging of Plant Tissue**

Sarah Ashbacher¹, David C. Muddiman¹, Jeffrey G. Manni² *North Carolina State University*, ²*JGM Associates, Inc.*

(Tue-P14) **Biopolymer Analysis by Laser-Assisted Micro-Pyrolysis Flowing Atmospheric-Pressure Afterglow High-Resolution Mass Spectrometry**

Daniela Barroso¹, Ejoke Akatugba², Bibek R. Bhattarai¹, Songyue Shi³, Gerardo Gamez⁴
¹*Department of Chemistry and Biochemistry,*

Texas Tech University, Lubbock, Texas 79409-1061, US, ²*Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409-1061 US*, ³*Proteomics Core Facility, UT Southwestern Medical Center, Dallas, Texas 75390, US*, ⁴*Texas Tech University*

(Tue-P15) **Optimizing Absolute Quantification Strategies for IR-MALDESI MSI**

Emily R. Bruce¹, Yunxin Ouyang², Tatiana Segura², David C. Muddiman¹ *North Carolina State University*, ²*Duke University*

Tue-P16) **Hair Metabolome in 5xFAD Mice and Patients with Alzheimer’s Disease Using High Resolution Mass Spectrometry Approaches**

Chih-Wei Chang¹, Pao-Chi Liao¹ *National Cheng Kung University*

(Tue-P17) **Obtaining Single Mammalian Cell Spatial Resolution with a 2940 nm Laser by IR-MALDESI Mass Spectrometry Imaging**

Seth Eisenberg¹, Alena N. Joignant¹, Kevan T. Knizner¹, Jeffrey Manni², David C. Muddiman¹
¹*North Carolina State University*, ²*JGM Associates, Inc.*

(Tue-P18) **Alternative mid-IR Absorbing Matrices for Reflection and Transmission Mode IR-MALDESI Mass Spectrometry Imaging**

Sierra N. Hunter¹, Mary F. Wang¹, David C. Muddiman¹ *North Carolina State University*

(Tue-P19) **Development of a protocol for the elemental analysis of tire marks in road crime forensics**

John G. Lucchi¹, Micaela Hernandez¹, Matthieu Baudelet¹ *University of Central Florida*

(Tue-P20) **Supervised Machine Learning Approaches to System Suitability Testing for Mass Spectrometry Imaging**

Russell R. Kibbe¹, Alexandria L. Sohn¹, David C. Muddiman¹ *North Carolina State University*

(Tue-P21) **Broadband Tandem Mass Spectrometry Through the Use of 2D Correlation and Direct Analysis in Real Time Ionization**

Garon H. Lowke¹, Elly Breves¹, Jacob T. Shelley¹
¹*Rensselaer Polytechnic Institute*

(Tue-P22) **Topographic Mass Spectrometry Imaging of Brassica oleracea Leaves by Infrared Matrix-Assisted Laser Desorption Ionization with Automatic z-Axis Correction**

Quinn Mills¹, Sarah Ashbacher¹, Alexandria L. Sohn¹, David C. Muddiman¹ *North Carolina State University*

(Tue-P23) **Extending a Bayesian Method for Inferring Constituent Information using MS/MS Data**

Taichi Tomono¹, Satoshi Hara², Junko Iida³, Takashi Washio⁴ *AI Solution Unit,*

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Technology Research Laboratory, Shimadzu Corporation, ²Graduate School of Informatics and Engineering, The University of Electro-Communication, ³Life Science Business Department, Analytical & Measuring Instruments Division, Shimadzu Corporation, ⁴Faculty of Business and Commerce, Kansai University

(Tue-P24) Vibrational Spectroscopy and Mass Spectrometry Studies using ¹³C-labeled N-Heterocyclic Carbene-functionalized Nanoparticles

Shayanta Chowdhury¹, Gaohe Hu², Isabel Jensen³, Alyssa Santos⁴, David Jenkins³, Lasse Jensen⁵, Jon Camden¹ ¹University of Notre Dame, ²The Pennsylvania State University, ³The University of Tennessee, Knoxville, ⁴St. Bonaventure University, ⁵Pennsylvania State University

(Tue-P25) Enhancing Robustness of Cl Elemental Detection in Post-ICP Chemical Ionization Orbitrap-MS

Zahra Afsharsaveh¹, Kaveh Jorabchi¹
¹Georgetown University

(Tue-P26) Detection of bromide and iodide anions with the liquid sampling – atmospheric pressure glow discharge / Orbitrap coupling

Dehlia Lang¹, Joesph V. Goodwin¹, Cameron J. Stouffer¹, R. Kenneth Marcus¹ ¹Clemson University

(Tue-P27) Metal-Organic Frameworks Analysis via Laser-Assisted Micro-pyrolysis Coupled with Flowing Atmospheric-Pressure Afterglow High-Resolution Mass Spectrometry

Bibek R. Bhattarai¹, Ejoke Akatugba², Daniela Barroso¹, Songyue Shi³, Gerardo Gamez⁴
¹Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409-1061, US, ²Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas 79409-1061 US, ³Proteomics Core Facility, UT Southwestern Medical Center, Dallas, Texas 75390, US, ⁴Texas Tech University

(Tue-P28) Characterization of organic carbon molecular networks in Martian meteorites using mass spectrometry and 2D-correlation techniques

Elly Breves¹, Garon H. Lowke¹, Andrew Steele², Robert B. Cody³, Caroline Freissinet⁴, Jacob T. Shelley¹ ¹Rensselaer Polytechnic Institute, ²Carnegie Institution for Science, ³JEOL USA, Inc., ⁴LATMOS/IPSL, UVSQ University Paris-Saclay, Sorbonne University, CNRS

(Tue-P29) Use Your Time (Domain) Wisely: Streamlined Analysis of Complex Mixtures with Pulsed-Laser Techniques

Josefin Hufgard¹, Yi You¹, Jens Riedel¹ ¹Federal Institute for Materials Research and Testing (BAM)

(Tue-P30) Make PFAS Detectable Again: An Exploration of Ionization-Source-Induced Modification of Perfluoroalkyl Substances (PFAS) to Improve Detectability

Marisa Moss¹, Jacob T. Shelley¹ ¹Rensselaer Polytechnic Institute

(Tue-P31) Development of an Optical Particle Trap for Atomic and Molecular Characterization of Extraterrestrial Particles via Raman, LIBS, and Mass Spectrometry

Carlos Eduardo Nogales Herrera¹, Jacob T. Shelley¹, George Chan² ¹Rensselaer Polytechnic Institute, ²Lawrence Berkeley National Laboratory

(Tue-P32) Recirculated Microdroplets Increase RNA Oligomer Length Measured by MALDI-TOF MS

Samantha E. Pryor¹, Vincent S. Riggi¹, Karyn L. Rogers¹, Morgan F. Schaller¹, Jacob T. Shelley¹ ¹Rensselaer Polytechnic Institute

(Tue-P33) Comparison of cleaning techniques for the elemental analysis of bones

Magdalena E. Jackson¹, John Lucchi¹, Kristen Livingston¹, Matthieu Baudalet ¹University of Central Florida

(Tue-P34) Students Exploring Raman Spectroscopy: Developing Outreach Efforts and Training Young Scientists via Surface-Enhanced Raman Spectroscopy (SERS)

Julia Danischewski¹, Jared Viggers¹, Abdulsobur Fagbenro², Jacob T. Shelley¹ ¹Rensselaer Polytechnic Institute, ²Albany High School

(Tue-P35) Development of a Microwave-Enhanced Glow Discharge Atomic Emission Spectrophotometer

Steven Ray¹, Mitchell Stry¹, Gerardo Gamez²
¹SUNY Buffalo Dept of Chemistry, ²Texas Tech University

(Tue-P36) Glow Discharge Coded Aperture Optical Emission Spectroscopy (GOCAS)

Rajendra Joshi¹, Harshhit Agrawaal¹, Gerardo Gamez¹ ¹Texas Tech University

(Tue-P37) Optimization of Solution-Cathode Glow Discharge for Improved Molecular and Atomic Emission

Nadia Radomski¹, Michael R. Webb¹ ¹University of North Carolina Wilmington

(Tue-P38) Glow Discharge Optical Emission Coded Aperture Elemental Mapping (GOCAM) For Single-Shot Characterization of Nanoscale Materials

Rajendra Joshi¹, Harshhit Agrawaal¹, Gerardo Gamez¹ ¹Texas Tech University

(Tue-P39) Peri-Pump Analysis: An Automated Calibration Method for Induced Coupled Plasma Optical Emission Spectroscopy

Austin F. Read¹, Willis B. Jones², Bradley T. Jones¹ ¹Wake Forest University, ²University of North Florida

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(Tue-P40) Atomic Isotope Analysis of Lithium with Spatial Heterodyne Spectrometry and Lineshape Recovery through Deconvolution

Xunyu Li¹, Jens Riedel¹, Yi You¹ ¹*Federal Institute for Materials Research and Testing (BAM)*

(Tue-P41) Laser-Induced Plasma Diagnostics to Elucidate the Effects of Applied Microwave Interactions

Ezekiel Branch¹, Aryanna Monroe¹, Buddhika T. Kumara², Steven Ray³, Gerardo Gamez¹ ¹*Texas Tech University*, ²*The State University of New York at Buffalo*, ³*SUNY Buffalo Dept of Chemistry*

(Tue-P42) Exploration of the VNIR Region for Detection of Sulfur in Planetary Applications

Kelsey L. Williams¹, Carey Legett¹, Ronald K. Martinez¹, Samuel M. Clegg¹ ¹*Los Alamos National Laboratory*

(Tue-P43) Elemental Analysis in Yeast Cells and Microplastics by ICP-MS with Automated Micro-Flow Sample Introduction

Yan Cheung¹, Emmett Soffey¹ ¹*Agilent Technologies*

(Tue-P45) Multi-Channel Dilution Analysis

Taylor Dessoff¹, Willis B. Jones¹, Bradley T. Jones², Robbie Huff¹, Adam Richardson¹, Sophie Lewis¹, Abigail J. Crossman¹, Alexandria Eddy¹ ¹*University of North Florida*, ²*Wake Forest University*

(Tue-P46) Modeling Momentum Change from Laser Ablation for Space Debris Removal

Jaden E. Dougal¹, Prasoon K. Diwakar² ¹*South Dakota Mines*, ²*South Dakota School of Mines and Technology*

(Tue-P47) Correction of Carbon-Based Matrix Effects in Mip-Oes

Beatriz M. Fontoura¹, Bradley T. Jones¹, George L. Donati¹, Joaquim A. Nóbrega² ¹*Wake Forest University*, ²*Federal University of Sao Carlos*

(Tue-P48) Materials Testing in Lithium-Ion Battery Production: A Simplified Dilute-and-Shoot Approach for Trace Elemental Impurities in Electrolytes by ICP-OES

Ana Sarahi Garcia Gonzalez¹, Christopher Conklin¹ ¹*Agilent Technologies*

(Tue-P49) Elemental analysis of complex matrix samples by means microwave-sustained inductively coupled atmospheric-pressure plasma optical emission spectrometry

Guillermo Grindlay¹, Jorge Pérez¹, Paula Gras¹, Raquel Serrano¹, Luis Gras¹, Juan Mora¹ ¹*University of Alicante*

(Tue-P50) SPIDER Probe: An Integrated Sensor for Real-Time Molten Salt Monitoring

Kayla Hahn¹, Davis Bryars², Munmun Jahan³, Alina Jugan², Ammon Williams⁴, Alex W. Bataller³ ¹*Graduate Student at NC State University*, ²*NC State*, ³*North Carolina State University*, ⁴*Idaho National Lab*

(Tue-P51) Analysis of Infant Formula Using Calibration by Proxy

Beatriz M. Fontoura¹, Willis B. Jones², Bradley T. Jones¹, Hanieh Helli¹ ¹*Wake Forest University*, ²*University of North Florida*

(Tue-P52) Multi-Channel Dilution Analysis Using a Single Pump Channel

Robbie M. Huff¹, Willis B. Jones¹, Bradley T. Jones² ¹*University of North Florida*, ²*Wake Forest University*

(Tue-P53) A Novel Hand-Held Sensor for Elemental and Isotopic Quantification Using Atmospheric Plasma Glow Discharge

Munmun Jahan¹, Alex W. Bataller¹ ¹*North Carolina State University*

(Tue-P54) Standards in the Rinse

Nicholas B. Judd¹, Willis B. Jones², Bradley T. Jones¹ ¹*Wake Forest University*, ²*University of North Florida*

(Tue-P55) Post-column hydride generation followed by in-situ preconcentration in a dielectric barrier discharge: a simple approach to arsenic speciation analysis by atomic absorption spectrometry

Jan Kratzer¹, Matěj Plecháč¹, Gilberto Coelho¹, Milan Svoboda¹, Stanislav Musil¹, Tomáš Matoušek¹ ¹*Czech Academy of Sciences, Institute of Analytical Chemistry*

(Tue-P56) Determination of Antimony and Bismuth in Tea Leaves by Slurry Sampling Hydride Generation Atomic Absorption Spectrometry

Jerzy Mierzwa¹ ¹*Tennessee State University, Agriculture*

(Tue-P57) Tips for Creating Stable & Accurate Elemental Standards at Working Concentrations

Mike Booth¹ ¹*Inorganic Ventures*

(Tue-P58) A rapid speciation method for determining methylmercury and inorganic mercury in whole blood by isocratic Liquid Chromatography coupled to Vapor Generation Inductively Coupled Plasma Tandem Mass Spectrometry

Emily Pacer¹, Christopher Palmer², Patrick J. Parsons² ¹*University at Albany*, ²*New York State Department of Health / University at Albany*

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(Tue-P59) **Analysis of Organometallic Compounds and Metallic Particles in Specialty Gases by Direct Injection Using Gas Exchange Device (GED) Coupled to Inductively Coupled Plasma-Mass Spectrometry (ICP-MS)**

Chady Stephan¹, Aaron Hineman¹ ¹*PerkinElmer US LLC*

(Tue-P60) **Leveraging ICP-MS/MS technology: A generational step in human placenta analyses**

Joseph R. Teson¹, Pamela C. Kruger², Patrick J. Parsons² ¹*University at Albany*, ²*New York State Department of Health / University at Albany*

(Tue-P61) **Ozone reaction providing multiple ionic species for quantitation of aluminum by tandem quadrupole inductively coupled plasma mass spectrometry**

Yanbei Zhu¹, Daiki Asakawa¹ ¹*National Institute of Advanced Industrial Science and Technology*

(Tue-P62) **Strategies for Improving the Detection Limits of Selenium Nanoparticles via Single Particle ICP-MS Analysis**

Aaron Hineman¹, Ruth Merrifield¹, Chady Stephan¹, Liyan Xing¹ ¹*PerkinElmer US LLC*

(Tue-P63) **Lithium Mining Processing - Elemental Characterization of Lithium Brines Using an Agilent ICP-OES**

Ana Sarahi Garcia Gonzalez¹, Christopher Conklin¹ ¹*Agilent Technologies*

(Tue-P64) **GLOW DISCHARGE SPECTROSCOPY ATOMIC & MOLECULAR NANOSCALE LAYER ANALYZERS – OES, MS-TOF, QMS & MAGNETIC SECTOR.**

Ben Johns¹ ¹*Spectrometer Experts USA*

(Tue-P65) **HIGH-RESOLUTION NANOSCALE PROBING OF ANTI-PSEUDOMONAL BACTERIOPHAGES UNDER ENVIRONMENTAL STRESS**

Yue Cao¹, Dipesh Khanal², Hak-Kim Chan³, Mark M. Banaszak Holl⁴, Sandra Morales⁵ ¹*University of Sydney*, ²*The University of Sydney*, ³*Advanced Drug Delivery Group, Sydney Pharmacy School, Faculty of Medicine and Health, The University of Sydney, NSW, Australia*, ⁴*Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA* ⁵*Division of Pulmonology, Allergy, and Critical Care Medicine, Heersink School of Medicine, University of Alabama at Birmingham, Birmingham, USA*, ⁶*Phage Consulting*

(Tue-P66) **IR-TAMS: A New Automated Goniometer for Variable Angle Spectroscopy in Infra-red Range**

Dr. Aniket¹ ¹*PerkinElmer*

(Tue-P67) **Study of electronic structure of adamantane in condensed phase by far-ultraviolet spectroscopy**

Tomoyuki Komoto¹, Yusuke Morisawa² ¹*Kinki graduate school*, ²*Kindai University*

(Tue-P68) **Experimental and Theoretical Investigation of Functional PAH Precursors for Potential Nanoporous Graphene Growth**

Ahmed Hewail¹, Dale L. Perry², Djamilia Hourlier¹, David Guerin¹, Christophe Krzeminski¹, Thierry Melin¹, Eric Faulques¹, Nataliya Kalashnyk¹ ¹*Univ. Lille, CNRS, Centrale Lille, Univ. Polytechnique Hauts-de-France, UMR 8520 -IEMN – Institut d'Electronique, de Microélectronique et de Nanotechnologie, F-59000 Lille, France*, ²*Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720 USA*

(Tue-P69) **In-Situ Screening of Soybean Cultivars for Critical Quality Attributes**

Cameron C. Rich¹, Luis Rodriguez-Saona¹ ¹*The Ohio State University*

(Tue-P70) **Unravelling dynamics of water-soluble carbohydrates in wheat stem by NIR Spectroscopy under different irrigation regimes**

Deepti Sharma¹, Sonia Sheoran², Sulekha Chahal¹ ¹*Department of Biotechnology, Kurukshetra University, Kurukshetra, Haryana, India*, ²*ICAR-Indian Institute of Wheat & Barley Research, Karnal, Haryana*

(Tue-P72) **RaFLIM: A Multimodal Platform Combining Raman and Fluorescence Lifetime Imaging Microscopy**

Angela Flack¹, Samantha Redes¹ ¹*Edinburgh Instruments*

(Tue-P73) **Analysis of different anodes materials for batteries using Raman spectroscopy**

Carlos Morillo¹ ¹*JASCO Inc*

(Tue-P75) **Comparative Analysis of Recalled Metformin Using SIFT-MS and Liquid Chromatography**

Tucker Kitchengs, Leslie Silva¹, Vaughan Langford², Colin Hastie³, Mark Perkins³ ¹*Syft Technologies Inc.*, ²*Syft Technologies Ltd*, ³*Element Materials Technology*

(Tue-P76) **Using high-resolution mass spectrometry to identify potential targets of the drug metformin**

Dalton Hilovsky¹, Wei-chen Chang¹, Xiaojing Liu¹ ¹*North Carolina State University*

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Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

24AES04: Electrokinetic Fundamentals | 306C

Chair: Victor Ugaz, Texas A&M University
Co-Chair: Alaleh Vaghef-Koodehi, Rochester Institute of Technology

10:30 AM (AES-04.1) Nonlinear Electrophoresis Effects in Microfluidic Devices

Blanca H. Lapizco-Encinas¹ *Rochester Institute of Technology*

10:50 AM (AES-04.2) Neural network enabled multiparametric impedance signal templating for high throughput single-cell deformability cytometry

Javad Jarmoshti¹, Abdullah-Bin Siddique¹, Federica Caselli², Nathan S. Swami¹ *University of Virginia*, ²*Tor Vergata University of Rome*

11:10 AM (AES-04.3) Electro-antibacterial Therapy (EAT) to enhance intracellular bacteria clearance in pancreatic cancer cells

Josie L. Duncan¹, Raffae Ahmad², Hunter Danesi², Daniel Slade², Rafael V. Davalos¹, Scott Verbridge² *Georgia Tech*, ²*Virginia Tech*

11:30 AM (AES-04.4) Microfluidic analytical systems for assaying dynamic cellular secretions

Michael Roper¹, Joshua Davis¹, James Thornham¹, Viviana James¹, Nicholas Pazos¹, Farhad Zahedi¹ *Florida State University*

11:50 AM (AES-04.5) Electrokinetic Fundamentals in the Characterization and Manipulation of Biologically Relevant Systems

Tayloria N.G. Adams¹, Tunglin Tsai², Kiara Lacy², Sujeung Lim², Emil Lundqvist², Herdeline Ardoña², Lexi L. Crowell-Simpkins¹, Luis Henriquez¹, Mary Tran¹, Prema Vyas², Destiney Ward², Yufan Qin², Angie Castro² *University of California, Irvine*, ²*University of California Irvine*

24ATOM04: Laser Based Applications I | 305A

Co-Chair: Jhanis Gonzalez, Applied Spectra Inc

10:30 AM (ATOM-04.1) Fully self-calibrated compact Laser Induced Breakdown Spectroscopy for the volcano monitoring and space exploration

Alessandro De Giacomo¹, Aya Taleb¹, Marcella Dell'Aglio², Rosalba Gudiuso¹ *University of Bari*, ²*IFN-CNR*

10:50 AM (ATOM-04.2) From LIXS to HELDI: New Laser Methods to Crack the Low-Periodic-Table Code

Davide Bleiner¹ *Empa*

11:10 AM (ATOM-04.3) NASA CLPS mission: In situ chemical analysis of lunar regolith using LIMS

Andreas Riedo¹, Peter Keresztes Schmidt¹, Peter Wurz¹, UBE CLPS-LIMS Team¹ *University of Bern*

11:30 AM (ATOM-04.4) Single particle excitation and atmospheric debris clearing mechanisms of femtosecond laser filaments

Kyle S. Latty¹, Kyle C. Hartig¹ *University of Florida*

11:50 AM (ATOM-04.5) Advancing Nuclear Safeguards with Field-Deployable Laser Induced Breakdown Spectroscopy

George Chan¹ *Lawrence Berkeley National Laboratory*

24AWD08: FACSS Charles Mann Award | 301B

Chair: Jürgen Popp, Leibniz Institute of Photonic Technology
Co-Chair: Nicholas Stone, University of Exeter

10:30 AM (AWD-08.1) Spatially offset high wavenumber Raman spectroscopy for physiological hydration assessment in vivo

Anita Mahadevan-Jansen¹ *Vanderbilt University*

10:50 AM (AWD-08.2) Scaling metabolomics down to the single cell level with O-PTIR spectroscopy

Roy Goodacre¹, Cassio Lima¹, Howbeer Muhamadali¹ *University of Liverpool*

11:30 AM (AWD-08.4) Applications of Raman microscopy in breast cancer surgery: towards intra-operative assessment of surgical margins and sentinel lymph nodes

Ioan Notingher¹ *University of Nottingham*

11:50 AM (AWD-08.5) Full fingerprint hyperspectral imaging of prostate cancer tissues within clinical timeframes using Quantum Cascade Laser systems

Peter Gardner¹, Douglas Ferguson², Niels Kroeger-Lui³, Domenic Dreisbach⁴, Ashwin Sachdeva¹ *University of Manchester*, ²*University of Exeter Medical School*, ³*Bruker Scientific*, ⁴*Bruker Optics GmbH & Co. KG*

24BIM03: Optical Technologies and Companion Diagnostics in Healthcare Management | 302A

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

10:30 AM (BIM-03.1) Spatially Offset Raman Spectroscopy (SORS): Chemical Analysis through Sealed Containers as Rapid Detection of Falsified Medical Products

Sara Mosca¹, Qianqui Lin², Robert Stokes³, Tehmina Bharucha⁴, Bevin Gangadharan⁴, Rebecca Clarke⁵, Laura Gomez Fernandez⁴, Micheal deats⁶, John Walsby-Tickle⁵, Benediktus Yohan Arman⁴, Shrikrishna R. Chunekar⁷, Kundan D. Patil⁷, Sunil Gairola⁷, Kerlijn Van Assche⁶, Susanna Dunachie⁸, Hamid A. Merchant⁹, Rutendo Kuwana¹⁰, Alexandrine Maes¹⁰, James McCullagh⁵, Celine Caillet⁶, Nicole Zitzmann⁴, Paul N. Newton⁶, Pavel Matousek¹ *STFC - UKRI*, ²*University of Twente*, ³*agilent*, ⁴*Department of Biochemistry, University of Oxford*, ⁵*Department of Chemistry, University of Oxford*, ⁶*Nuffield Department of Medicine*,
Next year: October 5-10, 2025 • Northern Kentucky Convention Center

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Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

University of Oxford, ⁷Serum Institute of India, ⁸NHS Foundation trust, ⁹Department of Pharmacy, University of Huddersfield, ¹⁰Regulation and Safety Unit, World Health Organization (WHO)

10:50 AM (BIM-03.2) **Profiling Serum Bile-Acids with a Synthetic Receptor Array for the Diagnosis of Alcoholic Hepatitis**

Liam T. Wilson¹, Luke Tyson², Mark Thursz², William Rosenberg³, William Peveler⁴ ¹University of Glasgow, ²Faculty of Medicine, Imperial College London, ³University College London, ⁴Department of Chemistry, University of Glasgow

11:10 AM (BIM-03.3) **Core-Satellite Assembly Facilitated Enzyme-Free, Isothermal Amplification Sensing**

Samuel Mabbott¹ ¹Texas A&M University

11:30 AM (BIM-03.4) **In vivo Raman Spectroscopy Detects Cervical Biochemical Changes with Establishment of Pregnancy**

Christine M. O'Brien¹, Emily Spurlin¹, Katy Belcher¹, Jennifer Esteves¹, Patricia Jimenez¹ ¹Washington University in St. Louis

11:50 AM (BIM-03.5) **Intravital Microscopy for Mechanistic Study of Synergistic Immuno Photothermal Nanotherapy (SYMPHONY) for Cancer Treatment**

Yang Liu¹, Khang Hoang¹, Ericka Chorniak¹, Wiguins Etienne¹, Paolo Maccarini¹, Gregory Palmer¹, Brant Inman¹, Tuan Vo-Dinh¹ ¹Duke University

Christopher D. Brown¹ ¹908 Devices

24FORENS02: Food Forensics | 303

Chair: Luis Rodriguez-Saona

10:30 AM (FORENS-02.1) **Understanding Novel NIR Instrumentation Technology for Portable Applications**

John Gilmore¹ ¹Hamamatsu Corporation

10:50 AM (FORENS-02.2) **Engineering advancement of handheld near infrared sensors: opportunities and challenges**

Christopher D. Ball¹, Luis Rodriguez-Saona² ¹The Ohio State University / ElectroScience Laboratory, ²The Ohio State University

11:10 AM (FORENS-02.3) **OPPORTUNITIES OF HANDHELD RAMAN TECHNOLOGY FOR QUALITY CONTROL AND SAFETY APPLICATIONS IN THE FOOD INDUSTRY**

Luis Rodriguez-Saona¹ ¹The Ohio State University

11:30 AM (FORENS-02.4) **Precision Analysis of Bacterial Biomarkers Using Surface-Enhanced Raman Spectroscopy and Machine Learning**

AMIT KUMAR¹, Redwan Islam¹, Susu M. Zughair², Xianyan Chen³, Yiping Zhao¹ ¹The University of Georgia, ²College of Medicine, Qatar University, ³University Of Georgia

11:50 AM (FORENS-02.5) **Raman spectroscopy in food forensics**

Alexander Rzhveskii

24CHEM03: Chemical Data Science in the 21st Century: Where We Might Be Going | 305B

Chair: Karl Booksh, University of Delaware

10:30 AM (CHEM-03.1) **The Future of Molecular-Scale Measurements Enabled by Chemical Data Science – an NSF-funded workshop report**

Sharon L. Neal¹, Barry K. Lavine², Karl S. Booksh¹ ¹University of Delaware, ²Oklahoma State University

10:50 AM (CHEM-03.2) **Propagating Correlated Errors to Determine Confidence Intervals for Class Boundaries in Multivariate Classification**

Karl S. Booksh¹, Helder V. Carneiro¹, Caelin Celani¹ ¹University of Delaware

11:10 AM (CHEM-03.3) **Self-Modeling Curve Resolution Analysis of Raman Spectra from Mixed Deuterated and Protiated Phospholipid Membranes Reveals Isotopically-Segregated Lipid Domains**

Jay P. Kitt¹ ¹University of Utah - Chemistry

11:30 AM (CHEM-03.4) **Convolutional Neural Networks to Enhance Investigative Lead Information from Automotive Clear Coats**

Barry K. Lavine¹, Collin G. White¹, Douglas G. Heisterkamp¹ ¹Oklahoma State University

11:50 AM (CHEM-03.5) **Operation Extrapolation: Improving the Inductive Capacity of Chemometric / Data Science Tools for Complex Analytical Spaces**

24IR04: Materials Science Applications of Optical Photothermal IR Spectroscopy | 301A

Chair: Minghe Li, Boehringer Ingelheim

Co-Chair: Curtis Marcott, Light Light Solutions

10:30 AM (IR-04.1) **Advancing Microplastic Analysis through Machine Learning Techniques**

Junli Xu¹ ¹University College Dublin

10:50 AM (IR-04.2) **Widefield infrared photothermal imaging and spectroscopy**

Masaru Kuno¹ ¹University of Notre Dame

11:10 AM (IR-04.3) **Assessment of Fluticasone Propionate/Salmeterol Xinafoate/Lactose Particle Sizes and Co-Associations in Pharmaceutical Dry Powder Inhalation Products: A Photothermal Nanospectroscopic Study.**

Dipesh Khanal¹, Sheikh Tanzina Haque², Blessy Joseph², Elizabeth R. Bielski³, Bryan Newman³, Huzeyfe Yilmaz⁴, Snober Ahmed⁵, Susan Boc³, Hak-Kim Chan⁶, Mark M. Banaszak Holl⁷ ¹The University of Sydney, ²Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA, ³Division of Therapeutic Performance I, Office of Research and Standards, Office of Generic

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

Drugs, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD, USA, ⁴US Food & Drug Administration, ⁵Division of Pharmaceutical Quality Research II, Office of Pharmaceutical Quality Research, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO, USA, ⁶Advanced Drug Delivery Group, Sydney Pharmacy School, Faculty of Medicine and Health, The University of Sydney, NSW, Australia, ⁷Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA

11:30 AM (IR-04.4) **Widefield fluorescence detected photothermal infrared microscopy: high speed chemical analysis and dynamic imaging of biological materials**

Craig Prater¹, Eoghan Dillon¹, Mustafa Kansiz², Oxana Klementieva³, Rinuk E. Limurn⁴, Kathleen M. Gough⁴ ¹Photothermal Spectroscopy Corp., ²Photothermal Spectroscopy Corp., ³Lund University, ⁴University of Manitoba

11:50 AM (IR-04.5) **Advances in Biopharmaceutical Particulates/Sub-visible Analysis through Submicron IR (O-PTIR) Micro-spectroscopy**

Mustafa Kansiz¹, Miriam Unger², Craig Prater³, Kevin Dahl⁴ ¹Photothermal Spectroscopy Corp., ²Photothermal Spectroscopy Corp., GmbH, ³Photothermal Spectroscopy Corp., ⁴Particelse

24MASS06: **Breaking Boundaries in Mass Spectrometry: To Infinity and Beyond** | 306A

Chair: Jacob Shelley, Rensselaer Polytechnic Institute

10:30 AM (MASS-06.1) **The Long Neglected Cycloidal Mass Analyzer**

Jason J. Amsden¹, Rafael Bento Serpa¹, Elettra Piacentino¹, Kathleen Horvath¹, Raul Vyas¹, Tanouir Aloui¹, Charles B. Parker¹, James B. Carlson², Chris Zarzana³, Elizabeth LaBone⁴, Jonathon Andrus³, Nathan Stevens³, Rose Greer⁴, Kyle Samperton⁴, Danielle Mannion⁴, Justin Keogh⁵, Roger Sperline⁵, M. Luisa Sartorelli⁶, Brian R. Stoner¹, Gehm E. Michael¹, Glass T. Jeffrey¹, M. Bonner Denton⁵ ¹Duke University, ²RTI International, ³Idaho National Laboratory, ⁴Savannah River National Laboratory, ⁵University of Arizona, ⁶Universidade Federal de Santa Catarina

10:50 AM (MASS-06.2) **Analytical Characterization Approaches to Measure Prebiotic Synthesis Products in Very Salty Environments**

Maria Jesus Herrero Perez¹, Jacob T. Shelley¹, Karyn L. Rogers¹ ¹Rensselaer Polytechnic Institute

11:10 AM (MASS-06.3) **Versatility of a planetary science instrument prototype with a dual source linear ion trap integrated to an Orbitrap analyzer**

Adrian E. Southard¹, Lucas Andrews², Ryan Danell³, Friso Van Amerom⁴, Ricardo D. Arevalo², Steven Rogacki⁵, Emanuel Hernandez⁶, Diego Garcia Y Rosales⁷ ¹CRESST-II/University of Maryland, College Park and NASA GSFC, ²University of Maryland, College Park, ³Danell Consulting, Inc., ⁴Mini-Mass consulting, Inc., ⁵Space Research Physics Lab, ⁶NASA Goddard Space Flight Center, ⁷AMU Engineering Inc.

11:30 AM (MASS-06.4) **Expanding Our AIMs: Building on Acoustic Ion Manipulation (AIM) Capabilities through Changes to the Standing Acoustic Wave**

Julia Danischewski¹, Lauren Bauer¹, Yi You², Jens Riedel², Jacob T. Shelley¹ ¹Rensselaer Polytechnic Institute, ²Federal Institute for Materials Research and Testing (BAM)

11:50 AM (MASS-06.5) **Fluorine Detection by a High-Power Nitrogen Microwave Plasma (MICAP) Coupled to Chemical Ionization Mass Spectrometry**

Jordan L. Tanen¹, Kaveh Jorabchi¹ ¹Georgetown University

24PMA04: **Solving Industrial Problems with Vibrational Spectroscopy** | 306B

Chair: Patrick Wray, Bristol Myers Squibb

Co-Chair: James Kimber, Pfizer

10:30 AM (PMA-04.1) **Spectroscopic Mapping of 3D Printed Microfluidic Devices for High-Throughput Pharmaceutical Formulation Development**

Zoë Whalley¹, Patrick Wray², Tom Mills³, Richard Greenwood³ ¹University of Birmingham, Bristol Myers Squibb, ²Bristol Myers Squibb, ³University of Birmingham

10:50 AM (PMA-04.2) **Development of in-situ variable-temperature low- and mid-frequency Raman spectroscopy to elucidate closely related polymorphs**

Jaypee Quino¹ ¹Pfizer Inc.

11:10 AM (PMA-04.3) **Optimum Solution for a Calibration-Free Method: Understanding the Role of Numerical Solver Parameters on IOT Prediction of Active Ingredients in Pharmaceutical Powder Blends**

Md. Nahid Hasan¹, Zhenqi (Pete) Shi², Chen Mao², James K. Drennen¹, Carl A. Anderson¹ ¹Duquesne University, ²Genentech, Inc.

11:30 AM (PMA-04.4) **Developing spectroscopic calibrations in a bench simulator that transfer to manufacturing equipment**

Stephen V. Hammond¹ ¹Expo Process Analytics

11:50 AM (PMA-04.5) **Comparison of Calibration Burden for Partial Least Squares and Iterative Optimization Technology in Process Analytical**

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

Technology Applications

Adam J. Rish¹, Owen Rehrauer¹, Sebastian Sowinski², Uwe Kirschner² ¹*Sentronic US Corp*, ²*Sentronic GmbH*

¹*Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry*, ²*Joint Research Centre (JRC), European Commission (EC), Geel, Belgium*, ³*Joint Research Centre (JRC), European Commission (EC), Ispra, Italy*

24RAM04: SERS 4 | 302B

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

10:30 AM (RAM-04.1) Exploring the solid/solution interface of plasmonic colloidal nanoparticles for the direct SERS detection of biological analytes

Chiara Deriu¹, Laura Fabris¹ ¹*Politecnico di Torino*

10:50 AM (RAM-04.2) Surface-enhanced Raman Studies of Bacteria: In-situ Studies of Biofilms and Volatile Metabolites

Steven Bell¹, Wafaa Aljuhani¹, Qinglu Chen¹ ¹*Queen's University Belfast*

11:10 AM (RAM-04.3) Digital SERS-LFT Dipstick: Ultra-sensitive, Rapid Virus Quantification in Environmental Dust

Peter Vikesland¹, Wei Wang¹, Sonali Srivastava¹, Aditya Garg², Chuan Xiao¹, Seth Hawks¹, Jin Pan¹, Nisha Duggal¹, Gabriel Isaacman-VanWertz¹, Wei Zhou¹, Linsey Marr¹ ¹*Virginia Tech*, ²*Massachusetts Institute of Technology*

11:30 AM (RAM-04.4) Plasmon-induced Nanocavitation-enabled Nanogap Hotspot Regeneration for Long-term Wearable SERS Bioimaging in Protein-rich Biofluids

Aditya Garg¹, Meitong Nie², Peter Vikesland², Erin Gloag², Wei Zhou² ¹*Massachusetts Institute of Technology*, ²*Virginia Tech*

11:50 AM (RAM-04.5) SERS-sensing hydrogels for in-situ analysis in agricultural settings

Manisha Sheokand¹, Lyndsay N. Kissell¹, Pietro Strobbia¹, Niloufar Yavari¹ ¹*University of Cincinnati*

24RAM13: Applications of micro Raman Spectroscopy 302C

Chair: To Be Announced

10:50 AM (RAM-13.2) Evaluating Multilayer Polymers with Raman Spectroscopy: A comparison of depth profiling and cross-sectional analysis

Michelle N. Sestak¹, Fran Adar² ¹*HORIBA Instruments Incorporated*, ²*Horiba Scientific*

11:10 AM (RAM-13.3) Automated μ -Raman-based analysis of a candidate microplastics' reference material

Natalia P. Ivleva¹, Oliver Jacob¹, John Seghers², Rita La Spina², Gabriella Schirinzi³, Konstantinos Chatzipanagis², Andrea Held², Håkan Emteborg², Martin Elsner¹, Elżbieta Anna Stefaniak²

11:30 AM (RAM-13.4) Applicability of Stable Isotope Raman Microspectroscopy for Analysis of Microbial Degradation of Microplastics

Natalia P. Ivleva¹, Kara Müller¹, Martin Elsner¹ ¹*Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry*

11:50 AM (RAM-13.5) Low temperature Raman microscopy for high-sensitivity molecular imaging of rapidly frozen cells

Kenta Mizushima¹, Yasuaki Kumamoto², Shoko Tamura³, Masahito Yamanaka², Kentaro Mochizuki⁴, Menglu Li², Syusuke Egoshi⁵, Kosuke Dodo⁶, Yoshinori Harada⁴, Nicholas I. Smith⁷, Mikiko Sodeoka⁷, Hideo Tanaka⁸, Katsumasa Fujita¹ ¹*Department of Applied Physics, Osaka University*, ²*Osaka University*, ³*Tokyo Metropolitan Institute of Medical Science*, ⁴*Kyoto Prefectural University of Medicine*, ⁵*Synthetic Organic Chemistry Laboratory, Riken Cluster for Pioneering Research*, ⁶*Synthetic Organic Chemistry Laboratory, Cluster for Pioneering Research, RIKEN*, ⁷*Biophotonics Laboratory, Immunology Frontier Research Center, Osaka University*, ⁸*Kyoto University of Advanced Science, Kyoto Prefectural University of Medicine*

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

24AES05: Innovations in Device Fabrication & Applications 306C

Chair: Chris Easley

Co-Chair: Major Selemani, Saint Louis University

1:30 PM (AES-05.1) Adventures in 3D Printing Devices that Integrate Cell Culture with Analysis

Scott Martin¹ ¹*Saint Louis University*

1:50 PM (AES-05.2) Biased-Alternating Current Electrophoresis Method to Generate Biomolecules Gradient-based High-throughput Screening Platform

Qingrong He¹, Ran An¹, T. Randall Lee¹

¹*University of Houston*

2:10 PM (AES-05.3) Microfluidic paper-based analytical devices: Do-it-yourself approaches

Wendell Coltro¹, Lucas Sousa¹, Habdías Silva-Neto¹, Leyllanne Souza¹, Danielly Rocha¹

¹*Federal University of Goiás*

2:30 PM (AES-05.4) Quantifying the Force on Freely Diffusing Proteins in an Electric Field Gradient

Mark A. Hayes¹, Jerry Sheu¹, A K M Fazlul Karim Rasel¹ ¹*Arizona State University*

2:50 PM (AES-05.5) Microengineered Platforms for Neurochemical Monitoring Along the Gut-Brain Axis

Ashley Ross¹ ¹*University of Cincinnati*

24ATOM05: Laser Based Applications II | 305A

Co-Chair: Jorge Pisonero, University of Oviedo

Co-Chair: Ana Lores Padin, Ghent University

1:30 PM (ATOM-05.1) Detection of Li isotopes at remote distances

Vassilia Zorba¹, Sung-Uk Choi², Jose Chirinos², Changmin Kim², Xianglei Mao² ¹*UC Berkeley & Lawrence Berkeley National Lab*, ²*Lawrence Berkeley National Lab*

1:50 PM (ATOM-05.2) LA-ICP-MS and LIBS as a tool in epidemiology studies and their impact to understand environmental chemical exposure in human health.

Mauro Martinez¹, Manish Arora¹ ¹*Icahn School of Medicine at Mount Sinai*

2:10 PM (ATOM-05.3) Challenges and opportunities for laser-based approaches to Rb-Sr geochronology

Alicia Cruz-Uribe¹, Cemil Arkula¹, Joshua Garber², Teng Ee Yap³, Francois LH Tissot³ ¹*University of Maine*, ²*The Pennsylvania State University*, ³*California Institute of Technology*

2:30 PM (ATOM-05.4) Multielement analysis using short transient signals in spatially resolved LA-ICP-Q-MS analysis

Maximilian Podsednik¹, David K. Gibbs², Jakob Willner², Silvia Larisegger³, Michael Nelhiebel³, Andreas Limbeck² ¹*KAI GmbH*, ²*TU Wien*, ³*KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH*

2:50 PM (ATOM-05.5) Detection of metals in

microplastics by LIBS and LA-ICP-MS techniques

Pavel Porizka¹, Aida Fazlic¹, Pavlina Modlitbova¹, Gabriela Kalčíková², Lukas Brunnbauer³, Andreas Limbeck³, Jozef Kaiser¹ ¹*CEITEC Brno University of Technology*, ²*University of Ljubljana*, ³*TU Wien*

24AWD07: Spectroscopy Magazine Emerging Leader in Molecular Spectroscopy Award Session | 301B

Chair: Joseph Smith, Merck & Co

1:30 PM (AWD-07.1) Conformal Predictions: Assigning Meaningful Confidence Intervals in Multivariate Classification

Karl S. Booksh¹, Caelin Celani¹, Joseph P. Smith², Nicole Ralbovsky² ¹*University of Delaware*, ²*Merck*

1:50 PM (AWD-07.2) Infrared Imaging Applied to the Forensic Examination of Automotive Paints

Barry K. Lavine¹, Haoran K. Zhong¹, Elizabeth K. Donkor¹, Collin G. White¹, Thomas K. Hancewicz² ¹*Oklahoma State University*, ²*TMH Associates*

2:10 PM (AWD-07.3) Combining SERS with Machine Learning to Monitor Oxidative Stress

Bhavya Sharma¹, Wilson Garuba¹ ¹*University of Tennessee*

2:30 PM (AWD-07.4) Raman hyperspectroscopy combined with machine learning is a universal tool for disease diagnostics

Igor K. Lednev¹, Bhavik Vyas² ¹*University at Albany, SUNY*, ²*University at Albany*

2:50 PM (AWD-07.5) Chemometric methods for maple syrup grading

Jean-Francois Masson¹, Saba Bashir¹, Issraa Beniani¹, Malama Chisanga² ¹*Universite de Montreal*, ²*University of Montreal*

24CHEM06: Applications of AI and Chemometrics in Forensic Chemistry | 305B

Chair: Ruth Smith, Michigan State University

1:30 PM (CHEM-06.1) Application of transfer learning for GC/MS data classification in fire debris analysis

Ting-Yu Huang¹, Jorn Yu² ¹*Ming Chuan University*, ²*Sam Houston State University*

1:50 PM (CHEM-06.2) AI Opinions in Forensic Fire Debris Analysis

Michael E. Sigman¹ ¹*University of Central Florida*

2:10 PM (CHEM-06.3) Weeding out Cannabis Ingestion: Towards determination of Cannabis use biomarkers using high resolution mass spectrometry.

Rabi A. Musah¹, Niara Nichols¹ ¹*University at Albany-SUNY*

2:30 PM (CHEM-06.4) Developing a Semi-Supervised

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

Machine Learning Model for the Detection of Newly Emerging Street Drugs using Paper-Spray Mass Spectrometry

Allie Miskulin¹, Bruce Wallace¹, Chris Gill², Dennis Hore¹ ¹University of Victoria, ²Vancouver Island University

2:50 PM (CHEM-06.5) Advances in Cannabis sativa L. quality control - Handheld Near Infrared Sensor technology for in-situ analysis

Cameron M. Jordan¹, Luis Rodriguez-Saona¹, Eric S. Armstrong¹, M. Monica Giusti¹, Xinyue Fan¹, Silvia de Lamo Castellvi¹ ¹The Ohio State University

Abbe Center of Photonics, Jena, Germany., ²Photonic Data Science department, Leibniz Institute of Photonic Technology, Jena, Germany, ³Institute of Medical Microbiology, Jena University Hospital, Jena, Germany, ⁴Leibniz Institute of Photonic Technology, Jena, Germany., ⁵Friedrich Schiller University Jena and Abbe Center of Photonics, Institute of Physical Chemistry and Abbe Center of Photonics, Jena, Germany. Leibniz Institute of Photonic Technology, Jena, Germany

24CTPEARLY03: Rising Talents in Enhanced Raman Spectroscopy | 303

Chair: Lamyaa Almeahmadi, MIT

1:30 PM (CTPEARLY-03.1) Integrating AI-assisted Raman spectroscopy and Electrokinetics for Bacterial Identification in Wastewater

Yirui Zhang¹, Liam K. Herndon¹, Punnag Padhy¹, Alexander Al-Zubeidi¹, Baba Ogunlade¹, Alexandria Boehm¹, Jennifer Dionne¹ ¹Stanford University

1:50 PM (CTPEARLY-03.2) A multimodal spectroscopic approach combining mid-infrared and near-infrared for discriminating Gram-positive and Gram-negative bacteria

Thulya Chakkumpulakkal Puthan Veetil¹, Kamila Kochan², Galain Williams³, Kimberley Bourke⁴, Xenia Kostoulias⁵, Anton Peleg⁶, Dena Lyras⁶, Paul De Bank⁷, David Perez Guaita⁵, Bayden Wood⁶ ¹Monash University, ²lecturer, ³research fellow, ⁴research assistant, ⁵senior research fellow, ⁶professor, ⁷senior lecturer

2:10 PM (CTPEARLY-03.3) Toward a Surface-enhanced Raman spectroscopy and deep learning approach to bacterial wastewater monitoring

Liam K. Herndon¹, Yirui Zhang¹, Fareeha Safir², Baba Ogunlade¹, Punnag Padhy¹, Halleh Balch¹, Alexandria Boehm¹, Jennifer Dionne¹ ¹Stanford University, ²Pumpkinseed Technologies

2:30 PM (CTPEARLY-03.4) Plasmon-driven surface reactions and enzyme catalysis probed through surface-enhanced Raman spectroscopy

Ruchi Singh¹, Soumik Siddhanta², Vikas yadav¹ ¹Research Scholar, ²Assistant Professor

2:50 PM (CTPEARLY-03.5) Tip-enhanced Raman and nano-FTIR spectroscopy for virion screening

Tanveer Ahmed Shaik¹, Savelii Filipkov¹, Oleg Ryabchykov², Franziska Hornung³, Tanja Deckert-Gaudig⁴, Thomas W. Bocklitz⁴, Stefanie Deinhardt-Emmer³, Volker Deckert⁵ ¹Friedrich Schiller University Jena and Abbe Center of Photonics, Institute of Physical Chemistry and

24IR05: Novel laser based chemical sensing | 301A

Chair: Bernhard Lendl, TU Wien

1:30 PM (IR-05.1) High-throughput field-resolved infrared spectroscopy of cells in flow

Jan Ornik¹, Marinus Huber¹, Daniel Bausch¹, Holger Mirkes², Florian Lindinger¹, Mark Kielpinski¹, Thomas Henkel¹, Mihaela Zigman³, Ute Neugebauer¹, Max Naumann¹, Ferenc Krausz⁴, Jürgen Popp¹, Ioachim Pupeza⁵ ¹Leibniz Institute of Photonic Technology, ²Ludwig Maximilians University Munich, ³Ludwig-Maximilians-Universität München (LMU) & Max Planck Institute of Quantum Optics (MPQ), ⁴Max Planck Institute of Quantum Optics, ⁵Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau & Leibniz Institute of Photonic Technology

1:50 PM (IR-05.2) Infrared molecular fingerprinting to phenotype human health and disease

Mihaela Zigman¹, Philip Jacob², Marinus Huber², Liudmila Voronina², Frank Fleischmann², Tarek Eissa², Kosmas Kepesidis³, Thomas Kolben⁴, Michael Chaloupka⁴, Juergen Behr⁵, Nadia Harbeck⁴, Maximilian Reiser⁴, Christian Stief⁴, Birgit Linkohr⁶, Annette Peters⁶, Ioachim Pupeza⁷, Alexander Weigel², Ferenc Krausz³ ¹Ludwig-Maximilians-Universität München (LMU) & Max Planck Institute of Quantum Optics (MPQ), ²LMU, ³LMU, MPQ, CMF, ⁴LMU Clinics, ⁵LMU Clinics, Asklepios Clinics, ⁶Helmholtz Munich, ⁷Ludwig Maximilians University Munich, Max Planck Institute of Quantum Optics, a Leibniz Institute of Photonic Technology

2:10 PM (IR-05.3) QCL-IR Imaging of Live Cells: Monitoring the Total Mass of Biomolecules in Single Cells

Young Jong Lee¹, Yow-Ren Chang¹ ¹NIST

2:30 PM (IR-05.4) Sparse Signal Recovery in Mid-IR Imaging Systems

Viviana Arrunategui Norvick¹, Michael Wakin², Yamuna Phal² ¹Colorado School of Mines Phal Group, ²Colorado School of Mines

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

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2:50 PM (IR-05.5) **Next-generation Tm-fiber-based femtosecond laser for field-resolved infrared spectroscopy**

Jan Ornik¹, Daniel Bausch¹, Florian Lindinger¹, Aarya Arya¹, Lakshya Sharma¹, Max Kieker¹, Marinus Huber¹, Don Sajan², Christian Gaida², P. E. Collin Aldia³, Oliver H. Heckl³, Jens Limpert⁴, Ioachim Pupeza⁵ ¹*Leibniz Institute of Photonic Technology*, ²*Active Fiber Systems GmbH*, ³*Optical Metrology Group, Faculty of Physics, University of Vienna*, ⁴*Friedrich-Schiller-University Jena, Institute of Applied Physics, Abbe Center of Photonics*, ⁵*Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau & Leibniz Institute of Photonic Technology*

Bristol Myers Squibb, ²*Bristol Myers Squibb*, ³*University of Birmingham*

2:30 PM (PAT-03.4) **Chemometric Model Transfer: Offline Model Maintenance and Real-Time Model Updating**

Kexin Ling¹, Courtney Talicska¹, Nathan Linklater¹, Andrew S. Palm¹ ¹*Pfizer Inc*

2:50 PM (PAT-03.5) **Broad spectra fiber solutions for process-control in-line**

Alexander S. Novikov¹, Martin Warman², Andrea Teuber¹, Boris Mizaikoff³, Tatiana Sakharova¹, Alexey Bocharnikov¹, Haro Fritsche¹, Viacheslav Artyushenko¹ ¹*art photonics GmbH*, ²*Martin Warman Consultancy Ltd*, ³*Institute of Analytical and Bioanalytical Chemistry, Ulm University*

24MASS04: Advances in Mass Spectrometry-Based Glycomics | 306A

Chair: Gabe Nagy, University of Utah

1:30 PM (MASS-04.1) **Developing a Bioanalytical Toolbox for Human Milk Oligosaccharide Characterization**

Gabe Nagy¹ ¹*University of Utah*

1:50 PM (MASS-04.2) **Advancements in Glycomics and Glycoproteomics: Innovative Methods and Clinical Applications**

Yehia Mechref¹ ¹*Texas Tech University*

2:10 PM (MASS-04.3) **Making use of informative glycan-specific ions in glycopeptide MS/MS spectra**

Nicholas M. Riley¹ ¹*University of Washington*

2:30 PM (MASS-04.4) **glycoPATH: Correlating LC-MS/MS glycomic and RNAseq tran-scriptomic data to determine glycosylation pathways**

Michael Russelle S. Alvarez¹, Xavier Holmes¹, Armin Oloumi¹, Ryan Schindler¹, Sheryl Joyce Grijaldo-Alvarez¹, Qingwen Zhou¹, Carlito B. Lebrilla¹ ¹*University of California Davis*

2:50 PM (MASS-04.5) **Standards-Free Absolute Quantitation of Oxidizable Glycopeptides by Coulometric Mass Spectrometry**

Hao Chen¹ ¹*New Jersey Institute of Technology*

24PAT03: Novel PA Technologies & Applications | 302C

Chair: Alison Nordon, University of Strathclyde

1:30 PM (PAT-03.1) **In situ monitoring of solid form using low frequency Raman spectrometry**

Alison Nordon¹ ¹*University of Strathclyde*

1:50 PM (PAT-03.2) **Batch Statistical Process Monitoring: Inter- and Intra-Batch Monitoring**

Neal B. Gallagher¹ ¹*Eigenvector Research Inc*

2:10 PM (PAT-03.3) **Application of PAT Towards the Development of 3D Printed Pharmaceutics (and Beyond)**

Zoë Whalley¹, Patrick Wray², Tom Mills³, Richard Greenwood³ ¹*University of Birmingham*

24PMA05: Analysis of Biologicals In Blood 1 | 306B

Chair: John Marshall, Toronto Metropolitan University

Co-Chair: Thomas Kislinger, Princess Margaret Cancer Centre

1:30 PM (PMA-05.1) **N-Glycoproteomics of patient-derived xenografts for the discovery of novel cancer biomarkers**

Thomas Kislinger¹ ¹*Princess Margaret Cancer Centre*

2:10 PM (PMA-05.2) **Digital Detection of Proteins**

David C. Duffy¹ ¹*Quanterix Corporation*

2:30 PM (PMA-05.3) **Ion extraction of hydrogen rearrangements and heavy isotopes reduced the type II error rate of plasma proteomics**

John G. Marshall¹, Jaimie Dufresne², Zhuo Zhen Chen¹, John G. Marshall¹, John G. Marshall¹ ¹*Toronto Metropolitan University*, ²*YYZ PHARMATECH INC*

2:50 PM (PMA-05.4) **Overcoming Biopharmaceutical Interferents for Quantitation of Host Cell DNA Using an Automated, High-Throughput Methodology**

Mackenzie Smith¹ ¹*Merck & Co.*

24RAM05: IRDG | 302B

Chair: Karen Faulds, University of Strathclyde

1:30 PM (RAM-05.1) **Point of use SERS for Detection of Antimicrobial Resistance**

Duncan Graham¹, Waleed Hassanain¹, Chris Johnson², Neil Keegan², Karen Faulds¹ ¹*University of Strathclyde*, ²*University of Newcastle*

1:50 PM (RAM-05.2) **Detecting biomarkers with electrochemical surface-enhanced Raman spectroscopy**

Tabitha Jones¹, Sarah Sibug-Torres², Jeremy Baumberg¹ ¹*University of Cambridge*, ²*University Of Cambridge*

2:10 PM (RAM-05.3) **Surface-Enhanced Raman Spectroscopy and Machine Learning for Community-Based Drug Checking**

Next year: October 5-10, 2025 • Northern Kentucky Convention Center

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

Rebecca R. Martens¹, Lea Gozdziński¹, Bruce Wallace¹, Dennis Hore¹ ¹*University of Victoria*
2:30 PM (RAM-05.4) **Laser-Quick Diagnosis: SERS-LFIAs Allow for Rapid Insight into Drug Induced Liver Injury**

Benjamin A. Clark¹, Sian Sloan-Dennison¹, Karen Faulds¹, Duncan Graham¹, James Dear², Kathleen Scullion², David Creasey³, Cicely Rathmell³, Paul Fineran⁴, Joanne Mair⁴ ¹*University of Strathclyde*, ²*University of Edinburgh*, ³*Wasatch Photonics*, ⁴*Translational Healthcare Technologies*

2:50 PM (RAM-05.5) **SORS and advanced technologies for cultural heritage**

Alberto Lux¹, Claudia Conti¹, Alessandra Botteon¹, Sara Mosca², Pavel Matousek² ¹*CNR-ISPC*, ²*STFC - UKRI*

24SPSJ02: NIR Spectroscopy Multidimensional Approaches 302A

Chair: Akifumi Ikehata, NARO

Co-Chair: Mika Ishigaki

1:30 PM (SPSJ-02.1) **Chemometric-machine learning framework driven portable spectroscopy for non-invasive quality estimation of fruits**

ARUN SHARMA¹ ¹*Department of Food Engineering, National Institute of Food Technology Entrepreneurship and Management*

(NIFTEM), Haryana, India

1:50 PM (SPSJ-02.2) **Novel Near-Infrared Hyperspectral Imaging Systems for Endoscopic Composition Analysis**

Toshihiro Takamatsu¹, Seiya Hayashi², Naoto Kakuta², Hiroshi Takemura² ¹*National Institute of Advanced Industrial Science and Technology*, ²*Tokyo University of Science*

2:10 PM (SPSJ-02.3) **New trends in chemometrics for NIR spectroscopy**

Federico Marini¹ ¹*Dept. of Chemistry, University of Rome "La Sapienza"*

2:30 PM (SPSJ-02.4) **Hydrogen bonding state of water in high-concentrated aqueous solutions of alkali-metal salts probed by near-infrared spectroscopy**

Yusuke Morisawa¹ ¹*Kindai University*

2:50 PM (SPSJ-02.5) **Local Environment in Liquid Phase Amides: Carbonyl Stretching Band Examination via Lorentz Oscillator Model and Anharmonic Analysis of NIR and MIR spectra**

Justyna Grabska¹, Krzysztof B. Bec¹, Jerzy P. Hawranek², Christian W. Huck¹ ¹*University of Innsbruck*, ²*University of Wrocław*

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 3:50 PM – 5:30 PM | *Various Locations*

24AES06: Electrokinetic Bioanalysis | 306C

Chair: Lisa Flanagan, Departments of Neurology, Biomedical Engineering, Anatomy & Neurobiology, University of California Irvine

Co-Chair: Negar Farhang Doost, Chemical and Biomedical Engineering Department, West Virginia University

3:50 PM (AES-06.4) Assessing Plasticity in Prostate Cancer using Electrokinetic Techniques

Lexi L. Crowell-Simpkins¹, Mary Tran¹, Luis Henriquez¹, Juan Yakisich², Brian Aufderheide², Tayloria N.G. Adams¹ ¹University of California, Irvine, ²Hampton University

4:10 PM (AES-06.3) Diagnosis of Tick-Borne Rickettsial Infections through Dielectrophoresis

Negar Farhang Doost¹, Soumya K. Srivastava² ¹Chemical and Biomedical Engineering Department, West Virginia University, ²West Virginia University

4:30 PM (AES-06.4) Electrokinetic Microscale Separations Combining Linear and Nonlinear Effects

Blanca H. Lapizco-Encinas¹ ¹Rochester Institute of Technology

4:50 PM (AES-06.1) DEP electrophysiology: A potential marker for blood related health and disease

Emily Kruczek¹, John O'Neill², Andrew Beale², Krista Clarke¹, Oreoluwa Griffiths¹, Caroline Kingdon³, Jonathan Gibbins⁴, Elina Lacerda³, Debra Dunn-Walters¹, rebecca Lewis¹, Alexander Stewart¹, Rita Jabr⁵, Rula Abdallat⁶, Rashedul Hoque¹, Matthew Johnson⁷, Sarah Reece⁸, Petra Schneider⁸, Fatima Labeed⁹ ¹University of Surrey, ²MRC-LMB, ³LSHTM, ⁴University of Reading, ⁵UCL, ⁶Hashemite University, ⁷Khalifa University, ⁸University of Edinburgh, ⁹UAE University

5:10 PM (AES-06.5) Single Molecule Imaging Enhanced by Electrokinetic Ion Concentration Polarization for in situ Profiling of Gene Expression in Multicellular Organisms

Gongchen Sun¹ ¹University of Texas at San Antonio

24ATOM06: Atomic Based Imaging | 305A

Co-Chair: C. Derrick Quarles, Jr., Elemental Scientific, Inc.

Co-Chair: Beatriz Fernandez Garcia, University of Oviedo

3:50 PM (ATOM-06.1) Strategies to increase figures of merit in LA-ICP-QMS and -TOFMS

David Clases¹, Thomas Lockwood², Lukas Schlatt³, Raquel Gonzalez de Vega¹ ¹University of Graz, ²University of Technology Sydney, ³Ametek - Nu Instruments

4:10 PM (ATOM-06.2) From qualitative to quantitative protein bioimaging in individual cells by LA-ICP-MS; one step forward.

Paula Menero Valdés¹, Beatriz Fernández¹, Lydia Álvarez², Héctor González-Iglesias³, Rosario Pereiro¹ ¹University of Oviedo, ²Instituto

Oftalmológico Fernández-Vega, ³Instituto de Productos Lácteos de Asturias (IPLA-CSIC)

4:30 PM (ATOM-06.3) Multielemental Quantitative mapping of Biogenic Structures with LA-ICP-TOF-MS for Sclerochronological Research

Ana Lores-Padin¹, Thibaut Van Acker¹, Martin Wiech², Niels de Winter³, Frank Vanhaecke¹ ¹Ghent University, ²INSTITUTE OF MARINE RESEARCH, ³Vrije Universiteit Amsterdam

4:50 PM (ATOM-06.4) High speed particle mapping via LA-ICP-TOF-MS for the analysis of environmental samples

Benjamin T. Manard¹, Hunter B. Andrews¹, Brian Ticknor¹, Paula Cable-Dunlap¹, Josh Hewitt¹, Jordan Stanberry¹ ¹Oak Ridge National Laboratory

5:10 PM (ATOM-06.5) Investigating the Effect of Spatial Overlap of Shots in LIBS Imaging to Improve Spatial Resolution

David K. Gibbs¹, Jakob Willner¹, Silvia Larisegger², Michael Nelhiebel², C. Derrick Quarles Jr.³, Andreas Limbeck¹ ¹TU Wien, ²KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH, ³Elemental Scientific, Inc.

24BIM05: AI-Driven Multimodal Chemical Imaging for Biomedical Diagnostics | 302A

Chair: Juergen Popp, Leibniz Institute of Photonic Technologies

3:50 PM (BIM-05.1) Metabolic Nanoscopy

Lingyan Shi¹ ¹UC San Diego

4:10 PM (BIM-05.2) Spatial Single Cell Omics based on Spectrally Resolved Raman Imaging

Peter T. So¹, Koseki C. Kobayashi-Kirschvink¹, Jeon Woong Kang² ¹Massachusetts Institute of Technology, ²mas

4:30 PM (BIM-05.3) ML-enhanced Raman microscopy for rapid and high-sensitivity molecular diagnosis

Katsumasa Fujita¹ ¹Osaka University

4:50 PM (BIM-05.4) Photothermal and Fluorescence-detected Photothermal Infrared spectromicroscopic analyses of single cells

Kathleen M. Gough¹, Rinuk 'Limurn¹, David Hartry¹, Chalapathi Gajjala², Sabine Mai¹, Rohith Reddy³, Craig Prater⁴ ¹University of Manitoba, ²University of Houston, ³University of Houston, ⁴Photothermal Spectroscopy Corp

5:10 PM (BIM-05.5) Optical photothermal infrared spectroscopy of cortical and trabecular tissue sub-micron composition in bone biopsies

Sofia Mehmood¹, Isha Dev¹, Yana Bronfman², Edward DiCarlo², Nancy Pleshko³, William Querido³ ¹Temple University, ²Hospital for Special Surgery, ³Department of Bioengineering, Temple University

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 3:50 PM – 5:30 PM | *Various Locations*

24CHEM05: Chemometrics in Food & Agriculture | 305B

Chair: Mengliang Zhang, Ohio University
Co-Chair: Jianghao Sun, Food Composition and Methods Development Laboratory, BHNRC, ARS, USDA

3:50 PM (CHEM-05.1) Authentication and Discrimination of Infrared Spectra of Edible Oils Using Experimental and Digitally Blended Data for both Calibrated and Uncalibrated Adulterants

Barry K. Lavine¹, Elizabeth K. Donkor¹, Shiksha Tiwari¹, Isio Sota-Uba¹, Collin G. White¹, Thomas K. Hancewicz², Karl S. Booksh³
¹Oklahoma State University, ²TMH Associates, ³University of Delaware

4:10 PM (CHEM-05.2) Surveillance of Pathogenic Bacteria on a Food Matrix Using Machine-Learning-Enabled Paper Chromogenic Arrays

Zhen Jia¹, Boce Zhang¹ ¹University of Florida

4:30 PM (CHEM-05.3) A Tool for Evaluating the Impact of Genetics and Environment on Plant Metabolites

Jamea Harnly¹ ¹US Department of Agriculture

4:50 PM (CHEM-05.4) Raman-Based Quantification of Arsenic Toxicities in Rice

Dmitry Kurouski¹, Isaac AS Juarez¹ ¹Texas A&M University

5:10 PM (CHEM-05.5) Improving generalizability of deep learning models for hyperspectral data analysis

Bosoon Park¹, Taesung Shin² ¹United State Department of Agriculture, Agricultural Research Service, ²USDA, ARS

24FORENS01: Nuclear Forensics | 303

Chair: Robert Lascola, Savannah River National Laboratory
Co-Chair: William Gilbraith, Savannah River National Laboratory

3:50 PM (FORENS-01.1) On-Line Raman Hydrogen Isotope Detection for Fusion Accounting and Monitoring

William Gilbraith¹, Holly B. Flynn¹, Robert Lascola², Collin Malone¹ ¹Savannah River National Laboratory, ²SRNL, DOE

4:10 PM (FORENS-01.2) Online Monitoring of Hydrogen Processing using Hollow-Core Waveguide-Based Raman Spectroscopy

John T. Kelly¹, Robert Lascola¹, William Gilbraith² ¹SRNL, DOE, ²Savannah River National Laboratory

4:30 PM (FORENS-01.3) Tritium detection during depth-profiling of neutron irradiated Zircaloy using ultrafast LIBS

Sivanandan S. Harilal¹, Abdul K. Shaik¹, Elizabeth J. Kautz¹, Arun Devaraj¹ ¹Pacific Northwest National laboratory

4:50 PM (FORENS-01.4) Analysis of Subsurface Defects in National Ignition Facility (NIF) Optics Using fs-LA-ICPMS

Gregory L. Klunder¹, Paul Spackman¹, Christopher Mah¹ ¹Lawrence Livermore National Laboratory

5:10 PM (FORENS-01.5) Panel Discussion

24IR03: Life Science Applications of Photothermal IR Spectroscopy | 301A

Chair: Rohith Reddy, University of Houston
Co-Chair: Caitlin Davis, Yale University

3:50 PM (IR-03.1) Exploring Metabolism: Advanced Insights from Photothermal Infrared Microscopy in Biomedical Research

Yeran Bai¹ ¹University of Arizona

4:10 PM (IR-03.2) Advances in Biomedical Diagnostics using Photothermal Mid-infrared Spectroscopic Imaging

Chalapathi Gajjela¹, Ragib Ishrak², Xinyu Wu², Reza Reihani², David Mayerich², Rohith Reddy²
¹University of houston, ²Univ. of Houston

4:30 PM (IR-03.3) O-PTIR Spectral Imaging of Bone Composition at the Sub-micron Scale

Reshma Sudhesh¹, Pooja Arvind¹, Nancy Pleshko², William Querido² ¹Temple University, ²Department of Bioengineering, Temple University

4:50 PM (IR-03.4) Live cell metabolic imaging with sub-micron IR microscopy

Caitlin Davis¹, Hannah Castillo¹, Sydney Shuster¹
¹Yale University

5:10 PM (IR-03.5) OPTIR and SERS classification of magnetically sorted cancer cells

Blair Rist¹, Spencer Witte¹, Zachary D. Schultz¹
¹The Ohio State University

24PMA06: Generative AI and machine learning advancing pharmaceutical development with vibrational spectroscopy 306B

Chair: Michelle Raikes, Boehringer Ingelheim Pharmaceuticals

3:50 PM (PMA-06.1) Spectroscopic Applications for Pharmaceutical Development

John wasylyk¹, Robert Wethman¹, Ming Huang¹
¹Bristol Myers Squibb Co.

4:10 PM (PMA-06.2) Automation of Quantification and Classification of Raman samples through AI

Arelis Colon¹, Joseph Bonvallet¹, Ty Olmstead¹
¹Ocean Optics

4:30 PM (PMA-06.3) Hyper-spectra imaging analysis of PLGA microspheres via machine learning enhanced Raman spectroscopy

Minghe Li¹ ¹Boehringer Ingelheim

TECHNICAL PROGRAM - TUESDAY, OCTOBER 22, 2024

Oral Symposia | 3:50 PM – 5:30 PM | *Various Locations*

4:50 PM (PMA-06.4) **Spectroscopy data-based machine learning predictive modeling in long-acting injectables drug formulation development**

Kenan Pandza¹, Karthik Raman¹, Max Brodie¹, Corina Badea-Mic badea-Mic¹ ¹*Persist AI*

5:10 PM (PMA-06.5) **Lasers for optical photothermal infrared microscopy for chemical selective imaging in the biomedical context**

Christoph Krafft¹, Juergen Popp² ¹*Leibniz Institute of Photonic Technology*, ²*Leibniz Institut of Photonic Technology*

24RAM06: Food | 302B

Chair: Roy Goodacre, University of Liverpool

3:50 PM (RAM-06.1) **Optimizing Beer Product Quality Control: Rapid Monitoring of Quality and Volatile Compounds by using Miniaturized Vibrational Spectroscopy**

Haona Bao¹, Yalan Wu¹, Luis Rodriguez-Saona² ¹*The Ohio State University*, ²*The Ohio State University*

4:10 PM (RAM-06.2) **Prediction of Barley Malt Quality Using ATR-FTIR Spectroscopy, Feature Selection Methods, and Automated Multivariate Regression Models**

Oudus A. Thanni¹, Peter de Boves Harrington¹, Oyeyemi Ajayi², Ramamurthy Mahalingam², Jason Walling² ¹*Ohio University*, ²*USDA-ARS Cereal Crop Research Unit*

4:30 PM (RAM-06.3) **Dethroning GC-MS: Bringing NIR, Raman, and SERS together for Rapid Edible Oil Analysis**

Adam J. Hopkins¹ ¹*Metrohm USA*

4:50 PM (RAM-06.4) **Opportunities of sustainable sources of protein and oil for the food industry through insect farming**

Silvia de Lamo Castellvi¹, Carmen Mendez², Celeste Matos-Gonzalez³, Yalan Wu³, Luis Rodriguez-Saona¹ ¹*The Ohio State University*, ²*Universitat Rovira i Virgili*, ³*The Ohio state university*

5:10 PM (RAM-06.5) **Rapid and in situ screening for key quality traits in pulse crops**

Alessandra F. Victorio Ramos¹, Luis Rodriguez-Saona² ¹*the ohio state university*, ²*The Ohio State University*

24RAM14: Industrial Raman | 302C

Chair: To Be Announced

3:50 PM (RAM-14.1) **Removing Bottlenecks to Real-Time Release in Biopharmaceuticals with Raman Spectroscopy**

Karin M. Balss¹, Erin Masucci¹, Colin Fitzpatrick¹ ¹*Janssen*

4:10 PM (RAM-14.2) **Raman Analysis for Analyte Determination in Metal Plating Baths**

Jonathon Duay¹, Graig Garman¹, Brenda Maes¹, Katrina Sadzewicz¹, Shailendra Parihar¹ ¹*Sandia National Laboratories*

4:30 PM (RAM-14.3) **Raman Spectroscopy as a PAT Tool for Quantifying Monoclonal Antibody Aggregates**

Christine Massie¹, Marina Hincapie² ¹*Sanofi - Process Analytical Technology – Mammalian Platform, Framingham, Massachusetts, USA*, ²*Sanofi, Process Analytical Technology – Mammalian Platform, Framingham, Massachusetts, USA*

4:50 PM (RAM-14.4) **Monitoring Live Cell Viability during Culturing Perturbation using Raman Spectroscopy**

Faizal¹, Keita Iwasaki¹, Kosuke Hashimoto¹, Hidetoshi Sato² ¹*Kwansei Gakuin University*, ²*School of Biological and Environmental Sciences, Kwansei Gakuin University*

5:10 PM (RAM-14.5) **Assessing the limit of detection and quantification of critical process parameter in Timegated Raman spectroscopy.**

Amuthachelvi Daniel¹, Jacopo Zini¹, Sofia Lane¹, Mari Tenhunen¹ ¹*Timegate Instruments Oy*

24SPR02: Young Investigators In Plasmonics | 306A

Chair: Laura Fabris, Politecnico di Torino

3:50 PM (SPR-02.1) **Colloids and Surfaces: Design and Experimental Strategies Towards Reproducible Microbial Plasmonic Sensing**

Malama Chisanga¹, Roy Goodacre², Jean-Francois Masson³ ¹*University of Montreal*, ²*University of Liverpool*, ³*Universite de Montreal*

4:10 PM (SPR-02.2) **Imaging Thermal Gradients from Plasmon Decay using Wavefront Microscopy**

Claire A. West¹, Stephan Link², Emilie Ringe³, Vladimir Lomonosov³, Tinglian Yuan² ¹*University of Illinois, Urbana-Champaign*, ²*University of Illinois, Urbana-Champaign*, ³*University of Cambridge*

4:30 PM (SPR-02.3) **Simultaneous Detection of Thrombin and VEGF with Gold Nanoprism-Enhanced SERS Aptasensor**

Pooja Anantha¹, Piyush Raj¹, Peng Zheng¹, Swati Tanwar¹, Ishan Barman¹ ¹*Johns Hopkins University*

4:50 PM (SPR-02.4) **High-Performance Nanoparticle-on-Liquid-Metal (NPoLM) SERS Sensors**

Peter Q. Liu¹, Shreyan Datta¹, Shoaib Vasini¹, Xianglong Miao¹ ¹*University at Buffalo*

5:10 PM (SPR-02.5) **Localizing chemical changes on nanostructures using spectrally resolved super-resolution SERS imaging**

Deben N. Shoup¹, Zachary D. Schultz² ¹*Ohio State University*, ²*The Ohio State University*

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Award & Plenary Lectures | 8:15 AM – 9:30 AM | *Ballroom A*

8:15 AM Award Presentation

8:30 AM ACS Analytical Division Award in Spectrochemical Analysis: Stimulated Raman Microscopy: From Scattering to Photothermal

Ji-Xin Cheng¹ *Boston University*

9:00 AM NESAS and SAS Lester W. Strock Award: Uranium particle analysis by ICP-MS-based approaches

Benjamin T. Manard¹ *Oak Ridge National Laboratory*

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Wednesday Poster Sessions | 9:30 AM – 10:30 AM | *Exhibit Hall B*

(Wed-P1) Implementation of stacked ensemble machine learning for detection of plutonium contamination in soil via LIBS

Paige Anderson¹, Janos I. Braun², Justin I. Borrero Negrón¹, Kyle C. Hartig¹, Ashwin Rao³ *University of Florida*, *New Mexico State University*, *Air Force Research Laboratory*

(Wed-P2) Isotopic analysis of lithium via acousto-optically gated high-repetition laser-induced breakdown spectroscopy and spatial heterodyne spectroscopy

Simon Blume¹, Xunyu Li¹, Jens Riedel¹ *Federal Institute for Materials Research and Testing (BAM)*

(Wed-P3) Machine Learning-Enhanced LIBS for Spectral Discrimination and Chemometric Analysis of Pu Oxalate Surrogates

Justin I. Borrero Negrón¹, Daniel Emrick², Paige Anderson¹, Janos Braun³, Eliel Villa-Aleman⁴, Ashwin P. Rao⁵, Kyle C. Hartig¹ *University of Florida*, *University of New Mexico*, *New Mexico State University*, *Savannah River National Laboratory*, *Space Vehicles Directorate, Air Force Research Laboratory*

(Wed-P4) Design and Optimization of a new microwave microreactor for Laser-induced breakdown spectroscopy (LIBS).

Buddhika T. Kumara¹, Steven Ray², Gerardo Gamez³ *The State University of New York at Buffalo*, *SUNY Buffalo Dept of Chemistry*, *Texas Tech University*

(Wed-P5) Application of LIBS and XRF to the analysis of heavy metals in shark blood

Audrey O. Caplow¹, Praseon Diwaker², Kristine Stump¹, Heather Marshall¹, Jake Jerome³ *Ransom Everglades High School*, *South Dakota School of Mines and Technology*, *University of Miami*

(Wed-P6) Rare Earth Element (REE) Measurement in Coal and Rock Mineral Matrices

CR BHATT¹, DANIEL A. HARTZLER², DUSTIN L. MCINTYRE² *NETL-LEIDOS*, *NETL*

(Wed-P7) Machine Learning assisted LIBS for mineral ore provenance determination

Hunter Paxton¹, Samuel E. Kessinger¹, Stirling Wallace¹, Ava Beck¹, Ava Hermes¹, Jon Kellar¹, Praseon K. Diwaker¹ *South Dakota School of Mines and Technology*

(Wed-P8) LIBS Signal Enhancement for Non-Metals by Application of Vacuum

David K. Gibbs¹, Patrick Tapler¹, Birgit Achleitner¹, Silvia Larisegger², Michael Nelhiebel² *TU Wien*, *KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH*

(Wed-P9) Elucidation of Energy and Mass Transfer Mechanisms of Optical Trapped Single, Micron-Sized Particles via Laser-Particle Interactions

Justin I. Borrero Negrón¹, Kyle S. Latty¹, Kyle C. Hartig¹ *University of Florida*

(Wed-P10) Precision Agriculture: Using LIBS and Drones Multispectral Imagery in Conjunction

Zachary Karg¹, Carson Daly¹, Rajesh Sani¹, Tanvi Govil¹, Praseon K. Diwaker² *South Dakota Mines*, *South Dakota School of Mines and Technology*

(Wed-P11) Laser-induced Breakdown Spectroscopy for Real-Time Monitoring of Molten Salts via Aerosol Formation

Zechariah B. Kitzhaber¹, Hunter B. Andrews¹, Daniel Orea¹, Joanna McFarlane¹ *Oak Ridge National Laboratory*

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Wednesday Poster Sessions | 9:30 AM – 10:30 AM | Exhibit Hall B

(Wed-P12) **Characterizing supported fresh catalysts by Laser-Induced Breakdown Spectroscopy (LIBS): from concept to routine analysis**

Francisco A. Lopez-Linares¹, Amanda Dos santos Augusto¹, Cesar F. Ovalles¹, Jinyi Han¹, Alexander Kuperman¹, Rachel E. Mohler¹
¹*Chevron*

(Wed-P13) **Understanding Li I 670.8 nm Self-Reversal in Laser Produced Plasmas through Complementary Monochromatic Imaging and Optical Emission spectroscopy**

Nusrat Karim¹, Elizabeth J. Kautz², Mathew P. Polek³, Sivanandan S. Harilal⁴ ¹*NC State university*, ²*NC State University*, ³*University of California, San Diego*, ⁴*Pacific Northwest National Laboratory*

(Wed-P14) **Simultaneous detection of different nanoparticle labels and their mutual influence in mixtures by Laser-Induced Breakdown Spectroscopy**

Jozef Kaiser¹, Pavel Porizka¹, Eva Zikmundová¹, Eva Kočí¹, Antonín Hlaváček² ¹*CEITEC Brno University of Technology*, ²*Institute of Analytical Chemistry of the Czech Academy of Sciences*

(Wed-P15) **Deep Learning-Based Classification of Rock Materials by Mineral Type and Geographic Origin Using LIBS**

Hunter Paxton¹, Prasoon K. Diwakar¹ ¹*South Dakota School of Mines and Technology*

(Wed-P16) **Fast and large-scale imaging in laser-induced breakdown spectroscopy experiments**

Maximilian Podsednik¹, Jakob Willner², Silvia Larisegger³, Michael Nelhiebel³, Andreas Limbeck² ¹*KAI GmbH*, ²*TU Wien*, ³*KAI Kompetenzzentrum Automobil- und Industrieelektronik GmbH*

(Wed-P17) **Effect of ultrafast GHz burst femtosecond laser ablation on elemental analysis with laser induced breakdown spectroscopy**

Veronica C. Bradley¹, Vassilia Zorba¹, Minok Park¹ ¹*Lawrence Berkeley National Laboratory*

(Wed-P18) **Differentiation of Regioisomeric 4-N-Methoxy- and Dimethoxybenzyl Derivatives of Methoxyphenylpiperazine via GC-MS and GC-IR**

Randall Clark¹, Younis Abiedalla² ¹*Auburn Univ.*, ²*Auburn University*

(Wed-P19) **Controlled Reaction Dynamics of Binary Hexafluorides to Explore New Chemical Signatures**

Austin L. Dorris¹, Louis McNamara¹, John T. Kelly², Abigail M. Waldron¹ ¹*Savannah River National Laboratory*, ²*SRNL, DOE*

(Wed-P20) **Method for pretreating blood in ethyl glucuronide(EtG) and ethyl sulfate(EtS) analysis**

Young-Hoon Jo¹, Miyeon Lee¹, Doyeon Lee¹, Min-Hui Son¹, Hyun Jee Kim¹ ¹*National Forensic Service*

(Wed-P21) **Forensic utility of carboxyhemoglobin levels in postmortem spleen specimens in South Korea**

Miyeon Lee¹, Young-Hoon Jo¹, Doyeon Lee¹
¹*National Forensic Service*

(Wed-P22) **Direct Analysis Of Glass Powder On Bullets by Laser Ablation ICP-MS**

Summer Garcia¹, Stan Holenda², Shirly Montero¹
¹*Arizona State University*, ²*Serva Energy*

(Wed-P23) **Improving the Classification of Natural and Synthetic Diamonds Using Fluorescence Analysis and Classification Models**

Niloufar Yavari¹, Elizabeth Shade², Daniel Sturmer², Craig Dietsch², Pietro Strobbia¹
¹*University of Cincinnati*, ²*Department of Geosciences|University of Cincinnati*

(Wed-P24) **Determining the Limit of Detection for a Universal Body Fluid Identification Method**

Riley Alpuché¹, Benjamin Taubner¹, Nathaniel Cady¹, Igor K. Lednev¹ ¹*University at Albany, SUNY*

(Wed-P29) **Removal of Allergenic Protein from Peanuts using Beaded Particles**

Nicholas C. Bright¹, Anselm Omoike² ¹*USC Upstate*, ²*University of South Carolina Upstate*

(Wed-P30) **Hyperspectral infrared (IR) absorption imaging with fluorescence photothermal detection**

Caitlin E. Dunlap¹, Gwendylan Turner¹, Aleksandr Razumtcev¹, Minghe Li², Michelle Cousineau¹, Daniel Herman³, Markus Mangold⁴, Lynne S. Taylor¹, Garth J. Simpson¹ ¹*Purdue University*, ²*Purdue University*, ³*IR Sweep*, ⁴*IR Sweep*

(Wed-P31) **FTIR microspectroscopy as a tool to elucidate the interaction between microplastics and mammalian cells**

Helena Friedrich¹, Sirawut Tubtim¹, Eric Auyang², Stephanie Wright², Hendrik Vondracek³, Gianfelice Cinque³, Ka Lung Andrew Chan¹
¹*King's College London*, ²*Imperial College London*, ³*Diamond Light Source*

(Wed-P32) **Environmental contributions and non-sample related impacts on the spectra from a handheld diffuse reflectance spectrometer**

Daniel Highland¹, Matthew Eady², David Jenkins² ¹*FHI 360*, ²*FHI360*

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Wednesday Poster Sessions | 9:30 AM – 10:30 AM | *Exhibit Hall B*

(Wed-P34) **Early Landmark Contributions to the Development of Infrared Spectroscopy at the Stamford CT R&I Labs**

Peter J. Larkin

(Wed-P36) **Investigating Structural and Vibrational Properties of Metal-Imidazole Complexes**

Dale L. Perry¹, Nataliya Kalashnyk², Stephanie Belin³, V. Ivanov⁴, Eric Faulques⁵ ¹*Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720 USA*, ²*Univ. Lille, CNRS, Centrale Lille, Univ. Polytechnique Hauts-de-France, UMR 8520 -IEMN – Institut d'Electronique, de Microélectronique et de Nanotechnologie, F-59000 Lille, France*, ³*Synchrotron SOLEIL, L'Orme des Merisiers, BP48, 91192 Gif-sur-Yvette Cedex, France*, ⁴*Faculty of Physics, University of Sofia, 5 James Bourchier Blvd, BG1147 Sofia, Bulgaria*, ⁵*Univ. Lille, CNRS, Centrale Lille, Univ. Polytechnique Hauts-de-France, UMR 8520 -IEMN, F-59000 Lille, France*

(Wed-P37) **Towards a quantitative interpretation of the vibrational spectra of iron oxide nanoparticles**

Mireia Sainz¹, Iñigo González de Arrieta¹, Telmo Echániz², Karam Nader³, Maite Insausti⁴, Gabriel Alejandro López¹ ¹*Physics Department, University of the Basque Country (UPV/EHU), E-48940 Leioa, Spain*, ²*Applied Mathematics, University of the Basque Country (UPV/EHU), E-48013 Bilbao, Spain*, ³*Organic and Inorganic Chemistry, University of the Basque Country (UPV/EHU), E-48940 Leioa, Spain*, ⁴*Organic and Inorganic Chemistry, University of the Basque Country (UPV/EHU), E-48940 Leioa, Spain*. *BCMaterials, Basque Center for Materials, Applications and Nanostructures, UPV/EHU Science Park, 48940 Leioa, Spain*

(Wed-P39) **Expanding the addressable chemical space with libraries of computed spectra**

Michelle D'Souza¹, Calvin Stevenson¹, Ty Abshear¹, Graeme Whitley¹ ¹*Wiley*

(Wed-P40) **Determining Absolute Configuration of Pharmaceutical Compounds Using Vibrational Circular Dichroism**

Laura Swanhall¹, Akshar Gupta¹ ¹*Vertex Pharmaceuticals*

(Wed-P43) **Mahina Color Camera: A Framing Multispectral Imager for Lunar Applications**

Jonathan Herringer¹, David Blewett², Brett Denevi², Heather Meyer², Charles Hibbitts², Stanley Ikpe², Bryan Maas², Shaughn London² ¹*Torrent Photonics LLC*, ²*Space Exploration Sector, Johns Hopkins University Applied Physics Laboratory*

(Wed-P41) **Investigating Gas Dynamics and Reactions in Supersonic Jets**

Abigail M. Waldron¹, Austin L. Dorris¹, John Kelly¹, Louis McNamara¹ ¹*Savannah River National Laboratory*

(Wed-P42) **Application of infrared spectroscopy technology in the authentication and quality screening of Pisco distillates**

Yalan Wu¹ ¹*The Ohio State University*

(Wed-P44) **Emergent Surface-Specificity in Incoherent Spectroscopy of Ordered Chiral Assemblies**

Garth J. Simpson¹ ¹*Purdue University*

(Wed-P45) **Synthesis and biological evaluation of orally active anti-Trypanosoma agents**

Fatma M. Salem¹, Eman Mohamed¹, Bin Su¹ ¹*Cleveland State University*

(Wed-P46) **Formation of an unreported form of methemoglobin from deoxyhemoglobin during thermal treatment**

Alessandro Bossi¹, Paola Saccomandi², Antonio Pifferi¹ ¹*Politecnico di Milano, Dipartimento di Fisica*, ²*Politecnico di Milano*

(Wed-P47) **Assessing the Efficacy of Near Infrared Spectroscopy to Monitor the Maturation of Intraoral Bone Grafts**

Rocco A. Di Pede¹, Nancy Pleshko² ¹*Temple University*, ²*Department of Bioengineering, Temple University*

(Wed-P48) **Development of a Low-Cost Cartilage Optical Phantom for Vis-NIR Fiber Optic Probe Spectroscopy Validation**

Shu-jin Kust¹, Nancy Pleshko² ¹*Temple University*, ²*Department of Bioengineering, Temple University*

(Wed-P49) **High precision measurements of molecular terrains: local conformation, energetics, and thermostability in biomolecular complexes**

Hao-Che Peng¹, Isaiah Odeyemi², Allison L. Stelling³ ¹*unclear*, ²*UT Dallas*, ³*UT Arlington*

(Wed-P50) **Molecular Sensing using Silicon Photonic-based Chip**

Lamyaa Almeahadi¹ ¹*MIT*

(Wed-P51) **Effects of CBN-Binding on DNA Aptamer Higher Order Structure Analyzed by Circular Dichroism Spectroscopy**

Forrest R. Empey-Kohl¹, Satoko Suzuki², Ai Yamane³, Taiji Oyama³, Ken-ichi AKAO², Takehiko Wada⁴ ¹*Jasco Inc*, ²*JASCO Corporation*, ³*Jasco Corporation*, ⁴*Tohoku University*

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Wednesday Poster Sessions | 9:30 AM – 10:30 AM | *Exhibit Hall B*

(Wed-P52) Revolutionizing Blood Banking: Exploring the Benefits of Normoglycemic Storage Techniques

Morgan Geiger¹, Logan D. Soule¹, Stephen Branch¹, Yunong Wang², Lane Baker², Dana Spence¹ ¹Michigan State University, ²Texas A&M

(Wed-P53) Characterization of Electrochemical Aptamer-Based Sensors for the Detection of Neuropeptide Y

Hailey Pruitt¹, Evelyn Carreto Guevara², Rebecca Y. Lai² ¹Department of Chemistry and Biochemistry, University of North Georgia, ²Department of Chemistry, University of Nebraska-Lincoln

(Wed-P54) Metformin Enhances Fructose Uptake and Catabolism in Mouse Intestine and Mitigates Hepatic Steatosis

Joshua C. Hartsell¹, Grace Scheidemantle¹, Mareca Lodge¹, Dalton Hilovsky¹, Arion Kennedy¹, Xiaojing Liu¹ ¹North Carolina State University

(Wed-P55) SpectroChip: An Optical System-on-Chip Enabling Ultra-portable Devices for Broad Industrial Sensing Applications

Xiaoxu Sean Lin¹, Jyun-Wei Wen², Chitsung Hong², Margaret Jiang¹, Cheng-Hao Ko² ¹SPU Optics Inc, ²Spectrochip Inc

(Wed-P56) Bugs as Drugs: Vehicles for Cancer Therapeutics

Jianen Lyu¹, Wyatt Paulishak², Michael VanNieuwenhze³, Laurence Wood² ¹Indiana University, ²Texas Tech University Health Science Center, ³Baylor University

(Wed-P57) Electron-Multiplying Cameras Increase Sensitivity in High-Speed Coherent Anti-Stokes Raman Scattering Imaging

Adam J. Wise¹, Yusuke Murakami², Niels Klement³, Wesley Browne³, Hideaki Kano² ¹Oxford Instruments Andor, ²Kyushu University, ³University of Groningen

(Wed-P59) Atomic Force Microscope-Infrared Spectroscopy as a Powerful Tool to Study the Distribution of Fluticasone Propionate/Salmeterol Xinafoate/Lactose Monohydrate in Advair Diskus 100/50 Formulations.

Blessy Joseph¹, Dipesh Khanal², Elizabeth R. Bielski³, Bryan Newman³, Huzeyfe Yilmaz⁴, Snober Ahmed⁵, Susan Boc³, Hak-Kim Chan⁶, Mark M. Banaszak Holl⁷ ¹Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA, ²The University of Sydney, ³Division of Therapeutic Performance I, Office of Research and Standards, Office of Generic Drugs, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, Silver Spring, MD, USA, ⁴US Food & Drug Administration, ⁵Division of Pharmaceutical

Quality Research II, Office of Pharmaceutical Quality Research, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO, USA, ⁶Advanced Drug Delivery Group, Sydney Pharmacy School, Faculty of Medicine and Health, The University of Sydney, NSW, Australia, ⁷Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA Division of Pulmonology, Allergy, and Critical Care Medicine, Heersink School of Medicine, University of Alabama at Birmingham, Birmingham, USA

(Wed-P60) Near-infrared transmission spectrometer system for rapid inspection of tablet samples

Kazuhiko Fujiwara¹, Masashi Fukuhara¹, Hiroshi Satozono¹ ¹Hamamatsu Photonics

(Wed-P61) Considerations for Analytical Methods used in Cleaning Validation of Advanced Therapy Medicinal Products

Brian Bosso¹ ¹STERIS Corp

(Wed-P62) Simultaneous Separation of Cardiovascular Medications in Their Combination Drugs Using Micellar Liquid Chromatography

Ibrahim A. Alothaim¹, Yahya M. ALSHEHRY¹ ¹Saudi Food and Drug Authority

(Wed-P63) Innovative Measurement approaches in UV VIS for Biotech downstream process analysis

Fabien Chauchard¹, Davinia Brouckaert² ¹INDATECH CHAUVIN ARNOUX, ²INDATECH

(Wed-P64) Raman-based bioprocess control with

generalizable de novo multivariate modeling

Christopher D. Brown¹, Colin Gavin¹, Steve Driscoll¹, Morgan Siegmann¹ ¹908 Devices

(Wed-P65) Tuberculosis medications and non-destructive compliance screening with comparison of handheld and benchtop diffuse reflectance spectrometers

Matthew Eady¹, Daniel Highland², David Jenkins¹ ¹FHI360, ²FHI 360

(Wed-P66) Comparison of Generic and Name Brand Dry Powder Inhalers: Advanced Insights Using Optical Photothermal Infrared Microscopy

Sheikh Tanzina Haque¹, Blessy Joseph¹, Elizabeth R. Bielski², Bryan Newman², Huzeyfe Yilmaz³, Snober Ahmed⁴, Susan Boc², Dipesh Khanal⁵, Hak-Kim Chan⁶, Mark M. Banaszak Holl⁷ ¹Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA, ²Division of Therapeutic Performance I, Office of Research and Standards, Office of Generic Drugs, Center for Drug Evaluation and Research, U.S.

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Wednesday Poster Sessions | 9:30 AM – 10:30 AM | *Exhibit Hall B*

Food and Drug Administration, Silver Spring, MD, USA, ³US Food & Drug Administration, ⁴Division of Pharmaceutical Quality Research II, Office of Pharmaceutical Quality Research, Office of Pharmaceutical Quality, Center for Drug Evaluation and Research, U.S. Food and Drug Administration, St. Louis, MO, USA, ⁵The University of Sydney, ⁶Advanced Drug Delivery Group, Sydney Pharmacy School, Faculty of Medicine and Health, The University of Sydney, NSW, Australia, ⁷Department of Mechanical and Materials Engineering, University of Alabama at Birmingham, Birmingham, USA Division of Pulmonology, Allergy, and Critical Care Medicine, Heersink School of Medicine, University of Alabama at Birmingham, Birmingham, USA

(Wed-P67) Validation of a Combined Thin-Layer Chromatography/Digital Image Analysis Method using ImageJ for the Quantitation of Metronidazole in Tablets

Christopher L. Harmon¹, Sean Butts², Mary Beth Sowers¹, Ed Bethea¹, David Jenkins¹ ¹FHI360, ²FHI360, North Carolina State University

(Wed-P68) Particle tracking analysis and Raman microspectroscopy for the characterization of different lipid nanoparticle formulations

Maximilian J. Huber¹, Henry Dehne², Julia Klüpfel³, Natalia P. Ivleva¹ ¹Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry, ²Particle Metrix GmbH, ³ISAR Bioscience GmbH

(Wed-P69) Enhancing bioprocess monitoring: Optimization of time gate in timegated Raman spectroscopy for accurate metabolite detection in high cell density perfusion process

Jacopo Zini¹, Mari Tenhunen¹, Amuthachelvi Daniel¹ ¹Timegate Instruments Oy

(Wed-P70) A novel instrument platform for structure identification, process optimization, and impurity monitoring with molecular rotational resonance spectroscopy

Justin L. Neill¹, Alex Mikhonin¹ ¹BrightSpec, Inc.

(Wed-P72) Shining Light on Pharma: The Raman Microscopy Advantage

Samantha Redes¹, Angela Flack¹ ¹Edinburgh Instruments

(Wed-P73) Observation of solid-state structure transition at room temperature by frequency-domain terahertz spectroscopy, DSC and PXRD

Kei Shimura¹, Kenji Aiko¹, Mizuki Mohara¹, Hiroki Ohshima², Ryuta Koike² ¹Hitachi High-Tech Corporation, ²Mitsubishi Tanabe Pharma Corporation

(Wed-P75) Characterization of drug-polymer miscibility in amorphous solid dispersion (ASD) systems using sub-micron IR (O-PTIR) spectroscopy and imaging

Miriam Unger¹, Mustafa Kansiz², Eoghan Dillon³ ¹Photothermal Spectroscopy Corporation, ²Photothermal Spectroscopy Corp., ³Photothermal Spectroscopy Corp

(Wed-P76) Identification of A Trace Impurity in TFA by UPLC-PDA-MS and SPME-GC-MS

Mark Wang¹, Scott Huffman¹, Ravi Kalyanaraman¹ ¹Bristol Myers Squibb

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

24AES07: Commercialization & Industry Applications 306C

Chair: Rafael Davalos, Georgia Tech
Co-Chair: Lexi Crowell-Simpkins, University of California,
Irvine

10:30 AM (AES-07.1) Acoustofluidics: merging acoustics and fluid mechanics for biomedical applications

Tony Jun Huang¹ ¹Duke University

10:50 AM (AES-07.2) Adaptive, In-Situ 3D Printing Using Multiphase Microfluidic Control Enables Multi-Material Integration in Electrokinetic Ionic Circuits

Guillermo Ramirez¹, Gabriel Garibaldi¹,
Gongchen Sun¹ ¹University of Texas at San Antonio

11:10 AM (AES-07.3) Electrical biomarkers in blood

Erin Henslee¹ ¹Wake Forest University

11:30 AM (AES-07.4) Machine learning-driven analysis of electrochemical measurements for improved predictions in a microfluidic sensor.

Sreerag Kaalivectil¹, Nellone Reid¹, Joshua Young¹, Sagnik Basuray¹ ¹New Jersey Institute of Technology

11:50 AM (AES-07.5) Label-Free Cell Enrichments on the CytoR1: Improving Viability, Sustaining Phenotype, and Maximizing Cell Recovery

Alexandra R. Hyler¹, Dean E. Thomas¹,
Kyle S. Kinskie¹, Kyle M. Brown², Josie L. Duncan³, Rafael V. Davalos³, Nathan S. Swami⁴
¹CytoRecovery, Inc., ²Cytorecovery, ³Georgia Tech, ⁴University of Virginia

24ATOM09: Non-traditional Plasmas | 305A

Chair: Ken Marcus, Clemson University

10:30 AM (ATOM-09.1) The Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD) Microplasma Ionization Source: Large Levels of Versatility in a VERY Small Package

R. Kenneth Marcus¹ ¹Clemson University

10:50 AM (ATOM-09.2) Plasma Assisted Reaction Chemical Ionization: An Adaptable Strategy for Elemental MS

Kaveh Jorabchi¹, Frenio Redeker¹, Jordan L. Tanen¹, Kelsey O'Malley¹, William McMahon¹
¹Georgetown University

11:10 AM (ATOM-09.3) Analyte Incorporation Studies in the Scgd Using Atomic Absorption Detection

Jaime Orejas¹, Yinchenxi Zhang¹, María del Mar Gonzalez del Campo¹, Jorge Pisonero¹, Nerea Bordel¹ ¹University of Oviedo

11:30 AM (ATOM-09.4) Elemental and Isotopic Analysis with Solution-Cathode Glow Discharge Mass Spectrometry for Geochronological Dating

Jared Viggers¹, Jacob T. Shelley¹, Garrett M.

MacLean¹ ¹Rensselaer Polytechnic Institute
11:50 AM (ATOM-09.5) A Case Study for a High-Resolution Mass Spectrometry Approach: The Determination of Neodymium Isotope Ratios with the Liquid Sampling –Atmospheric Pressure Glow Discharge (LS-APGD) Ion Source Coupled with an Orbitrap

Suraj Shrestha¹, Joseph V. Goodwin¹, Benjamin T. Manard², Brian Ticknor², Paula Cable-Dunlap², R. Kenneth Marcus¹ ¹Clemson University, ²Oak Ridge National Laboratory

24ATOM12: Novel Approaches to and Applications of LIBS 302B

10:30 AM (ATOM-12.1) Lunar Surface Exploration with Laser-Induced Breakdown Spectroscopy (LIBS)

Samuel M. Clegg¹, Kelsey L. Williams¹, Ronald K. Martinez¹, Carey Legett¹ ¹Los Alamos National Laboratory

10:50 AM (ATOM-12.2) LIBS Plasmas on Mars: Temperature and Electron Density with SuperCam over a large range of distances, rock compositions, and morphologies

Henry Manelski¹, Roger Wiens¹, Susanne Schröder², Bruno Bousquet³, Peder Hansen², Anthony Nelson⁴, Samuel M. Clegg⁴, Ronald Martinez⁴, Noah Martin⁴, Ann Olilla⁴, Agnes Cousin⁵ ¹Purdue University, ²Deutsches Zentrum für Luft- und Raumfahrt (Berlin), ³University of Bordeaux, ⁴Los Alamos National Laboratory, ⁵Institut de Recherche en Astrophysique et Planetologie

11:10 AM (ATOM-12.3) Is LIBS ready for the future? The potential impact of today's technology to tackle tomorrow's material flows

Jens Riedel¹, Yi You¹, Simon Blume¹, Li Xunyu²
¹Federal Institute for Materials Research and Testing (BAM), ²BAM

11:30 AM (ATOM-12.4) High-resolution measurements of uranium using tunable laser absorption spectroscopy of laser produced plasmas

Ryland G. Wala¹, Mathew P. Polek², Sivanandan S. Harilal³, R. Jason Jones⁴, Mark C. Phillips⁴
¹University of Arizona, ²University of California, San Diego, ³Pacific Northwest National Laboratory, ⁴The University of Arizona

11:50 AM (ATOM-12.5) Improving analytical merits of laser-induced breakdown spectroscopy of hydrogen isotopes using an orthogonal double-pulsing scheme

Elizabeth J. Kautz¹, Mathew P. Polek², Ewa Rönnebro³, Sivanandan S. Harilal³ ¹NC State University, ²University of California, San Diego, ³Pacific Northwest National Laboratory

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Oral Symposia | 10:30 AM – 12:10 PM | *Various Locations*

24AWD03: ACS Analytical Division Award in Spectrochemical Analysis Award Session | 301B

Campbell¹ ¹University of Edinburgh, ²University of Glasgow

Chair: Ji-Xin Cheng, Boston University

10:30 AM (AWD-03.1) **Advancing spectroscopic imaging by probing complementary absorption and scattering vibrational modes**

Delong Zhang¹, Pengcheng Fu¹, Yongqing Zhang¹, Hyeon Jeong Lee¹ ¹Zhejiang University

10:50 AM (AWD-03.2) **Functional Bond-Selective Microscopy for Subcellular Biology at the Single-Molecule Level**

Lu Wei¹ ¹California Institute of Technology

11:10 AM (AWD-03.3) **Hyperspectral IR absorption imaging with fluorescence photothermal detection**

Garth J. Simpson¹ ¹Purdue University

11:50 AM (AWD-03.5) **Surface-Area Enhanced Raman Spectroscopy of DNA: A Quantitative and Reproducible Alternative to Plasmonic-Based SERS**

Grant J. Myres¹, Jay P. Kitt¹, Joel M. Harris²
¹University of Utah - Chemistry, ²University of Utah

24BIM04: Optical Point-of-Use Technologies for Automated Biomedical and Life-Sciences Analysis | 302A

Chair: Ute Neugebauer, Friedrich Schiller University Jena

10:30 AM (BIM-04.1) **In vivo flow cytometry: blood cell analysis without drawing blood**

Charles P. Lin¹ ¹Massachusetts General Hospital, Harvard Medical School

10:50 AM (BIM-04.2) **Ex vivo label-free immune cell analysis**

Ute Neugebauer¹, Max Naumann², Rustam Guliev², Leah Haase², Simone Eiserloh², Oleg Ryabchykov³, Uwe Glaser², Ignacio Rubio⁴, Thomas W. Bocklitz⁵, Iwan Schie², Juergen Popp², Aikaterini Pistiki², David Vazquez Pinzon²
¹Friedrich Schiller University Jena, ²Leibniz Institute of Photonic Technology, ³Photonic Data Science department, Leibniz Institute of Photonic Technology, Jena, Germany, ⁴Jena University Hospital, ⁵Leibniz Institute of Photonics Technology

11:10 AM (BIM-04.3) **Fluorescent probes for real-time bacterial detection**

Mark Bradley¹ ¹Queen Mary University of London, PHURI

11:30 AM (BIM-04.4) **New High-Throughput Liquid Screening Devices Based on Raman Spectroscopy**

Ryan Senger¹, Amr Sayed-Issa¹, John Robertson²
¹Virginia Tech, ²Rametrix Technologies, Inc.

11:50 AM (BIM-04.5) **Incorporation of Optical Biosensors into a Live Cystic Fibrosis (CF) Airway-on-chip Device to Study Therapy Response**

Bilgi Kip¹, Vinayak Nirmale¹, Prasad Aradhya¹, Robert Gray², Norbert Radacsi¹, Colin J.

24FORENS03: Forensics Analysis in the Lab and at the Crime Scene | 303

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

Co-Chair: Marisia Fikiet, University of New Haven

10:30 AM (FORENS-03.1) **Forensic Science R&D Funding Programs at the National Institute of Justice**
Frances Scott¹, Greg Dutton¹ ¹National Institute of Justice

10:50 AM (FORENS-03.2) **A critical evaluation of miniaturized Near-Infrared and Raman Spectrophotometers in Forensic Analytical Science**
Christian W. Huck¹ ¹University of Innsbruck

11:10 AM (FORENS-03.3) **Exploring bloodstain aging on interfering substrates exposed to stimulated indoors and outdoors environmental conditions by ATR-FTIR spectroscopy**

Entesar Alhetlani¹, Mohamed O. Amin², Meshari Al-Qalfas¹, Salma Alantari¹, Igor K. Lednev³
¹Kuwait University, ²University at Albany, ³University at Albany, SUNY

11:30 AM (FORENS-03.4) **Investigating Counterfeit Cannabis Edibles using Vibrational Spectroscopy**

Marisia A. Fikiet¹, Lindsey B. Weinger², Jill Carreiro³, Jeff Rawson⁴, Josep DeAlcaraz-Fossoul¹, Richard A. Crocombe, Pauline E. Leary⁵, Brooke W. Kamrath ¹University of New Haven, ²Platinum CEM, ³Carriero Consulting, ⁴Institute of Cannabis Science, ⁵Noble, Inc.

11:50 AM (FORENS-03.5) **Unmasking Gunshot Residue Deposition and Transference Mechanisms using Laser Sheet Scattering, High-speed Videography, Atmospheric Particle Analysis, and Spectrometric Analytical Techniques**

Thomas D. Ledergerber¹, Kourtney Dalzell¹, Matthew Staymates², Luis Arroyo¹, Tatiana Trejos¹ ¹West Virginia University, ²National Institute of Standards and Technology

24IR07: Advances in nanoscale spectroscopy from mid-IR to beyond | 301A

Chair: Andrea Centrone, NIST

10:30 AM (IR-07.1) **Recent Development of Simultaneous AFM-IR and Kelvin Probe Force Microscopy**

Xiaoji Xu¹, Amirhossein Zahmatkeshsaredorahi², Devon Jakob¹ ¹Lehigh University, ²Lehigh University

10:50 AM (IR-07.2) **Understanding Signal Intensity and Spatial Resolution in Resonance-Enhanced AFM-**

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IR: Experimental and Theoretical Insights.

Andrea Centrone¹, Jeffrey Schwartz¹, Devon Jakob¹, Georges Pavlidis¹ ¹NIST

11:10 AM (IR-07.3) **Understanding the AFM-IR signal**

Georg Ramer¹, Yide Zhang¹, Ufuk Yilmaz¹, Bernhard Lendl¹ ¹TU Wien

11:30 AM (IR-07.4) **Customized infrared nanospectroscopy platform to monitor electric-field induced effects**

Valeria Giliberti¹, Maria Eleonora temperini², Raffaella Polito², Tommaso Venanzi³, Leonetta Baldassarre², Huatian Hu⁴, Cristian Ciraci⁴, Marialilia Pea⁵, Andrea Notargiacomo⁵, Francesco Mattioli⁵, Michele Ortolani² ¹Italian Institute of Technology, Center for Life Nano- & Neuro-Science, ²Physics Department, Sapienza University of Rome, ³Italian Institute of Technology, Center for Life Nano- and Neuro-Science, ⁴Italian Institute of Technology, Center for Biomolecular Nanotechnologies, ⁵IFN-CNR

24MASS05: Novel Instrumentation, Analysis Tools, and Chemistry in Mass Spectrometry | 306A

Chair: Jacob Shelley, Rensselaer Polytechnic Institute

10:30 AM (MASS-05.1) **Unintended ion-molecule reactions between residual water and indazole-containing fragments of synthetic cannabinoids in tandem mass spectrometry.**

Glen P. Jackson¹, McKenna R. Oaks¹, Emanuel Ubana², Fabien Goulay², Christopher S. Poulos² ¹West Virginia University, ²WVU

10:50 AM (MASS-05.2) **Handheld mass spectrometry analysis of surface-dwelling and airborne fentanyl analogs and CWA**

Christopher D. Brown¹, Matt Aernecke¹, Robert Green¹ ¹908 Devices

11:10 AM (MASS-05.3) **Analysis of Petroleum Nitrogen Compounds Using Tandem Mass Spectrometry**

Jaya Paudel¹, Dylan Carter¹, Lauren Davis¹, Benjamin Bythell¹, Peter de Boves Harrington¹ ¹Ohio University

11:30 AM (MASS-05.4) **Cheminformatics tools and chemistry data underpinning mass spectrometry analyses at the US Environmental Protection Agency**

Antony J. Williams¹ ¹United States Environmental Protection Agency

11:50 AM (MASS-05.5) **Virtual Slit Cycloidal Mass Spectrometry for Isotopic Measurements of Actinide Particles**

Rafael Bento Serpa¹, Charles B. Parker¹, Elizabeth D. LaBone², Christopher A. Zarzana³, Justin Keogh⁴, Jonathon Andrus³, Nathan Stevens³, Rosalie Greer², Kyle Samperton², Danielle Mannion², Joseph Mannion², Glass T. Jeffrey¹, M. Bonner Denton⁴, Jason J. Amsden¹ ¹Duke University, ²Savannah River National

Laboratory, ³Idaho National Laboratory, ⁴University of Arizona

24PAT04: In Situ Spectroscopy for industrial R&D | 302C

Chair: Mark Rickard, DuPont

10:30 AM (PAT-04.1) **In-situ Raman Spectroscopy Enable Safe Process Scale-Up**

Xiaoyun (Shawn) Chen¹, Michael Telgenhoff², Brian Rekken³ ¹Dow Chemical, ²Dow, ³dow

10:50 AM (PAT-04.2) **Preprocessing Vibrational Spectra Containing Overlapping Non-target Peaks in Nuclear Waste Process Monitoring**

Steven H. Crouse¹, Ronald Rousseau¹, Martha Grover¹ ¹Georgia Institute of Technology

11:10 AM (PAT-04.3) **Rapid Screening of feedstock using spectroscopy, chemometrics and machine learning (ML)**

Yusuf Sulub¹ ¹SABIC

11:30 AM (PAT-04.4) **Circular economy in the pulp and paper industry promoted by process intensification**

Karin Wieland¹, Miranda Eisenköck¹, Barbara Weiß¹, Anna Katharina Schwaiger², Wolfgang Fuchs², Bernhard Lendl³, Michael Harasek³ ¹Competence Center CHASE GmbH, ²Sappi Europe, ³TU Wien

11:50 AM (PAT-04.5) **PAT Discussion Panel: Technology, Best Practices, Current Challenges, and Future Developments**

24PMA07: Frontiers in Drug Sensing and Nanoendoscopic Theragnostic | 306B

Chair: Malama Chisanga, University of Montreal

10:30 AM (PMA-07.1) **Advancing Point-of-care Therapeutic Drug Monitoring with Surface-enhanced Raman Spectroscopy**

Yaman Goksel¹, Gohar Soufi¹, Roman Slipets¹, Isidro Badillo Ramirez¹, Anja Boisen¹ ¹Technical University of Denmark

10:50 AM (PMA-07.2) **Quantitative SERS analysis of drug precursors**

Li-Lin Tay¹ ¹National Research Council Canada

11:10 AM (PMA-07.3) **The integration of electrophysiology and Raman spectroscopy as a novel label-free platform for structural and functional toxicity**

Christian Tentellino¹, Marta D'Amora², Rustamzhon Melikov¹, Giuseppina Iachetta¹, Giulia Bruno¹, Francesco Tantussi¹, Michele Dipalo¹, Francesco De Angelis¹ ¹Italian Institute of Technology, ²Italian Institute of Technology and University of Pisa

11:30 AM (PMA-07.4) **Integrating Vibrational Spectroscopy and Machine Learning for Fentanyl Screening from Human Nails**

Lenka Halamkova¹, Aubrey Barney¹, Jeremy Lawrence¹ ¹Texas Tech University

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11:50 AM (PMA-07.5) **Surface Enhanced Raman Spectroscopy for Field Forward Forensics of Fentanyl Laced Illicit Pills**

Phillip G. Wilcox¹, Ashish Tripathi¹, Erik D. Emmons¹, Roberta Xega¹, Elizabeth Dhummakupt¹, Bruce King¹, Daniel Carmany², Andrew Walz¹, Neal Kline¹, Emily Lockhart³, Joseph Bozenko³, Jason Guicheteau¹ ¹*U.S. Army DEVCOM Chemical Biological Center*, ²*Excet, Inc.*, ³*U.S. Drug Enforcement Administration*

24SPECIAL04: Spectrochimica Acta Part B award | 305B

Chair: Alessandro De Giacomo, University of Bari

10:30 AM (SPECIAL-04.1) **Laser-induced XUV spectroscopy: From fundamentals to application for high-precision LIBS**

Daive Bleiner¹ *Empa*

10:50 AM (SPECIAL-04.2) **DIAGNOSIS AND CORRECTION METHODS FOR SPECTRAL INTERFERENCE IN THE FRAMEWORK OF LIBS IMAGING**

Ludovic Duponchel¹, Vincent Motto-Ros²
¹*University of Lille*, ²*ILM*

11:10 AM (SPECIAL-04.3) **Atmospheric pressure plasma discharges as hydride atomizers for trace element analysis by atomic spectrometry**

Jan Kratzer¹ *Czech Academy of Sciences, Institute of Analytical Chemistry*

11:30 AM (SPECIAL-04.4) **The current role of X-ray fluorescence spectrometry in the analytical chemistry field: an overview of recent trends and applications**

Eva Margui¹ *University of Girona*

11:50 AM (SPECIAL-04.5) **Glow discharge emission spectroscopy: how useful, how exciting!**

Zdenek Weiss¹ *FZU - Inst. of Physics of the Czech Academy of Sciences*

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Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

24AES08: Future 50: AES Innovations | 306C

Chair: Soumya Srivastava, West Virginia University
Co-Chair: Guillermo Ramirez, University of Texas at San Antonio

1:30 PM (AES-08.1) **Dielectric behavior of cells exposed to simulated microgravity**

Sai Deepika Reddy Yaram¹, Soumya K. Srivastava¹ *West Virginia University*

1:50 PM (AES-08.2) **Electrospun nanofiber mats for micro/nanoscale electrokinetics**

Tonoy K. Mondal¹, Jacob West¹, Stuart J. Williams¹ *University of Louisville*

2:10 PM (AES-08.3) **Pneumatic Circuit Modeling and Design for Plug-and-Play Microfluidics and Biosensing Applications**

Christopher J. Easley¹, Joanne Y. Seow¹, Md Mohibullah¹, Sabita Dangol¹, Joshua G. Howell¹ *Auburn University*

2:30 PM (AES-08.4) **A Novel Dielectrophoretic-based Microfluidic Diagnostic Tool for Stage IV Breast Cancer using PBMCs**

Christopher J. Smith¹, Raphael O. Oladokun¹, Timothy Eubank¹, Soumya K. Srivastava¹ *West Virginia University*

2:50 PM (AES-08.5) **A modular, point-of-care, microfluidic bio-detection system for zoonotic diseases**

Niranjana Haridas Menon¹, Yu hsuan Cheng¹, Autumn Maruniak², Brady Clapsaddle², Girish Srinivas², Sagnik Basuray¹ ¹*New Jersey Institute of Technology*, ²*TDA Research*

24ATOM08: sp- and sc-ICP-MS | 305A

Chair: Antonio Montoro Bustos, NIST

1:30 PM (ATOM-08.1) **Transport efficiency assessment for nanomaterials characterization by means spICPMS: still an unsolved problem**

Guillermo Grindlay¹, Daniel Torregrosa¹, Luis Gras¹, Juan Mora¹ *University of Alicante*

1:50 PM (ATOM-08.2) **Improved sensitivity: A key for accurate sc-ICP-MS characterization of cell populations**

Beatriz Fernández¹, Paula Menero Valdés¹, Alicia Villa-Vazquez¹, Lydia Álvarez², C. Derrick Quarles Jr.³, Héctor González-Iglesias⁴, Rosario Pereiro¹ ¹*University of Oviedo*, ²*Instituto Oftalmológico Fernández-Vega*, ³*Elemental Scientific, Inc.*, ⁴*Instituto de Productos Lácteos de Asturias (IPLA-CSIC)*

2:10 PM (ATOM-08.3) **Studying the degradation and released of plastic particles by SP ICP-MS: method development and applications**

Raquel Gonzalez de Vega¹, Thebny Moro², Bernhard Grüner³, Tatiane de Andrade Maranhão², Maximilian J. Huber⁴, Natalia P. Ivleva⁴, Etienne Skrzypek¹, Joerg Feldmann⁵, David Clases¹ ¹*University of Graz*, ²*Universidade Federal de Santa Catarina*, ³*University of Muenster*, ⁴*Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry*, ⁵*University Of Graz*

2:30 PM (ATOM-08.4) **Using SP ICP-TOF-MS to investigate the roles Hg nanoparticles can play in the**

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

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bioaccumulation of Hg in the ocean

Lhiam Paton¹, Nick Marczinczik², Thomas Lindsay³, Thebny Moro⁴, Raquel Gonzalez de Vega⁵, David Clases⁵, Joerg Feldmann¹
¹University Of Graz, ²University of Muenster,
³University of Aberdeen, ⁴Universidade Federal de Santa Catarina, ⁵University of Graz

2:50 PM (ATOM-08.5) Extending the Linear Dynamic Range of Single Particle ICP-MS for the Quantification of Microplastics

Antonio R. Montoro Bustos¹, George C. Caceres², Monique E Johnson³, John L Molloy³, Sang Bok lee⁴ ¹Guest Researcher, ²NIST/UMD, ³NIST, ⁴UMD

24AWD05: NESAS Lester W. Strock Award Session | 301B

Chair: Benjamin Manard, Oak Ridge National Laboratory

1:30 PM (AWD-05.1) Can Ultra-high Mass Resolution Mass Spectrometry Eliminate Chemical Separations for Isotope Ratio Mass Spectrometry?

R. Kenneth Marcus¹ ¹Clemson University

1:50 PM (AWD-05.2) What Does 15 Years, and Counting, of Collaboration Look Like?

C. Derrick Quarles Jr.¹ ¹Elemental Scientific, Inc.

2:10 PM (AWD-05.3) Electrothermal vaporization (ETV) as a new method for safeguards.

Cole R. Hexel¹, Benjamin T. Manard¹, Cyril Thompson¹, N. Alex Zirakparvar¹ ¹Oak Ridge National Laboratory

2:30 PM (AWD-05.4) Laser ablation-based approaches to the analysis of solid samples: A path to unexpected but lifelong friendships

Jhanis J. Gonzalez¹ ¹Applied Spectra Inc./ Principal Scientific Engineering Associate

2:50 PM (AWD-05.5) Laser-Induced Collaboration - An Overview of Laser Ablation Research at a Multidisciplinary National Laboratory

Hunter B. Andrews¹ ¹Oak Ridge National Laboratory

24CHEM07: Answering Age Old Questions with Data: Chemometrics in Art Conservation | 305B

Chair: Maria Delgado Cornelio, University of Delaware

1:30 PM (CHEM-07.1) Multivariate Classification Techniques for Heritage Scientists

Richard G. Brereton¹ ¹University of Bristol

1:50 PM (CHEM-07.2) Revealing secrets of the past: chemometrics in the study of artistic heritage materials

Marc Vermeulen¹ ¹The National Archives, UK

2:10 PM (CHEM-07.3) Optimization of Gaussian Mixtures Model Factors in Hyperspectral Imaging Data of Archaeological Paintings

Helder V. Carneiro¹, Roxanne Radpour¹, Karl S. Booksh¹ ¹University of Delaware

2:30 PM (CHEM-07.4) Accuracy of Machine Learning Classification Algorithms for Laser-Induced Breakdown Spectroscopy Data in Geological Applications

Prasoon K. Diwakar¹, Jon Kellar¹, Margaret Thompson¹, Samuel E. Kessinger¹, Hunter Paxton¹ ¹South Dakota School of Mines and Technology

3:50 PM (CHEM-07.5) Classification of Pinus ponderosa Ash Origin Using Elemental Fingerprinting and Multivariate Classification

Maria F. Delgado Cornelio¹, Caelin Celani¹, Michael E. Ketterer², James Jordan³, Karl S. Booksh¹ ¹University of Delaware, ²Northern Arizona University, ³United States Geological Survey

24FORENS04: Pharmaceutical Micro and Macro Forensics I | 303

Co-Chair: Ravi Kalyanaraman, Bristol Myers Squibb

Co-Chair: Adam Lanzarotta

1:30 PM (FORENS-04.1) Analytical Field Testing for Rapid Forensic Counterfeit Analysis of Pharmaceuticals

David Ferrizzi¹, Gary Pond¹ ¹Colorcon Inc.

1:50 PM (FORENS-04.2) Spectroscopic sleuthing: the use of vibrational spectroscopy to investigate quality and safety concerns in pharmaceuticals

Stephan Woods¹, Mike Bradley² ¹Thermo Fisher Scientific, ²Thermo Fisher Sci

2:10 PM (FORENS-04.3) Forensic analysis of CAR-T products

Rafael Masitas¹ ¹Bristol Myers Squibb

2:30 PM (FORENS-04.4) Pharmaceutical Forensic Microscopy and Anti-Counterfeit Measures

Dale K. Purcell

2:50 PM (FORENS-04.5) The Analysis of Unknown Particles Isolated from Compounded Pharmaceutical Products Using Optical Microscopy, FT-IR and Raman Micro Spectroscopy.

Mark R. Witkowski¹ ¹US FDA / Forensic Chemistry Center

24IR08: Vibrational Nano-Imaging Of Molecular Structure, Coupling, And Dynamics | 301A

Chair: Markus Raschke, University of Colorado

1:30 PM (IR-08.1) Measuring local chemical environment through infrared nanospectroscopy

Eric A. Muller¹ ¹Colgate University

1:50 PM (IR-08.2) Contactless Quantitative Local Conductivity Imaging of Semiconductor Nanostructures

Joanna M. Atkin¹ ¹University of North Carolina Chapel Hill

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2:10 PM (IR-08.3) **Viewing interfacial chemistry through a graphene window with broadband infrared nanospectroscopy**

Hans A. Bechtel¹ *Lawrence Berkeley National Laboratory*

2:30 PM (IR-08.4) **Quantum vibrational coupling as molecular ruler for nano-imaging from structural disorder to energy dissipation**

Markus Raschke¹ *University of Colorado*

2:50 PM (IR-08.5) **Realization and spatial mapping of strong vibrational coupling to surface phonon polariton near-fields**

Oliver Hirschmann¹, Andrew C. Jones², Wei Xiong³, Wilton Kort-Kamp², Ruggero Emmanuele², Harsh Bhakta⁴ *University of California-San Diego*, ²*Los Alamos National Laboratory*, ³*Univeristy of California- San Diego*, ⁴*University of California San Diego*

24PMA08: Measuring quality in complex raw materials used in biotech and biopharma: spectroscopic methods of analysis | 306B

Chair: Alan Ryder, Nanoscale Biophotonics Laboratory, University of Galway
Co-Chair: Brittany Rauzan

1:30 PM (PMA-08.1) **Collaborative Approaches to Achieve Consistency in Complex Raw Materials**

Chris Wiedel¹, Garrett Tisdell¹ *Nu-Tek BioSciences*

1:50 PM (PMA-08.2) **Heavy Metals in Fertilizer by X-Ray Fluorescence and Atomic Emission Techniques**

Andrew F. Callender¹, Sydney Decatur¹, Bryant J. Davis¹ *Tennessee Technological University*

2:10 PM (PMA-08.3) **Forensic techniques to identify and mitigate particle sources in pharma industry raw materials, drug substances or cell therapies.**

Pascal Chalus¹, Katja Schulze¹, Patrick Favrod¹, Michael Jahn¹, Abbas Razvi¹ *Lonza AG*

2:30 PM (PMA-08.4) **Stability testing of cellulose-based excipients using semi-quantitative spectroscopic and non-linear chemometric methods**

Nirzari Gupta¹, Jason D. Rodriguez¹ *US Food and Drug Administration*

2:50 PM (PMA-08.5) **Analytical efficacy of conventional Raman spectroscopy compared with shifted excitation Raman difference spectroscopy (SERDS) in the presence of dominant/varying fluorescence**

Mahsa Zarei¹, Edward Grant² *University of British Columbia*, ²*Professor*

24RAM08: Raman Imaging/Microscopy/SRS/CARS | 302B

Chair: Katsumasa Fujita, Osaka University

1:30 PM (RAM-08.1) **Current Developments in**

Intraoperative Raman Spectroscopy for Tumor Diagnostics: A Spectral Histopathology Perspective

Juergen Popp¹ *Friedrich Schiller University Jena, Institute of Physical Chemistry and Abbe Center of Photonics*

1:50 PM (RAM-08.2) **Analysis of redox states of cytochromes and myoglobin during the cardiac cycle by combining resonance Raman spectroscopy and tissue cryofixed techniques**

Wenjin Ho¹, Yoshinori Harada¹, Masahito Yamanaka², Yasuaki Kumamoto², Shoko Tamura³, Kentaro Mochizuki¹, Katsumasa Fujita², Hideo Tanaka⁴ *Kyoto Prefectural University of Medicine*, ²*Osaka University*, ³*Tokyo Metropolitan Institute of Medical Science*, ⁴*Kyoto University of Advanced Science, Kyoto Prefectural University of Medicine*

2:10 PM (RAM-08.3) **Correlative quantitative Raman imaging in mouse NASH model reveals direct relationships between diet and resultant liver pathology**

Alison Hobro¹, Takatoshi Sakaguchi¹, Shizuo Akira¹, Nicholas I. Smith² *Osaka University*, ²*Biophotonics Laboratory, Immunology Frontier Research Center, Osaka University*

2:30 PM (RAM-08.4) **Revealing Insights into White and Brown Adipocyte Differentiation through Optical Diffraction Tomography and Raman Spectroscopy**

Pooja Anantha¹, Piyush Raj¹, Zhenhui Liu¹, Ishan Barman¹ *Johns Hopkins University*

2:50 PM (RAM-08.5) **Panel Discussion**

24RAM15: Raman in Regenerative Medicine | 302C

Chair: Ioan Notingher, University of Nottingham

1:30 PM (RAM-15.1) **Raman Spectroscopy for Osteoarthritis Diagnostics and Monitoring Cartilage Regeneration**

Michael Albro¹, Erik Ersland², Dev Mehrotra², Masumeh Kazemi², Madeline Boyes³, Hsin Han⁴, J. Todd Lawrence⁵, Thomas Schaefer³, Mark Grinstaff², Brian Snyder⁶, Mads S. Bergholt⁷ *Boston University, Mechanical Engineering*, ²*Boston University*, ³*University of Pennsylvania*, ⁴*Drexel University*, ⁵*Children's Hospital of Philadelphia*, ⁶*Beth Israel Deaconess Medical Center*, ⁷*King's College London*

1:50 PM (RAM-15.2) **Raman Chemical Imaging as a Tool to Characterize Polymer-based Nanoparticle Gene Delivery Mechanisms in Cells**

David Punihao¹ *University of Vermont*

2:10 PM (RAM-15.3) **Optimisation Of Diffuse Raman Spectroscopy For In-vivo Quantification Of The Fibrotic Tissue Response in Small Animal Models**

Max Jordan Dooley¹, Pavel Matousek², hamid dehghani³, jeni Lucket⁴, amir ghaemmaghami⁵,

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Morgan Alexander⁵, Ioan Notingher⁶ ¹*University of Nottingham*, ²*STFC - UKRI*, ³*University of Birmingham*, ⁴*University of Nottingham*, ⁵*University of Nottingham*, ⁶*University of Nottingham*

2:30 PM (RAM-15.4) Non-destructive Diagnosis of Osteoarthritis with Depth Profiling: Unveiling Cartilage Health through Spatially Offset Raman Spectroscopy

Piyush Raj¹, Lintong Wu¹, Craig Almeida¹, Lauren Conway¹, Swati Tanwar¹, Jill Middendorf¹, Ishan Barman¹ ¹*Johns Hopkins University*

2:50 PM (RAM-15.5) High-throughput cellular imaging with reduced out-of-focus background in multiline illumination Raman microscopy

Tomoaki Okumura¹, Yasuaki Kumamoto¹, Katsumasa Fujita¹ ¹*Osaka University*

24SPR05: Applications of AI in plasmonics | 306A

Chair: Malama Chisanga, University of Montreal

1:30 PM (SPR-05.1) Deep Learning-Assisted Surface Plasmon Resonance Imaging for Enhanced Biosensing and Discrimination of Small Molecules

Thomas Hirsch¹, Simon Jobst², Rudolf Bierl² ¹*University of Regensburg*, ²*Regensburg University of Applied Sciences*

1:50 PM (SPR-05.2) Machine learning tools for plasmonic sensing and synthesis of nanoparticles

Jean-Francois Masson¹, Malama Chisanga², Hannah Williams¹, Saba Bashir¹, Jason Malenfant¹ ¹*Universite de Montreal*, ²*University of Montreal*

2:10 PM (SPR-05.3) Machine Learning Using Convolutional Neural Networks for SERS Analysis of Biomarkers in Medical Diagnostics

Joy Q. Li¹, Priya Dukes¹, Hsin-Neng Wang¹, Aidan J. Canning¹, Alejandro Gaona¹, Bridget M. Monaco¹, Kathrine Garman², Walter Lee², Michael Sarkis¹, Tuan Vo-Dinh¹ ¹*Duke University*, ²*Duke University School of Medicine*

2:30 PM (SPR-05.4) Expediting the Development of SERS Sensors through Machine Learning for Detection of Trace Analytes

Andrea N. Giordano¹, Rahul Rao¹ ¹*Air Force Research Laboratory*

2:50 PM (SPR-05.5) Methods for characterization of wafer scale SERS substrates

Matthew Singer¹, Ryan Priore², Longfei Ye² ¹*Thorlabs Inc.*, ²*Thorlabs Spectral Works*

24SPSJ03: Ultraviolet resonance Raman spectroscopy | 302A

Chair: Igor K. Lednev

Co-Chair: Barbara Rossi, Elettra-Sincrotrone Trieste

1:30 PM (SPSJ-03.1) DUV Resonance Raman effects in water: a probe of H-bonding properties in aqueous media

Barbara Rossi¹, Matteo Tommasini², Paolo Ossi², Marco Paolantoni³ ¹*Elettra-Sincrotrone Trieste*, ²*Politecnico di Milano*, ³*Department of Chemistry, Biology and Biotechnology, University of Perugia*

1:50 PM (SPSJ-03.2) Study on N-acetylamino saccharides with ATR-FUV and UV resonance Raman spectroscopies.

Hidetoshi Sato¹, Kosuke Hashimoto¹, Fatima Matroodi², Barbara Rossi³, Yusuke Morisawa⁴, Yukihiro OZAKI⁵ ¹*School of Biological and Environmental Sciences, Kwansai Gakuin University*, ²*Elettra - Sincrotrone*, ³*Elettra-Sincrotrone Trieste*, ⁴*Kindai University*, ⁵*Kwansai Gakuin University*

2:10 PM (SPSJ-03.3) UV resonance Raman spectroscopy of serum proteins

Janina Kneipp¹, Cecilia Spedalieri¹, Julian Plaickner², Norbert Esser², Eugen Speiser² ¹*Humboldt-Universität zu Berlin*, ²*ISAS e.V. Berlin*

2:30 PM (SPSJ-03.4) UVRR: From Supramolecular Chemistry to Kerr-gating and Site-Specific Labeling of Peptides

Stephan Niebling¹, Tim Holtum², Till Reichenauer², Luca Supovec², Sara Luz Gomez Maya³, Carsten Schmuck², Julien Bloino³, Vincenzo Barone³, Chiara Cappelli³, Sebastian Schlücker⁴ ¹*EMBL (c/o DESY)*, ²*University of Duisburg-Essen (UDE)*, ³*Scuola Normale Superiore (SNS)*, ⁴*University of Duisburg-Essen*

2:50 PM (SPSJ-03.5) Exploring the Self-Assembly of Biomolecules Using a Multi-Length Scale Approach

Sara Catalini¹, Sara Venturi², Barbara Rossi³, Fatima Matroodi³, Renato Torre⁴, Andrea Lapini⁵, Paolo Foggi⁶, Alessandro Di Michele¹, Paola Sassi⁶, Marco Paolantoni⁶ ¹*Department of Physics and Geology, University of Perugia*, ²*European Laboratory for Non-Linear Spectroscopy*, ³*Elettra-Sincrotrone Trieste*, ⁴*Department of Physics and Astronomy, University of Florence*, ⁵*Department of Chemical, Life and Environmental Sustainability Sciences, University of Parma*, ⁶*Department of Chemistry, Biology and Biotechnology, University of Perugia*

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24ART01: Student Research in Archaeological Chemistry | 306C

Chair: Kristen Livingston, University of Central Florida

3:50 PM (ART-01.1) **Exploring the benefits of LA-ICP-MS/MS for low-cost, high resolution strontium ratio measurements on animal tooth enamel**

Alexander D. Symons¹ ¹*Cornell University*

4:10 PM (ART-01.2) **Rethinking Panchavarna: Technical Investigation of the Pigments used in the Kerala Murals**

Moupi Mukhopadhyay¹ ¹*University of California, Los Angeles*

4:30 PM (ART-01.3) **Investigation of carbon-based black pigments with pump-probe microscopy**

Heidi V. Kastenholz¹, David Grass¹, Michael Topper², Martin Fischer¹, Warren Warren¹ ¹*Duke University*, ²*University of Colorado Boulder*

4:50 PM (ART-01.4) **Thermal decomposition of dolomite: Raman spectroscopy as a thermometric tool for the analysis of carbonates in mortar binders**

Moritz T. Zöllner¹, Jens Riedel¹, Thomas Schmid¹, Petra Dariz² ¹*Federal Institute for Materials Research and Testing (BAM)*, ²*Heritagelab*

5:10 PM (ART-01.5) **Unearthing Chemical Answers: LIBS Profiling of Skeletal Remains from the “Lost Churches” of Transylvania**

Kristen Livingston¹, Katie Zejdlik-Passalacqua², Jonathan Bethard³, Zsolt Nyaradi⁴, Matthieu Baudelet ¹*University of Central Florida*, ²*Western Carolina University*, ³*University of South Florida*, ⁴*Haaz Rezso Museum*

24ATOM07: Time-of-Flight Spectrometry | 305A

Chair: David Clases, University of Graz

3:50 PM (ATOM-07.1) **Optimizing LA-ICP-TOF-MS Workflows for Biological Samples: From Sample Preparation to Data Analysis**

Keith MacRenaris¹, Soo Ahn¹, Niharika Sinha¹, Andrew Crawford¹, Thomas O'Halloran¹ ¹*Michigan State University*

4:10 PM (ATOM-07.2) **New research on old ice: Understanding polar ice core chemistry at the micro-scale using laser ablation and ICP-TOFMS**

Pascal Bohleber¹ ¹*Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research*

4:30 PM (ATOM-07.3) **Quantification and characterisation of mineral nanoparticles in bio-indicators (Dreissenae) by micro-injection spICP-ToF-MS**

Francine Wang¹, Marc Benedetti¹, Mickael Tharaud¹ ¹*Institut de physique du globe de Paris / Université Paris Cité*

4:50 PM (ATOM-07.4) **Single-particle ICP-TOFMS**

analysis of aerosol particulate matter released by fused deposition modeling 3D printers

Tristen L. Taylor¹, Madison Strait¹, Alexander Gundlach-Graham¹ ¹*Iowa State University*

5:10 PM (ATOM-07.5) **Exploration into the advantages of combining LIBS with ICP-TOF-MS for high-speed imaging**

C. Derrick Quarles Jr.¹, Benjamin T. Manard², Hunter B. Andrews², Keith MacRenaris³ ¹*Elemental Scientific, Inc.*, ²*Oak Ridge National Laboratory*, ³*Michigan State University*

24BIM06: Biomedical Spectroscopy and Imaging (CLIRSPEC) | 302A

Chair: Nick Stone, University of Exeter

3:50 PM (BIM-06.1) **Identifying Consistent Spectral Features in Brain Tumor Tissue: Analysis of Data from a Raman Probe and Microscopy System**

Kerstin Ramser¹, Joel Wahl², Dirce Pineda Vazquez², Elisabeth Klint³, Johan Richter⁴, Jan Hillman⁴, peter milos⁴, Karin Wårdell⁴ ¹*Department of Engineering Sciences and Mathematics*, ²*Dep. of Engineering Sciences and Mathematic*, ³*Biomedical Engineering*, ⁴*Department of Neurosurgery and Biomedical and Clinical Sciences*

4:10 PM (BIM-06.2) **Identification of Biochemical Patterns in Liver and Kidney Diseases Using Infrared Spectroscopic Imaging**

Michael J. Walsh¹, Mikayla Hady², Blake Mathisen³, Zach Caterer², Katie Feucker², Aiesha Hamid¹, Suman Setty⁴ ¹*New York Institute of Technology*, ²*University of Wisconsin-Eau Claire*, ³*University of Wisconsin - Eau Claire*, ⁴*University of Illinois at Chicago*

4:30 PM (BIM-06.3) **Investigating glycogen distribution in myoblasts through Raman imaging**

Eva Krois¹, Stefan Hintze², Benedikt Schoser², Peter Meinke², Karin Wieland³, Christoph Haisch¹ ¹*Chair of Analytical Chemistry and Water Chemistry, Technical University of Munich*, ²*Friedrich-Baur-Institute at the Department of Neurology, Ludwig-Maximilians-University*, ³*Competence Center CHASE GmbH*

4:50 PM (BIM-06.4) **Raman spectroscopy for analysis of circulating extracellular vesicles biomarkers of sepsis in burn patients**

Hannah J. O'Toole¹, Neona Lowe¹, Vishalakshi Arun¹, Anna V. Kolesov¹, Tina L. Palmieri², Nam K. Tran³, Randy P. Carney¹ ¹*University of California, Davis*, ²*Division of Burn Surgery & Reconstruction, Department of Surgery, University of California, Davis Health, Firefighters Burn Institute Regional Burn Center*, ³*Department of Pathology and Laboratory Medicine, University of California, Davis*

5:10 PM (BIM-06.5) **Monitoring of Therapy Response**

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in 3D Cancer Tissue Models Using Surface-Enhanced Raman Scattering Biosensors

Bilgi Kip¹, Norbert Radacsi¹, Colin J. Campbell¹
¹University of Edinburgh

24IR09: NanoIR in Biosciences | 301A

Chair: F. Simone Ruggeri

3:50 PM (IR-09.1) Nano-chemical analysis via infrared nanospectroscopy to unravel protein interactions and transitions

Francesco Simone Ruggeri¹ ¹Wageningen University

4:10 PM (IR-09.2) Probing the aducanumab amyloid- β 42 protein aggregate interface using atomic force microscopy and infrared spectroscopy

Nico Kummer¹, Peter Nirmalraj² ¹Empa - Swiss Federal Laboratories for Materials Science and Technology, ²Empa - Swiss Federal Institute for Materials Science and Technology

4:30 PM (IR-09.3) Nanoscale Structural Characterization of Amyloid Beta 1-42 Oligomers and Fibrils Grown in the Presence of Fatty Acids

Dmitry Kurouski¹ ¹Texas A&M University

4:50 PM (IR-09.4) Electric-field induced effects on proteins probed by means of infrared nanospectroscopy

Valeria Giliberti¹ ¹Italian Institute of Technology, Center for Life Nano- & Neuro-Science

5:10 PM (IR-09.5) Maximizing the performance and selectivity of photothermal AFM-IR through parameter optimization and control

Chunzeng Li¹, Cassandra Phillips¹, Qichi Hu¹, Peter De Wolf¹, Alexandre Dazzi² ¹Bruker Nano, ²Université Paris-Saclay

24IR14: Recent Advances in Near-Infrared Spectroscopic Sensing | 301B

Chair: Christian Huck, University of Innsbruck

Co-Chair: Krzysztof Bec, University of Innsbruck

3:50 PM (IR-14.01) Handheld NIR Spectroscopy for Identification and Quantitation of Materials: Development of Robust and Instrument-Independent Calibrations

Heinz W. Siesler¹, Marina De Gea Neves¹, Frank Pfeifer¹ ¹University Duisburg-Essen

4:10 PM (IR-14.02) Principal Advances in Miniaturized NIR Spectroscopy Including Theoretical Attempts

Christian W. Huck¹ ¹University of Innsbruck

4:30 PM (IR-14.03) Practical Microplastic Analysis in Environmental Matrices: On-Site Identification and Quantification of Microplastics in Soil Samples Using Miniaturized NIR Spectroscopy

Krzysztof B. Bec¹, Justyna Grabska¹, Frank

Pfeifer², Heinz W. Siesler², Christian W. Huck¹
¹University of Innsbruck, ²University Duisburg-Essen

4:50 PM (IR-14.04) Exploration of oversampling strategy to secure robust prediction in determining component concentrations in solid mixtures under varying packing densities

Haeseong Jeong¹, Seungjee Yang¹, Jomjai Peerapattana², Hocil Chung¹ ¹Hanyang University, ²Khon Kaen University

5:10 PM (IR-14.05) Frustratingly Easy Unsupervised Calibration Transfer and Maintenance

Erik Andries¹, Ramin Nikzad-Langerodi² ¹Central New Mexico Community College / University of New Mexico, ²Software Competence Center Hagenberg GmbH

24PAT05: AI in PAT | 302C

Chair: Neal Gallagher, Eigenvektor Research Inc

Co-Chair: Jim Rydzak

3:50 PM (PAT-05.1) Recasting Chemometrics for a Machine Learning World

Brian G. Rohrback¹ ¹Infometrix, Inc.

4:10 PM (PAT-05.2) Enhancing Calibration Models in NIR Spectroscopy through Variable Selection: Unartificial Intelligence

Johannes Hougaard¹ ¹Novo Nordisk A/S

4:30 PM (PAT-05.3) Outlier Diagnostics in PAT Deployments: Expectations Versus Reality

Charles E. Miller¹ ¹Aspen Technology

4:50 PM (PAT-05.4) Catching Chaos: Calibration Statistics for Evaluating Predictions on Inappropriate Data Using Partial Least Squares and Iterative Optimization Algorithms

Carl A. Anderson¹, James K. Drennen¹ ¹Duquesne University

5:10 PM (PAT-05.5) Product Identification Model Utilizing a Support Vector Machine classifier on Fluorescence Data: Journey and Best Practices for Deployment

Ryan Wall¹ ¹Johnson and Johnson

24PMA09: Making Spectroscopy Deployable On-Line Innovations and Trends in BioPharm PAT | 306B

Chair: Mark Kemper

3:50 PM (PMA-09.1) Novel Flow Cell for Raman Measurements

Ilkka J. Lahdesmaki¹ ¹FIAlab Instruments, Inc.

4:10 PM (PMA-09.2) Label-Free Electrokinetics-Modulated Surface-Enhanced Raman Spectroscopy (EK-SERS) for Viral Detection Using Micro/Nano-Optoelectrodes (MNOE)

Chuan Xiao¹, Sonali Srivastava¹, Nickolay Lavrik², Peter Vikesland³, Wei Zhou¹ ¹Virginia

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Tech, ²*Oak Ridge National Laboratory*, ³*Professor*
4:30 PM (PMA-09.3) **Solving the epitope mapping enigma for drug discovery, drug design and pre-clinical candidate selection: A transformative solution for the biopharma industry**

Belinda Pastrana¹ *Protein Dynamic Solutions, Inc.*

4:50 PM (PMA-09.4) **Protein recovery and dye removal from wastewater via modified bubble column**

Ziqin Ni¹, Christopher E. Carr¹, Lydia Bourouiba², Uttoreo Saha¹ *Georgia Institute of Technology*, ²*Massachusetts Institute of Technology*

5:10 PM (PMA-09.5) **Model Transfer between Process Raman Spectrometers**

Shaun J. Fraser¹, Mark Kemper², Colin Couper³
¹*Bruker Corporation*, ²*Bruker Corp.*, ³*Bruker Corporation*

24RAM09: Spatially Offset Raman Spectroscopy (SORS) 302B

Chair: Pavel Matousek, STFC Rutherford Appleton Laboratory

3:50 PM (RAM-09.1) **Time Domain Diffuse Raman Spectroscopy based on Single Pixel Detection**

Alessandro Bossi¹, Antonio Pifferi¹, Valerio Gandolfi¹, Stefan Šušnjar², Sanathana Konugolu Venkata Sekar³, Renzo Vanna⁴, Fabrizio Martelli⁵, Andrea Farina⁴ *Politecnico di Milano*, *Dipartimento di Fisica*, ²*Spectracure*, ³*Biophotonics@Tyndall*, *Tyndall National Institute*, ⁴*Istituto Fotonica e Nanotecnologie - CNR*, ⁵*Università degli Studi di Firenze*, *Dipartimento di Fisica e Astronomia*

4:10 PM (RAM-09.2) **SORS-based direct quantification of ethanol contents of liquors in diverse glass bottles**

Sanghoon Cho¹, Sangjae Kim¹, Hoeil Chung²
¹*Hanyang University*, ²*Hanyang University*

4:30 PM (RAM-09.3) **Engineering vascularized optical phantom with skin-like properties for non-invasive Raman spectroscopy**

Lintong Wu¹, Piyush Raj¹, Saransh Arora¹, Raj Bhatt¹, Yi Zuo¹, Zhiwei Fang¹, Remco Verdoold², Tanja Koch², Luo Gu¹, Ishan Barman¹ *Johns Hopkins University*, ²*ams OSRAM Innovation and Engineering*

4:50 PM (RAM-09.4) **Plasmonic Caged Gold Nanostars for Theranostic Applications**

Aidan J. Canning¹, Tuan Vo-Dinh¹ *Duke University*

5:10 PM (RAM-09.5) **Bone tissue characterization through scattering media**

Hui Ma¹, Pranav Lanka¹, Suraj Kothuri², Carrie O'Flynn³, Patrick Henn⁴, Sanathana Konugolu Venkata Sekar¹, Stefan Andersson-Engels⁵, Rekha Gautam¹ *Biophotonics@Tyndall*, *Tyndall National Institute*, ²*Biophotonics@Tyndall*, *Tyndall National Institute*; *Department of Engineering Sciences*, *University College*

Cork, ³*ASSERT Center*; *College of Medicine and Health*, *University College Cork*, ⁴*ASSERT Center*; *College of Medicine and Health*, *University College Cork*, ⁵*Biophotonics@Tyndall*, *Tyndall National Institute*; *School of Physics*, *University College Cork*

24SPECIAL03: All in the Family: A Peaceful Gathering of Hieftje Descendants | 305B

Chair: Jacob Shelley, Rensselaer Polytechnic Institute

Co-Chair: Julia Danischewski, Rensselaer Polytechnic Institute

3:50 PM (SPECIAL-03.1) **How Do I Work This? From Molecular Spectroscopy to Aerogels**

Mary K. Carroll¹ *Union College*

4:10 PM (SPECIAL-03.3) **Leveraging Elemental Tools to Drive Innovation in R&D**

Denise McClenathan¹, Jennifer Morgan¹, Andrei Shauchuk¹, Samantha Carter¹, Christina Haven¹, Kelly Smith¹, Jenny Luna¹, Usa Rattanaudompol¹, Patrick Doyle¹, Lauren Duncan¹, Francisco Arias¹, Roy Dobson¹ *Procter & Gamble*

4:30 PM (SPECIAL-03.4) **Solution-cathode glow discharge as a source of atomic and molecular emission**

Michael R. Webb¹, Nadia Radomski¹ *University of North Carolina Wilmington*

4:50 PM (SPECIAL-03.4) **Synthetic and Natural Polymer Characterization and Imaging via Laser-Assisted Micro-Pyrolysis FAPA Mass Spectrometry**

Gerardo Gamez¹, Ejoke Akatugba², Daniela Barroso³, Bibek R. Bhattarai³, Songyue Shi⁴
¹*Texas Tech University*, ²*Department of Chemistry and Biochemistry*, *Texas Tech University*, *Lubbock, Texas 79409-1061 US*, ³*Department of Chemistry and Biochemistry*, *Texas Tech University*, *Lubbock, Texas 79409-1061, US*, ⁴*Proteomics Core*, *UT Southwestern Medical Center*

5:10 PM (SPECIAL-03.5) **From attempts to inject individual monodisperse droplets into an ICP 40 years ago to measuring millions of individual nano- and micro-particles entrapped in glacial ice now**

John Olesik¹, Madeleine Lomax-Vogt¹, Lucas Carter¹, Kutuzov Stanislav², Paolo Gabrielli³
¹*The Ohio State University*, ²*The Ohio University*, ³*Honeybee Robotics*

24SPR01: Plasmonic sensors | 306A

Chair: Jean-Francois Masson, University of Montreal

3:50 PM (SPR-01.1) **A Plasmonic Nanoledge Array for Sensing Cardiovascular Disease Biomarker in Blood**

JIANJUN WEI¹, Frank Tukur¹, Taylor Mabe¹
¹*UNC Greensboro*

TECHNICAL PROGRAM - WEDNESDAY, OCTOBER 23, 2024

Oral Symposia | 3:50 PM – 5:30 PM | *Various Locations*

- 4:10 PM (SPR-01.2) **DNA Origami Self-assembled Plasmonic Nanoprobes for Targeted Cancer Imaging**
Lintong Wu¹, Swati Tanwar¹, Gagandeep Kaur¹, Siddhi Date¹, Linika Goel¹, Arnab Chatterjee¹, Patty McGuiggan¹,
Ishan Barman¹ ¹*Johns Hopkins University*
- 4:30 PM (SPR-01.3) **Developing nanotags for higher throughput single nanoparticle dual colour imaging and tracking in suspension**
Hannah L. Taysum¹, Alastair W. Wark² ¹*University of Strathclyde*, ²*University Of Strathclyde*
- 4:50 PM (SPR-01.4) **Development of a sensitive, in-vivo surface-enhanced Raman scattering (SERS) mapping technique of cellular changes following H1N1-infection using a SERS-active printable hydrogel**
Delicia Gonsalves¹, Sonali Srivastava², Peter Vikesland³ ¹*Virginia Polytechnic Institute and State University*, ²*Virginia Tech*, ³*Professor*
- 5:10 PM (SPR-01.5) **Gold Nanocrowns: Synthesis and Application in Dual-Modal Colorimetric and Surface-Enhanced Raman Scattering for Lateral Flow Immunoassay**
Yuanhao Zhao¹, Supriya Atta², Tuan Vo-Dinh² ¹*Tuan Vo-Dinh's Lab at Duke University Biomedical Engineering Department*, ²*Duke University*

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Award & Plenary Lectures | 8:15 AM – 9:30 AM | *Ballroom A*

8:15 AM **Award Presentation**

8:30 AM **SAS and Applied Spectroscopy William F. Meggers Award: Quantitative analysis of tissue by Raman microscopy: from quantifying pharmaceuticals in tissue to intra-operative diagnosis during cancer surgery**
Ioan Notingher¹ ¹*Universtiy of Nottingahm*

9:00 AM **Coblentz Society Clara Craver Award: Coherent Raman Scattering Pharmacokinetic and Pharmacodynamic Tomography**
Conor Evans¹ ¹*Massachusetts General Hospital*

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Thursday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom Foyer*

(Thur-P1) **Increased Sensitivity of InAs/InAsSb Superlattice Long Wave Infrared Detectors with Large Quantities of Thin Absorbers**

Jędrzej Mijas¹, Daniel Hirsh¹, Michael Baez¹
¹*VIGO Photonics*

(Thur-P2) **Infrared spectrochemical analysis of collagen in control and aged parchments**

Kathleen M. Gough¹, Danylo M. Kruk¹, Rinuk E. 'Limurn¹, Fatemeh Jamshidzadehtaleshi², David Hartry¹, Laurent Bozec³, Mehrnoosh Neshatian³, Hans A. Bechtel⁴, Stephanie N. Gilbert Corder⁴
¹*University of Manitoba*, ²*Department of Chemistry, University of Manitoba*, ³*University of Toronto*, ⁴*Lawrence Berkeley National Laboratory*

(Thur-P3) **Correlated micro-spectroscopy to analyze microplastics.**

Carlos Morillo¹ ¹*JASCO Inc*

(Thur-P4) **Removal and Desorption of Peanut (Arachis hypogaea) Allergens 1-3 Using Magnetic Nanoparticles for**

Application in Immunotherapy

Viyah H. Morrow¹, Jeanette Gaffney¹, Tamar Layens¹, Anselm Omoike¹ ¹*University of South Carolina Upstate*

(Thur-P5) **Towards Multiplexed Nucleic Acid Delivery for Genetic Engineering Using Electroporation**

Alexia K. Cash¹, Mike B. Sano², Robert Williamson² ¹*NC State University*, ²*North Carolina State University*

(Thur-P6) **Manganese, Nickel, and Copper(II) N,N'-Diphenylazodioxide Complexes: Synthesis and Structural Characterization**

Ahmed M. Salem¹, W. Christopher Boyd²
¹*Cleveland State University*, ²*Department of Chemistry, Cleveland State University*

(Thur-P7) **Tunable 3D Nanoconfinement via PDMS Diaphragm Collapse in Bead-Array Microfluidic Platforms for Enhancing Biomolecular Binding Kinetics**

Abdullah-Bin Siddique¹, Jui-Hong Weng², Deng-Kai Yang², Chia-Fu Chou², Nathan S. Swami¹

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Thursday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom Foyer*

¹University of Virginia, ²Institute of Physics, Academia Sinica, Taiwan

(Thur-P8) **A tailor-made bio-nano catcher for precise capture of APE1/Ref-1 protein within living cells: Insights for mechanistic study and cancer therapy**

Ruilan Zhang¹, Meiping Zhao¹ ¹College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China

(Thur-P10) **Improving Oral Healthcare via Incorporating LFA with SERS**

Adewale A. Adehinmoye¹, Lyndsay N. Kissell¹, Daewoo Han¹, Der Vang¹, Andrew Steckl¹, Pietro Strobbia¹ ¹University of Cincinnati

(Thur-P11) **Comparative Spectroscopic Analysis of ¹³C-Enriched and Naturally Abundant Carbon Quantum Dots**

Cody W. Soper¹, Robert V. Chimenti, Nicholas Whiting¹ ¹Rowan University

(Thur-P12) **Chemometrics Assisted Gas Chromatography Analysis of Fatty Acids in Blood Plasma Under Varying Dietary Conditions Towards Clinical Applications**

Mohamed O. Amin¹, Nouf Aldhafiri², Fatemah J Bahman³, Entesar Alhetlani⁴, Rasheed Ahmad³ ¹University at Albany, ²Biological Sciences Department, Faculty of Science, Kuwait University, P.O. Box 5969, Safat 13060, Kuwait, ³Immunology & Microbiology Department, Dasman Diabetes Institute, Dasman 15462, Kuwait, ⁴Kuwait University

(Thur-P13) **Multiplexing Reagentless SERS Sensors for the Simultaneous Detection of Multiple Respiratory Diseases**

Steven M. Quarin¹, Lyndsay N. Kissell¹, Pietro Strobbia¹ ¹University of Cincinnati

(Thur-P14) **Investiating the Relationships of Optical Element, Plasmon, and Excitation Wavelength in the Performance of Optoplasmonic Materials**

Alexander Cikanek¹, Malama Chisanga², Jean-Francois Masson³ ¹University of Rochester, ²University of Montreal, ³Universite de Montreal

(Thur-P15) **Characterization of thermally activated plasmonic nanocomposites as an optical detection platform**

Casey Folks¹, Laura Casto-Bogges¹ ¹University of North Carolina at Charlotte

(Thur-P17) **Nondestructive analysis of the differentiation of iPS cells using Raman spectroscopy —Development of a monitoring method for urea cycle disorders—**

Yukina Hiramatsu¹, Mika Ishigaki², mai okano³, hirofumi hitomi³ ¹Shimane University, Graduate School of Natural Sciences, Life Sciences, ²Shimane University, ³Kansai Medical University

(Thur-P18) **Material-Agnostic Characterization of Spatially Offset Raman Spectroscopy in Turbid Media via Monte Carlo Simulations**

Zuriel Erikson V. Joven¹, Piyush Raj¹, Ishan Barman¹ ¹Johns Hopkins University

(Thur-P19) **Chick sexing based on the blood analysis using Raman spectroscopy**

Sana Matsumoto¹, Mika Ishigaki¹, Akane Ogino², Kai Onoe², Juichiro Ukon³ ¹Shimane University, ²NABEL Co., Ltd., ³UKON Craft Science Ltd., CEO

(Thur-P20) **A SERS-based living biosensor**

Ryan Senger¹, Hunter Flick¹ ¹Virginia Tech

(Thur-P21) **Water Lensing Effect in Remote Raman Spectroscopy**

Paige K. Williams¹, Whitney Schuler¹, Micheal Myrick¹, Caitlyn English¹, Zechariah Kitzhaber¹, Tammi Richardson¹ ¹University of South Carolina

(Thur-P22) **Evaluating Raman Spectroscopy for Gas-Phase Monitoring to Support the Uranium Science and Technology Center**

Avery L. Wood¹, Daniel E. Felton¹, Luke R. Sadergaski², Jennifer N. Neu¹, Tyler Sherwood², Jason Richards², Job Bello³, Roger J. Kapsimalis¹ ¹Oak Ridge National Lab, ²Oak Ridge National Laboratory, ³Spectra Solutions Inc.

(Thur-P23) **Spectroscopic Characterization at the Uranium Science and Technology Center**

Jennifer N. Neu¹, Daniel E. Felton¹, Luke R. Sadergaski², Avery L. Wood¹, Roger J. Kapsimalis¹ ¹Oak Ridge National Lab, ²Oak Ridge National Laboratory

(Thur-P24) **Stable picosecond infrared/green wavelength laser with ultra-narrow spectral linewidth for time-resolved Raman spectroscopy application.**

Evgeny Savelyev¹, Anatoly Makarov¹, Andrey Chumachenko¹, Andrei Gurovich¹, Vasilii Ustimchik¹, Valery Filippov¹ ¹Ampliconyx Oy

(Thur-P25) **Photoactivated plasmonic nanohybrid fibers with prolonged trapping of excited charge carriers for SERS analysis of biomolecules**

ARTI SHARMA¹, tripti ahuja², Shubhangi majumdar³, Jatin yadav⁴, Soumik Siddhanta⁵ ¹Research Scholar at Indian Institute of Technology Delhi, ²Post doctrate, ³Phd Student, ⁴MRPL, ⁵Assistant Professor

(Thur-P26) **Spectrally Resolved Super Resolution Raman Imaging of pH Probes**

Kate V. Sherlock¹, Deben N. Shoup², Abigail E. Smith¹, Zachary D. Schultz¹ ¹The Ohio State University, ²Ohio State University

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Thursday Poster Sessions | 9:30 AM – 10:30 AM | *Ballroom Foyer*

(Thur-P27) Towards an efficient online Raman detector for field flow fractionation

Maximilian J. Huber¹, Marcel Klotz¹, Ulrich Rupp², Stefan Kreissl², Miriam Boehmler², Natalia P. Ivleva¹ ¹*Technical University of Munich, Institute of Water Chemistry, Chair of Analytical Chemistry and Water Chemistry,* ²*Oxford Instruments WITec*

(Thur-P28) Mapping Refractive Index of Graded Index Optics Using Confocal Raman Microscopy

Jamison D. Engelhardt¹, Joseph F. Stanzione¹, Robert V. Chimenti¹ ¹*Rowan University*

(Thur-P29) Multiwavelength laser platform utilizing monolithic gratings

Luukas Kuusela¹, Timo Aho¹, Riina Ulkuniemi¹, Mika Mähönen¹, Jussi Hämelähti¹, Andreas Schramm¹, Soile Talmila¹, Pekko Sipilä¹, Petteri Uusimaa¹ ¹*Modulight Corporation*

(Thur-P30) Raman study for development of a diagnostic method of carcinoma in situ of the bladder

Hiroko Matsuyoshi¹, Kotaro Oka², Makito Miyake³, Hidetoshi Sato⁴ ¹*Tokai Gakuen University,* ²*Kwansei Gakuin University,* ³*Nara Medical University,* ⁴*School of Biological and Environmental Sciences, Kwansei Gakuin University*

(Thur-P31) QC solution for carbon materials: A Raman approach

Peng Miao¹ ¹*HORIBA Instruments Incorporated*

(Thur-P32) Raman spectroscopic quantification of various microplastic particles in water using polydimethylsiloxane-coated nickel foam as a particle-capturing platform

Sangjae Kim¹, Sanghoon Cho¹, Yunjung Kim¹, Hoeil Chung² ¹*Hanyang university,* ²*Hanyang University*

(Thur-P33) Pathlength and Height Dependence of Remote Water Raman Scattering

Whitney Schuler¹, Paige K. Williams¹, Zechariah Kitzhaber¹, Caitlyn English¹, Tammi Richardson¹, Nikos Vitzilaios¹, Micheal Myrick¹ ¹*University of South Carolina*

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 10:30 PM – 12:10 PM | *Various Locations*

24ART02: LA-ICP-MS Applications in Art and Archaeology | 306C

Chair: Andrew Zipkin, Eurofins | EAG Laboratories

10:30 AM (ART-02.1) Twenty years of LA-ICP-MS analysis at the Elemental Analysis Facility at the Field Museum

Laure Dussubieux¹ ¹*Field Museum*

10:50 AM (ART-02.2) Show me your passport please: trading networks of glass beads in the Province of Quebec (16th - 19th century)

Adelphine Bonneau¹, Bernard Gratuze², Jean-François Moreau³ ¹*Université de Sherbrooke,* ²*Centre Ernest-Babelon, IRAMAT – UMR7065, Université d'Orléans et CNRS,* ³*Université du Québec à Chicoutimi*

11:10 AM (ART-02.3) A Millennium of Craft, Conquest, and Collapse: Laser Ablation Inductively Coupled Plasma Mass Spectrometry analyses of archaeological ceramics from southern Peru

Nicola O. Sharratt¹, P. Ryan Williams², Donna Nash², Sofia Chacaltana Cortez³ ¹*Georgia State University,* ²*Arizona State University,* ³*Universidad Antonio Ruiz de Montoya*

11:30 AM (ART-02.4) Tales of golden glass and viking treasures

Gry H. Barfod¹ ¹*Aarhus University*

11:50 AM (ART-02.5) Exploring ceramic provenance and resource utilization in Igbo Ukwu (7th - 13th Century CE) Southeastern Nigeria.

Elizabeth Adeyemo¹, Mark Golitko¹ ¹*University of Notre Dame*

24ATOM10: Multi-Collector ICP-MS | 305A

Co-Chair: Benjamin T. Manard, Oak Ridge National Laboratory

Co-Chair: Daniel Dunlap, Oak Ridge National Laboratory

10:30 AM (ATOM-10.1) Next Generation Isotopic Analyses by MC-ICP-MS/MS

Daniel R. Dunlap¹, Benjamin T. Manard¹, N. Alex Zirakparvar¹, Matt Darnell¹, Cole R. Hexel¹ ¹*Oak Ridge National Laboratory*

10:50 AM (ATOM-10.2) Lithium isotopes as indicators of aging in lithium-ion batteries

Carlos Abad¹, Dalia Morcillo², Alexander Winckelmann³, Jhanis J. Gonzalez⁴, Ana

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 10:30 PM – 12:10 PM | *Various Locations*

Guilherme Buzanich², Marcus Oelze², Jochen Vogl², Silke Richter³, Sebastian Recknagel⁵
¹Bundesanstalt für Materialforschung und –prüfung (BAM), ²Federal Institute for Materials Research and Testing (BAM), ³Bundesanstalt für Materialforschung und -prüfung (BAM), ⁴Applied Spectra Inc./ Principal Scientific Engineering Associate, ⁵Bundesanstalt für Materialforschung und -prüfung (BAM),

11:10 AM (ATOM-10.3) **Applications and analytical boundaries of thallium isotopes**

Chadlin M. Ostrander¹ ¹University of Utah

11:30 AM (ATOM-10.4) **Application of high-spatial resolution LA-MC-ICP-MS in planetary materials**

Jacob B. Setera¹, Justin I. Simon², Rosalind M.G. Armytage³, Wayne P. Buckley³ ¹University of Texas at El Paso - Jacobs JETS II at NASA JSC, ²NASA Johnson Space Center, ³Jacobs JETS II at NASA JSC

11:50 AM (ATOM-10.5) **Direct Analysis of Nanoparticles on Solid Surfaces by MicroExtraction-ICP-MS**

Jordan Stanberry¹, Benjamin T. Manard¹, Brian Ticknor¹, Hunter B. Andrews¹, Cyril Thompson¹
¹Oak Ridge National Laboratory

24AWD04: Applied Spectroscopy William F. Meggers Award Award Session | 301B

Chair: Ioan Notingher, University of Nottingham

10:30 AM (AWD-04.1) **Spatially Offset Raman Spectroscopy (SORS) – Recent Developments**

Pavel Matousek¹, Sara Mosca¹, MEGHA MEHTA², William H. Skinner², Benjamin Gardner², Francesca Palombo², Nicholas Stone²
¹STFC - UKRI, ²University of Exeter

10:50 AM (AWD-04.2) **Identification of environmental microplastics using Raman spectroscopy**

Dustin Shipp¹, Eliza Ballantyne¹, Alexandra Cruz¹, Sally Rocks¹ ¹Utah Valley University

11:30 AM (AWD-04.4) **Development of an integrated forward viewing Raman spectroscopy and optical coherence tomography probe for endoscopy**

Mads S. Bergholt¹, Jianrong Qiu¹ ¹King's College London

11:50 AM (AWD-04.5) **Exploring extremes: fast and slow Raman microscopy for maximizing full spectroscopic potential**

Katsumasa Fujita¹ ¹Osaka University

24BIM07: Nanotheranostics: Diagnosis and Treatment of Disease Using Nanomaterials | 302A

Chair: Samuel Mabbott, Texas A&M University

10:30 AM (BIM-07.1) **Culture-free Detection of Bacteria in Biofluids**

Andrea Locke¹, Alec Walters¹, Anna Funderburg¹, Sophia Juarez¹ ¹Vanderbilt University

10:50 AM (BIM-07.2) **SESORRS Imaging Reveals Deep-Seated Tumors in Pre-Clinical Mouse Models of Cancer**

Fay Nicolson¹, Bohdan Andreiuk², Eunah Lee³, Bridget O'Donnell⁴, Andrew Whitley⁵, Scott Rudder⁶, Samuel Mabbott⁷, Kevin Haigis² ¹Dana-Farber Cancer Institute and Harvard Medical School, ²Dana-Farber Cancer Institute, ³HORIBA Instruments Inc, ⁴Honeywell, ⁵HORIBA Scientific, ⁶Opto Sigma, ⁷Texas A&M University

11:10 AM (BIM-07.3) **Advancing Reagentless SERS Sensors towards the Point-of-Care using Lyophilization**

Lutfun Naher¹, Steven M. Quarin¹, Der Vang¹, Pietro Strobbia¹ ¹University of Cincinnati

11:30 AM (BIM-07.4) **Machine Learning Methods in Exosomes Analysis with Surface-Enhanced Raman Spectroscopy (SERS) for Label-Free Cancer Detection**

Der Vang¹, Maria S. Kelly¹, Manisha Sheokand¹, Manju Sharma¹, Leyla Esfandiari¹, Ruxandra I. Dima¹, Pietro Strobbia¹ ¹University of Cincinnati

11:50 AM (BIM-07.5) **Multimodal Imaging Platform for Characterising Transition Metal Dichalcogenides in Bioapplications**

Angela Flack¹, Samantha Redes¹ ¹Edinburgh Instruments

24FORENS06: Pharmaceutical Micro and Macro Forensics 2 | 303

Chair: Ravi Kalyanaraman, Bristol Myers Squibb
Co-Chair: Adam Lanzarotta

10:30 AM (FORENS-06.1) **Recent Developments by FDA's International Mail Facility Satellite Laboratories Equipped with Rapid Screening Devices for Detecting Active Pharmaceutical Ingredients in Unknown (Unlabeled/Mislabeled) Drug Products**

Adam C. Lanzarotta¹, Sara Kern¹, JaCinta Batson¹, Brian Boyd¹, Lisa Lorenz¹, Michael Thatcher¹, Megan Sterling¹, Hannah LaRoy¹, Melissa Collins¹, Anvi Patel¹, Marie Marseille¹, Brandon Reyes¹, Christina Fernandez¹, Adiel Perez¹ ¹FDA Forensic Chemistry Center

10:30 AM (FORENS-06.2) **Application of Portable Spectrometers in Pharmaceutical Forensics**

Brittany Handzo¹, Ravi Kalyanaraman¹ ¹Bristol Myers Squibb

10:50 AM (FORENS-06.3) **Evolution and Current Trends in the Forensic Particulate Analysis of Pharmaceuticals**

David Exline¹ ¹Gateway Analytical

11:10 AM (FORENS-06.4) **Pharmaceutical Forensic Analysis Factors for Success**

Gretchen L. Shearer¹ ¹McCrone Associates

11:30 AM (FORENS-06.5) **Micro spectroscopy for pharmaceutical forensics.**

Sergey Mamedov¹ ¹HORIBA Scientific

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 10:30 PM – 12:10 PM | *Various Locations*

24IR10: Advances in QCL-IR Spectroscopy | 301A

Chair: Young Jong Lee

10:30 AM (IR-10.1) **External cavity quantum cascade laser vibrational circular dichroism spectroscopy (EC-QCL-VCD) for analysis of proteins at low concentrations**

Bernhard Lendl¹, Daniel-Ralph Hermann¹, Georg Ramer¹ ¹TU Wien

10:50 AM (IR-10.2) **Methods to Derive the Complex Refractive Indices of Different Hydration States for Solid Materials**

Tanya L. Myers¹, Michael Wilhelm¹, Kelly Peterson¹, Jeremy D. Erickson¹, Timothy J. Johnson¹ ¹Pacific Northwest National Laboratory

11:00 AM (IR-10.3) **Tissue Analysis by QCL-based Infrared Laser Imaging**

Peng Wang¹, Ethan Yang², Joshua Fischer¹, Domenic Dreisbach³, Thomas J. Tague¹ ¹Bruker Scientific LLC, ²Seer, ³Bruker Optics GmbH & Co. KG

11:30 AM (IR-10.4) **Microplastics Assessment in Intact Human Tissues by Infrared Spectroscopy**

Azita HassanMazandarani¹, John M. Masterson², Elad Ophir³, William Querido¹, Andrzej Steplewski⁴, Andrzej Fertala⁴, Yi Zhang⁵, Carissa Huynh⁵, Maurice M. Garcia², Nancy Pleshko¹ ¹Department of Bioengineering, Temple University, ²Department of Urology, Cedars-Sinai Medical Center, ³Bioengineering Department of Temple University, ⁴Department of Orthopedic Surgery, Thomas Jefferson University, ⁵Biobank and Research Pathology, Cedars-Sinai Medical Center

11:50 AM (IR-10.5) **Non-Destructive Glycan Analysis of Glycoproteins Using Sensitive IR Spectrophotometry**

Young Jong Lee¹, Seong-Min Kim¹ ¹NIST

24PMA10: Analysis Of Biologicals In Blood 2 | 306B

Co-Chair: John Marshall, Toronto Metropolitan University

Chair: David Muddiman, North Carolina State University

10:30 AM (PMA-10.1) **Fundamentals and Applications of IR Matrix-Assisted Laser Desorption Electrospray Ionization for Direct Analysis, Mass Spectrometry Imaging, and High Throughput and Phenotypic Screening**

David C. Muddiman¹ ¹North Carolina State University

10:50 AM (PMA-10.2) **Applications of Luminex xMAP Technology for Multiplexed Analysis of Blood-Based Biomarkers**

Sherry A. Dunbar¹ ¹Luminex, A Diasorin Company

11:10 AM (PMA-10.3) **Comparison of enzyme linked immunoassay detection by colorimetric, fluorescent, chemiluminescent and mass spectrometry**

Lloyd Johnson¹, Jaimie Dufresne², Zhuo Zhen

Chen¹, John G. Marshall¹ ¹Toronto Metropolitan University, ²YYZ PHARMATECH INC

11:30 AM (PMA-10.4) **Plasmonics-Enhanced Lateral-Flow Immunoassay**

Supriya Atta¹ ¹Duke University

24RAM10: Low Frequency Raman | 302B

Chair: Robert Chimenti

10:30 AM (RAM-10.1) **Old Polymorph, New Techniques: Assessing Ritonavir Crystallinity Using Low-Frequency Raman and Laser Directed Infrared Imaging**

Daniel Willett¹, Huzeyfe Yilmaz¹, Yeakub Zaker¹, Jason D. Rodriguez² ¹US Food & Drug Administration, ²US Food and Drug Administration

10:50 AM (RAM-10.2) **Low-frequency Raman spectroscopy studies on chiral phonons**

Rahul Rao¹ ¹Air Force Research Laboratory

11:10 AM (RAM-10.3) **Identification of Natural Minerals Using Infrared and Raman Spectroscopy Including Low-frequency Region**

Kohei TAMURA¹, Motohiro Tsuboi², Kuniyuki Furukawa³, Ken-ichi Aka¹, Harumi Sato⁴, Yukihiko Ozaki² ¹JASCO Corporation, ²Kwansei Gakuin University, ³Aichi University, ⁴Kobe University

11:30 AM (RAM-10.4) **Low-Frequency Raman Spectroscopy: Probing Order in Solid State Materials**

Keith C. Gordon¹ ¹University of Otago

11:50 AM (RAM-10.5) **Over 10 Years of Low Frequency Raman - A Look at the Evolution and Future of the Field**

James T. Carriere¹ ¹Coherent

24RAM16: Early Career Raman | 302C

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

Co-Chair: Bhavya Sharma, University of Tennessee, Knoxville

10:30 AM (RAM-16.1) **Bright Silica-encapsulated labelled Gold Nanoraspberries for Sensitive Detection.**

MEGHA MEHTA¹, Sara Mosca², William H. Skinner¹, Benjamin Gardner¹, Francesca Palombo¹, Pavel Matousek², Nicholas Stone¹ ¹University of Exeter, ²STFC - UKRI

10:50 AM (RAM-16.2) **Rapid Detection of Foodborne Pathogens by SERS**

Hayleigh May¹, Roy Goodacre², Duncan Graham¹, Karen Faulds¹ ¹University of Strathclyde, ²University of Liverpool

11:10 AM (RAM-16.3) **Deep Ultraviolet Raman Spectroscopy on Mars: Raman Bandwidth Calibration**

Next year: October 5-10, 2025 • Northern Kentucky Convention Center

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 10:30 PM – 12:10 PM | *Various Locations*

and Spectral Background Subtraction Provides Insights into the History of Jezero Crater

Ryan S. Jakubek¹, Rohit Bhartia², Kyle Uckert³, Richard Morris⁴, Sanford A. Asher⁵, Aaron Burton⁶, Andrea Corpolongo⁷, Andrew Czaja⁸, Marc Fries⁴, Kevin Hand³, Nikole Haney⁴, Joseph Razzell Hollis⁹, William Hug¹⁰, Carina Lee⁴, Francis McCubbin⁴, Michelle Minitti¹¹, Eva Scheller¹², Shiv Sharma¹³, Sunanda Sharma³, Sandra Siljeström¹⁴, Andrew Steele¹⁵ ¹Jacobs, NASA Johnson Space Center, ²Photon Systems, Inc., ³JPL, ⁴JSC, ⁵University of Pittsburgh, ⁶NASA, ⁷University of Cincinnati, ⁸Cincinnati, ⁹Natural History Museum, London, ¹⁰Photon Systems, ¹¹N/A, ¹²MIT, ¹³University of Hawai'i at Mānoa, ¹⁴RISE Research Institutes of Sweden, ¹⁵Carnegie Institution for Science

11:30 AM (RAM-16.4) Enhancing Ovarian Cancer Diagnostics: Integrating Raman Tag Labeling with ML-Enabled SERS of Extracellular Vesicles for Improved Transparency and Precision

Qing He¹, Hanna Koster¹, Justin O'Sullivan², Samantha Ono², Rachel Mizenko¹, Hannah J. O'Toole³, Marie Heffern², Randy P. Carney³ ¹University of California, Davis, Department of Biomedical Engineering, ²University of California, Davis, Department of Chemistry, ³University of California, Davis

11:50 AM (RAM-16.5) Chick sexing through blood analysis using Raman spectroscopy

Mika Ishigaki¹, Sana Matsumoto¹, Akane Ogino², Kai Onoe², Juichiro Ukon³ ¹Shimane University, ²NABEL Co., Ltd., ³UKON Craft Science Ltd., CEO

24SPECIAL01: Shootout at Hieftje's Atomic Spectroscopy Corral | 305B

Chair: Steve Ray, State University of New York at Buffalo
Co-Chair: Jacob Shelley, Rensselaer Polytechnic Institute

10:30 AM (SPECIAL-01.1) Back to the Future of Atomic Spectroscopy

Carsten Engelhard¹, Cristian Escobar-Carranza², Maximilian Heide², Manuel Heinelt², Annika Schardt², Johannes Schmitt², Désirée Schütz² ¹BAM & University of Siegen, ²University of Siegen

10:50 AM (SPECIAL-01.2) Nanomaterials Production: Exuberantly Undoing Decades of Gary Hieftje's Work

Vahid Majidi¹, Simona Murph¹ ¹Savannah River National Laboratory

11:10 AM (SPECIAL-01.3) From the Beginning

Richard (Rick) Russo¹ ¹Applied Spectra, Inc

11:30 AM (SPECIAL-01.4) Adventures in Characterizing the Low-Temperature Plasma Probe in the Hieftje Group: A Two-Sided View

George Chan¹, Carsten Engelhard², Jacob T. Shelley³ ¹Lawrence Berkeley National

Laboratory, ²BAM & University of Siegen, ³Rensselaer Polytechnic Institute

11:50 AM (SPECIAL-01.5) Famous Futurisms of Gary Hieftje - or -Why Application-Specific Simple Instrumentation is the Future of Plasma-Based Atomic Spectrometry

Steven Ray¹ ¹SUNY Buffalo Dept of Chemistry

24SPR03: New Plasmonic Materials And Architectures | 306A

Chair: Gregory Wallace, The University of Strathclyde

10:30 AM (SPR-03.1) Applied Magnesium Plasmonics

Andy Ten¹, Christina Boukouvala¹, Zeki Semih Pehlivan¹, Jodie Fergusson¹, Vladimir Lomonosov¹, Emilie Ringe¹ ¹University of Cambridge

10:50 AM (SPR-03.2) Discrimination of Genetic Biomarkers of Disease through Machine Learning-Based Hypothesis Testing of Direct SERS Spectra of DNA and RNA

Laura Fabris¹, Jinisha Chheda², Yating Fang², Ahmed Aziz Ezzat² ¹Politecnico di Torino, ²Rutgers University

11:10 AM (SPR-03.3) Reversible Assembly of Iron Oxide Nanoparticles on Gold Nanorods for Magnetic Alignment and Plasmonic Control

Mehedi H. Rizvi¹, Ruosong Wang², Jonas Schubert², William Crumpler¹, Christian Rossner², Amy L. Oldenburg³, Andreas Fery², Joseph B. Tracy¹ ¹North Carolina State University, ²Leibniz Institute for Polymer Research, ³University of North Carolina, Chapel Hill

11:30 AM (SPR-03.4) Imaging spatial and chemical distributions of plasmon induced effects

Zachary D. Schultz¹ ¹The Ohio State University

11:50 AM (SPR-03.5) Surfactant-Free Magnetic Gold Nanostars: Synthesis and SERS Sensing Application

Taylor L. Thorsen¹, Supriya Atta¹, Tuan Vo-Dinh¹ ¹Duke University

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

24ART03: Imaging Technologies for Cultural Heritage 306C

Chair: Roger L. Easton, Jr, Rochester Institute of Technology
Co-Chair: Juilee Decker, Rochester Institute of Technology

- 1:30 PM (ART-03.1) **Interactive Digital Preservation**
Atia Newman¹ *Rochester Institute of Technology*
- 1:50 PM (ART-03.2) **Revelation and Discovery in Biblical Manuscript Imaging: Enhancing Textual Data Collection for Critical Editions**
W. Andrew Smith¹ *Shepherds Theological Seminary*

- 2:10 PM (ART-03.3) **Preservation of Ancient Hindu Texts using Novel Technologies**
P.R. Mukund¹ *Rochester Institute of Technology*

- 2:30 PM (ART-03.4) **Overcoming Challenges in the Application of Multispectral Imaging to Illegible Ancient Manuscripts**
Michael Phelps¹ *Early Manuscripts Electronic Library (EMEL)*

- 2:50 PM (ART-03.5) **The growing role of imaging in conservation: impacts from conservation education to implementation and research**

24ATOM11: Elemental Analysis | 305A

Chair: Mesay Wolle, US Food and Drug Administration

- 1:30 PM (ATOM-11.1) **The Oh-Fish-AI Method for Measuring Methylmercury in Seafood: Method Development and Validation**
Jake A. Carter¹, Patrick Gray¹ *US FDA CFSAN*
- 1:50 PM (ATOM-11.2) **Use of imaging and counting techniques for the identification and analysis of metal particles in unused cannabis vaping products**
Zuzana Gajdosechova¹, Joshua Marleau-Gillette¹, Matthew J. Turnbull², Duane C. Petts³, Simon E. Jackson³, Daniele Regis³, Ivana Kosarac⁴, Guru Prasad Katuri⁴, Dharani Das⁴, Hanan Abramovici⁴, Andrew Wayne⁴, Ashley Cabecinha⁴
¹National Research Council Canada, ²University of Western Ontario, ³Natural Resources Canada, ⁴Health Canada

- 2:10 PM (ATOM-11.3) **Pushing the limits of ultra-trace element detection – Offline ExC and automated online ExC-IC-ICP-MS for the speciation analysis of technetium-99**
Maximilian Horstmann¹, C. Derrick Quarles Jr.², Steffen Happel³, Michael Sperling⁴, Andreas Faust⁵, David Clases⁶, Uwe Karst¹ *Institute of Inorganic and Analytical Chemistry, University of Münster*, ²Elemental Scientific, Inc., ³TrisKem International SAS, ⁴European Virtual Institute for Speciation Analysis (EVISA), ⁵European Institute for Molecular Imaging (EIMI), ⁶University of Graz

- 2:30 PM (ATOM-11.4) **LC-ICP-MS measurement of vitamin B12 in foodstuff at NIST**
Lee L. Yu¹ *National Institute of Standards and Technology*

- 2:50 PM (ATOM-11.5) **Considerations for Analysis of Food by ICP-MS**
Mark L. Kelinske¹, Jenny Nelson¹ *Agilent Technologies, Inc.*

24AWD06: Coblenz Society Clara Craver Award Session 301B

Chair: Conor Evans

- 1:30 PM (AWD-06.1) **Correlating in vivo spectral signatures with tissue biochemistry and architecture in eosinophilic esophagitis as a pathway to therapeutic monitoring**
Anita Mahadevan-Jansen¹ *Vanderbilt University*

- 2:10 PM (AWD-06.2) **Unveiling Deep-Seated Tumors with SESORRS**
Fay Nicolson¹, Bohdan Andreiuk², Eunah Lee³, Bridget O'Donnell⁴, Andrew Whitley⁵, Scott Rudder⁶, Samuel Mabbott⁷, Kevin Haigis²
¹Dana-Farber Cancer Institute and Harvard Medical School, ²Dana-Farber Cancer Institute, ³HORIBA Instruments Inc, ⁴Honeywell, ⁵HORIBA Scientific, ⁶Opto Sigma, ⁷Texas A&M University

- 2:30 PM (AWD-06.3) **Generating Single Cell Omics Data from Images with AI**

- Jian shu¹ *Harvard Medical School*
- 2:50 PM (AWD-06.4) **Pharmaceutical imaging with stimulated Raman scattering microscopy: from solid samples to cells**
Dan Fu¹ *University of Washington*

24FORENS05: Early Career Research in Forensic Sciences 303

Chair: Alexis Weber, SupreMETric

- 1:30 PM (FORENS-05.1) **Real-time spectroscopic monitoring of actinide-lanthanide oxide dissolution in organic solutions**
Chelsea M. Goetzman¹, Jarrod M. Gogolski¹, Tracy S. Rudisill¹, Robert Lascola² *Savannah River National Laboratory*, ²SRNL, DOE

- 1:50 PM (FORENS-05.2) **Multi-biochemical analysis of pollen grains for their identification in a forensic context**
Jack A. Trimble¹, Kaitlyn Cierpik¹, Camron Melendez¹, James McAleer¹, Matthieu Baudelet¹
¹University of Central Florida

- 2:10 PM (FORENS-05.3) **Direct Microextraction of Dried Blood Spots for Rapid, Multielement Quantification via ICP-MS**
Cameron J. Stouffer¹, R. Kenneth Marcus¹
¹Clemson University

Next year: October 5-10, 2025 • Northern Kentucky Convention Center

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

2:30 PM (FORENS-05.4) **Exploring a Novel Electrochemical Fabrication Method for Homogeneous Silica Reference Materials**

Peter S. Boone¹, Benjamin Jacobsen¹, Sharee Harris¹, Christina Ramon¹, Jennifer Shusterman¹, Andrew Pascall¹, Tashi Parsons-Davis¹ ¹*Lawrence Livermore National Laboratory*

2:50 PM (FORENS-05.5) **Towards a Stable Matrix-Matched Reference Material for the Analysis of Hair in Forensic Toxicology**

Kaitlyn A. Bonilla¹, Charlene Harris¹, Chloe Phillips¹, Ashley Fox¹, Matthieu Baudelet ¹*University of Central Florida*

Marina De Gea Neves¹ ¹*University Duisburg-Essen*, ²*Chevron*, ³*Chevron Technical Center*, ⁴*Eigenvector Research Inc.*,

1:50 PM (PAT-06.2) **Rapid Surface Chemical Imaging for Dedicated Process Monitoring Application**

Steven Barnett¹, James Chan² ¹*Barnett Technical Services and Soar Optics*, ²*Soar Optics*

2:10 PM (PAT-06.3) **Application of FT-IR Technology to Chevron's Crude Assay Program**

Sherry Alfonso¹ ¹*Chevron*

2:30 PM (PAT-06.4) **Quantification of Asphaltene in Crude Oil by NeoSpectra Handheld FT-NIR**

Marçal Plans Pujolras¹, Toni Miao², Cory McDaniel² ¹*Si-ware*, ²*Chevron*

2:50 PM (PAT-06.5) **CWA and TIC Library Generation and Laboratory Validation on Field Portable FTIR Systems**

Katelyn Koll¹, Evan Durnal¹, Sara Paalhar¹ ¹*MRIGlobal*

24IR11: Advanced Application of Vibrational Spectroscopy 301A

Chair: Michael George, University of Nottingham

1:30 PM (IR-11.01) **Engineering the Electron Transfer Dynamics of Donor-Acceptor Dyads Using Alkyne Bridges**

Kasun C. Mendis¹, Tong Ren², David Beratan³, Igor Rubtsov¹ ¹*Tulane University*, ²*Purdue University*, ³*Duke University*

1:50 PM (IR-11.02) **In-field, Vapor Threat Point Identification Using FT-IR Spectroscopy in Mounted or Dismounted Modalities**

David W. Schiering¹, John Seelenbinder¹, Gregg Ressler¹, Greger Andersson¹, Fred Tauro¹ ¹*908 Devices*

2:10 PM (IR-11.03) **3D Printer fumes: toxic or harmless?**

Sergey Shilov¹ ¹*Bruker*

2:30 PM (IR-11.04) **Detection and Quantification Mixtures of Gas-phase PFAS Mixtures Using Infrared Spectral Libraries and Chemometrics**

Kendall D. Hughey¹, Tracy J. Baker¹, Russell G. Tonkyn¹, Neal B. Gallagher², Nikita Thakur³, Christopher Thompson¹, Yuwei Zhao³, Timothy J. Johnson¹ ¹*Pacific Northwest National Laboratory*, ²*Eigenvector Research Inc.*, ³*APTIM*

2:50 PM (IR-11.05) **Visualization of the human ocular surface in participants with and without dry eye disease using infrared emissivity**

Douglas Borchman¹ ¹*University of Louisville*

24PAT06: PAT in petroleum and refinery industries 302C

Chair: Toni Miao, Chevron

1:30 PM (PAT-06.1) **On-Site Determination of the Total Petroleum Hydrocarbon Content of Soils by Handheld FT-NIR Spectroscopy: Development of a Global, Site- and Instrument-Independent Calibration**

Heinz W. Siesler¹, Toni Miao², Thomas Hoelen³, Barry M. Wise⁴, Frank Pfeifer¹, Cory McDaniel²,

24PMA11: Real time and offline analysis for bioprocessing 4.0 | 306B

Chair: Jason Dickens

1:30 PM (PMA-11.1) **Comprehensive Metals Mass Balance in CHO Cell Processes Using an Automated In-line LC-ICP-MS Platform**

Cameron J. Stouffer¹, Hannah McGrath¹, Sarah Wysor¹, R. Kenneth Marcus¹ ¹*Clemson University*

1:50 PM (PMA-11.2) **Portable Raman Spectrometers, Fluorescence and Lego Blocks**

Richard A. Crocombe, Pauline E. Leary¹, Brooke W. Kammrath ¹*Noble, Inc.*

2:10 PM (PMA-11.3) **LIBS-While-Drilling: A Breakthrough for Real-Time Downhole Analysis**

Pablo Sobron¹, Fredrik Rehnmark¹, Alian Wang², Jie Wei², Abhay Vidwans², Kris Zacny³ ¹*Impossible Sensing*, ²*Washington University in St. Louis*, ³*Honeybee Robotics*

2:50 PM (PMA-11.5) **Quality by design determined spectroscopic and spectrometric control strategies for drop-on-demand point-of-care pharmaceutical manufacturing**

Thomas P. Forbes¹, Greg Gillen¹, William Feeney¹, Johnny Ho¹ ¹*National Institute of Standards and Technology (NIST)*

24RAM11: Enhanced Raman Analysis via hybridization and multivariate approaches | 302B

Chair: NIST TBD

1:30 PM (RAM-11.1) **Analysis of the Early Responses of Viral Infection to Cells by Raman Spectroscopy**

Keita Iwasaki¹, Rheta Elkhaira¹, Hidetoshi Sato² ¹*Kwansei Gakuin University*, ²*School of Biological and Environmental Sciences, Kwansei*

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Oral Symposia | 1:30 PM – 3:10 PM | *Various Locations*

Gakuin University

1:50 PM (RAM-11.2) **Multimodal Confocal Microspectroscopy: Raman and Beyond...**

Angela Flack¹, Samantha Redes¹ ¹*Edinburgh Instruments*

2:10 PM (RAM-11.3) **Analyzing Leaf Pigmentation through Combined Raman and Photoluminescence Spectroscopy**

Matt Gabel¹ ¹*Thermo Fisher Scientific*

2:30 PM (RAM-11.4) **Multiplex SERS Detection of Polycyclic Aromatic Hydrocarbon (PAH) Pollutants in Water Samples Using Gold Nanostars and Machine Learning Analysis**

Joy Q. Li¹, Supriya Atta¹, Tuan Vo-Dinh¹ ¹*Duke University*

2:50 PM (RAM-11.5) **Advancing Raman spectroscopy through machine learning for molecular recognition and ultra-sensitive detection**

VIKAS YADAV¹, Soumik Siddhanta² ¹*Ph.D. Student*, ²*Assistant Professor*

24SPECIAL02: Shootout at Hieftje's Molecular Spectroscopy Corral | 305B

Chair: Jacob Shelley, Rensselaer Polytechnic Institute

1:30 PM (SPECIAL-02.1) **Dielectrophoretic and Thermophoretic Trapping and Guiding of Particles with Micro-Antenna Arrays Embedded in Microfluidic Devices**

Stephen C. Jacobson¹, Brigham L. Pope¹ ¹*Indiana University*

1:50 PM (SPECIAL-02.2) **Midlife Crisis of Gas Sensor Arrays: Signs, Causes, and Treatments**

Radislav Potyrailo

2:10 PM (SPECIAL-02.3) **How did I End Up in This Corral? Was It Because I Followed Hieftje's Advice or Ignored It?**

Michael Blades¹ ¹*The University of British Columbia*

2:30 PM (SPECIAL-02.4) **Atoms are very small... molecules are huge**

J Michael Ramsey¹ ¹*UNC-Chapel Hill*

2:50 PM (SPECIAL-02.5) **Droplets, Ions, and Plasmas: The Bare Necessities of Mass Spectrometry**

Jacob T. Shelley¹, Julia Danischewski¹, Yi You², Samantha E. Pryor¹, Courtney Walton¹, Garrett M. MacLean¹, Douglass Luke¹, Jens Riedel² ¹*Rensselaer Polytechnic Institute*, ²*Federal Institute for Materials Research and Testing (BAM)*

24SPR04: Photothermal plasmonics | 306A

Chair: Emilie Ringe, University of Cambridge

1:30 PM (SPR-04.1) **Vibrational Probing of Nonthermal Reactivity**

Prashant K. Jain¹ ¹*University of Illinois Urbana-Champaign*

1:50 PM (SPR-04.2) **Exploring the Mechanisms Behind the Mysterious Changes in the Optical Properties of Photothermally Irradiated Hollow Metallic Nanoshells**

Gregory Wallace¹, Jennifer Gracie², Amritpal Singh¹, Benjamin A. Clark¹, Ewen Smith¹, Tell Tuttle¹, Karen Faulds¹, Duncan Graham¹ ¹*University of Strathclyde*, ²*University of Edinburgh*

2:10 PM (SPR-04.3) **Ultrasensitive Photothermal Detection Modality for Gold Nanostar-Based Lateral-Flow Immunoassay**

Supriya Atta¹, Tuan Vo-Dinh¹ ¹*Duke University*

2:30 PM (SPR-04.4) **Caged Gold Nanostars Provide Improved Thermal and Photostability for Photothermal Monitoring via Full-view Photoacoustic Computed Tomography**

Aidan J. Canning¹, Tri Vu¹, Junjie Yao¹, Tuan Vo-Dinh¹ ¹*Duke University*

2:50 PM (SPR-04.5) **Panel Discussion**

24SPSJ04: Spectroscopy in Far Ultraviolet region | 302A

Chair: Yusuke Morisawa, Kindai University

Co-Chair: Nami Ueno, Rikkyo university

1:30 PM (SPSJ-04.1) **Influence of solvation structure variations induced by organic solvent molecular structures and salts on the electronic states of lithium electrolytes.**

Nami Ueno¹, Satoshi Kudo², Ichiro Tanabe² ¹*Rikkyo university*, ²*Rikkyo University*

1:50 PM (SPSJ-04.2) **Observing phase transitions in brine using the far-ultraviolet CTTS band of halogens**

Akifumi Ikehata¹, Yusuke Morisawa² ¹*NARO*, ²*Kindai University*

2:30 PM (SPSJ-04.4) **ATR-FUV spectroscopy for sugars and lipids**

Yusuke Morisawa¹, Yoshiki Hanjo², Sou Morimatsu² ¹*Kindai University*, ²*Graduate school of science and engineering, Kindai University*

2:50 PM (SPSJ-04.5) **Food analysis by catalytic kinetic method: Iodine contents in foods**

Surendra Prasad¹ ¹*The University of the South Pacific, Suva, Fiji*

TECHNICAL PROGRAM - THURSDAY, OCTOBER 24, 2024

Innovation Award Session | 3:30 PM – 5:30 PM | *Ballroom A*

3:30 PM **Calibration by Proxy**

Willis B. Jones¹, Abigail J. Crossman¹, Bradley T. Jones² ¹*University of North Florida*, ²*Wake Forest University*

4:30 PM **Advanced Repetition-Rate Modulation and Computational Strategies for Background-Free LIBS Using Non-Gated Spectrometers**

Yi You¹, Boyang Xue², Jens Riedel¹ ¹*Federal Institute for Materials Research and Testing (BAM)*, ²*Institute of Oceanographic Instrumentation, Qilu University of Technology (Shandong Academy of Sciences)*

5:00 PM **Development of Atomic Force Microscopy-Based Two-dimensional Infrared Nano-spectroscopy**

Xiaoji Xu¹, Qing Xie¹ ¹*Lehigh University*

5:30 PM **Entropically Induced Negative Absolute Temperature During Epoxy-Amine Polymerization**

Robert V. Chimenti, Samuel E. Lofland¹ ¹*Rowan University*

TECHNICAL PROGRAM - FRIDAY, OCTOBER 25, 2024

SciFri & Closing Sessions | 8:45 AM – 10:00 AM | *Room 304*

8:45 AM **Innovation Award Announcement**

24SCIFRI: SciFri Talks & SciX 2025 Preview

9:00 AM (SciFri-01.1) **Progress in computers, computer-controlled chemical instrumentation, and computer-assisted chemistry research**

Gary M. Hieftje¹ ¹*Retired*

9:30 AM (SciFri-01.2) **This Title Isn't AI Generated: Perspectives on AI, Machine Learning, and How They Will Revolutionize Chemical Analysis**

Caelin Celani¹, Karl S. Booksh¹ ¹*University of Delaware*

