

FACSS PRESENTS

SciX2019



National Meeting

AES Electrophoresis Society
The Coblenz Society
North American Society for Laser-Induced
Breakdown Spectroscopy (NASLIBS)
Society for Applied Spectroscopy (SAS)



RENAISSANCE

FINAL PROGRAM

OCTOBER 13 - 18

Palm Springs Convention Center - Palm Springs, CA

SciXconference.org

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

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SciX Conference and FACSS International Office

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(856) 224-4266 | facss@facss.org | scix@scixconference.org | www.scixconference.org | www.facss.org

WELCOME TO SciX 2019

On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) it is our pleasure to welcome you to the SciX 2019 Conference. We are excited to be in a brand-new venue for SciX in the Great American West – Palm Springs California – allowing us to expand the technical program, offer new workshops, and enable new networking opportunities.

We now have 15 FACSS member organizations from around the world working together to host a “right sized” conference. SciX 2019 is the National Meeting for the Society for Applied Spectroscopy, the AES Electrophoresis Society, the Coblenz Society, and the North American Society for Laser Induced Breakdown Spectroscopy. We would also like to welcome the newest FACSS member, the Society for Archaeological Sciences. As in the past, the heart of SciX is the technical program, this year organized under the leadership of the Program Chair, Garth Simpson. The Sunday Keynote speaker is our opening event and features Rohit Bhargava discussing the convergence of measurement and data sciences.

Kicking off every morning we have plenary talks featuring our award-winning colleagues, followed by award sessions throughout the day honoring their contributions. Award winners, their presentations, and sessions are prominently identified throughout the program and on the SciX mobile app (download the app for Android or iPhone for the most up-to-date information). Equally important are the poster sessions that feature everyone from students to early-career professionals to seasoned scientists and allow for more in-depth, but relaxed, discussions. Under the guidance of the Program Chair, the Section Chairs and Session Chairs have worked hard to organize symposia across many interesting topics and applications within the analytical sciences. The chairs also secure financial support from our sponsoring industrial partners. These funds go directly into the program to help bring in the best and brightest as our presenters. We also are pleased to honor the finalists in the competitive FACSS Innovation Award session on Thursday afternoon. We close out the technical program on Friday morning with special session entitled “Data Science Meets Measurement Science”.

A major goal for SciX is to support networking opportunities for every SciX attendee. Please be sure to check the program for all the networking opportunities that range from coffee breaks, lunches, poster sessions, and evening events. Everyone at SciX is welcome to put on their most Hollywood outfit and join us for the Wednesday night “A Night at the Oscars” all-inclusive event (food, drinks, entertainment).

SciX Conference is here to meet your needs – please let us know how we did and how we can improve by filling out the survey emailed to you after the conference ends. Also, every year many volunteers work behind the scenes to make the conference what it is – if you want to join the team, please contact FACSS, SciX, or your member society and volunteer! In addition, the SciX 2019 team thanks Kristin Burke, Tina Squillante, and Gina Pozielli at the FACSS / SciX International Office for their service and dedication.

Mark A. Hayes
SciX2019 General Chair



SciX 2019 General Chair
Mark Hayes
Arizona State University
mhayes@asu.edu



SciX 2019 Program Chair
Garth Simpson
Purdue University
gsimpson@purdue.edu



SciX 2019 Exhibits Chair
Michael Carrabba
Droplet Measurement Technologies
mcarrabba@rrslabs.com



SciX 2019 Workshops Chair
Robert Chimenti
RVC Photonics / Rowan University
rchimenti82@gmail.com



SciX 2019 Local Chair
Christopher Harrison
San Diego State University
charrison@sdsu.edu



FACSS & SciX Marketing Chair
John Wasylyk
Bristol-Myers Squibb
john.wasylyk@bms.com

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

2019 FACSS Executive Committee



Governing Board Chair: Fred LaPlant
3M Biopharmaceutical Purification Business Unit
 flaplant@mmm.com

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

Past Governing Board Chair: Steven Ray, *SUNY Buffalo*

Secretary: Glen Jackson, *West Virginia University*

Treasurer: Ian Lewis, *Kaiser Optical Systems*

Marketing Chair: John Wasyluk, *Bristol-Myers Squibb*

SciX 2019 Program Section Chairs

Awards	Mary Kate Donais , <i>Saint Anselm College</i>
LIBS	Francois Doucet , <i>Elemission</i>
AES	Sagnik Basuray , <i>New Jersey Institute of Technology</i>
Atomic Spectroscopy	Adam Woolley , <i>Brigham Young University</i>
Biomedical and Bioanalytical	Jorge Pisonero , <i>Universidad de Oviedo</i>
Chemometrics	Derrick Quarles Jr. , <i>Elemental Scientific</i>
Contemporary Issues in Analytical Science	Karen Esmonde-White , <i>Kaiser Optical Systems</i>
Forensics and Security	Juergen Popp , <i>Friedrich Schiller University Jena</i>
Mass Spectrometry	Peter Harrington , <i>Ohio University</i>
Molecular Spectroscopy (IR)	Rebecca Airmet , <i>Airmet Editing</i>
Nanotechnology	Greg Klunder , <i>Lawrence Livermore National Laboratory</i>
Pharmaceutical Analysis	Robert Lascola , <i>US Dept. of Energy, Savannah River National Laboratory</i>
Process Analytical Technology	Christopher Hendrickson , <i>National High Magnetic Field Laboratory</i>
Raman Spectroscopy	Glen Jackson , <i>West Virginia University</i>
Spectroscopical Society of Japan	Curt Marcott , <i>Light Light Solutions</i>
Special Sessions at SciX 2019	Michael George , <i>University of Nottingham</i>
Surface Plasmon Resonance	Bernhard Lendl , <i>TU Wien</i>
	Wei Zhao , <i>University of Arkansas at Little Rock</i>
	Anna Luczak , <i>Bristol-Myers Squibb</i>
	John Wasyluk , <i>Bristol-Myers Squibb</i>
	James Rydzak , <i>Specere Consulting</i>
	Xiaoyun (Shawn) Chen , <i>Dow Chemical</i>
	Duncan Graham , <i>University of Strathclyde</i>
	Ian R. Lewis , <i>Kaiser Optical Systems, Inc.</i>
	Pavel Matousek , <i>Rutherford Appleton Laboratory</i>
	Yukihiro Ozaki , <i>Kwansei Gakuin University</i>
	Shigeaki Morita , <i>Igor Lednev</i> , <i>Yusuke Morisawa</i> , and <i>Yuika Saito</i>
	Garth Simpson , <i>Purdue University</i>
	Robert Lascola , <i>Savannah River National Laboratory</i>
	Andrew Whitley , <i>HORIBA Scientific</i>
	Jean-Francois Masson , <i>Université de Montreal</i>
	Kateryna Artyushkova , <i>Physical Electronics</i>

GENERAL INFORMATION

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

CONFERENCE REGISTRATION / INFORMATION DESK is located in Mesquite G-H and hours are as follows:

Sunday	3:00 pm – 8:00 pm
Monday	7:00 am – 6:30 pm
Tuesday, Wednesday, Thursday	7:30 am – 5:00 pm
Friday (Renaissance Foyer)	7:30 am – 10:00 am

INTERNET ACCESS is available in all meeting areas. Select the FACSS_SciX network and use password scix2019 (all lower case).

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. See the registration desk if you need to preview your slides.

ORAL SYMPOSIA are scheduled Monday through Thursday.

Morning Session	Mon: 10:50 am – 12:30 pm
	Tu-Thu: 9:15 am – 10:55 am
Early Afternoon Session	1:30 pm – 3:10 pm
Late Afternoon Session	3:50 pm – 5:30 pm

POSTER SESSIONS

Sunday, Primrose Foyer

7:15 – 9:00 pm SAS Student Poster Session

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

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

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

Monday - Primrose Foyer

Hang posters for inspection between 8:30 am – 9:30 am

Attend poster: 9:45 am – 10:45 am

Attend poster: 3:10 pm – 3:50 pm

Remove poster by 4:00 pm

Tuesday and Wednesday - Exhibit Hall

Hang posters for inspection between 10:00 am – 10:45 am

Attend poster: 11:00 am – Noon

Attend poster: 3:10 pm – 3:50 pm

Remove poster by 4:00 pm

Thursday - Primrose Foyer

Hang posters for inspection between 10:00 am – 10:45 am

Attend poster: 11:00 am – Noon

Attend poster: 3:10 pm – 3:50 pm

Remove poster by 4:00 pm

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 36 for all course offerings.

EXHIBITS information is available on page 8. Hours are:

Monday (Opening Reception)	5:30 pm – 7:30 pm
Tuesday	10:00 am – 4:30 pm
Wednesday	10:00 am – 4:00 pm

WHAT'S HOT EXHIBITOR PRESENTATIONS

Sunday, 4:20 pm – 6:00 pm, *Primrose A*

Tuesday, 11:40 am – 1:10 pm, *Exhibit Hall*

Wednesday, 11:50 am – 1:00 pm, *Exhibit Hall*

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

BREAKS coincide with poster viewing sessions.

Monday breaks, *Primrose Foyer*

9:45 am – 10:45 am & 3:10 pm – 3:50 pm

Tuesday and Wednesday breaks, *Exhibit Hall*

11:00 am – 11:45 am & 3:10 pm – 3:50 pm

Thursday breaks, *Primrose Foyer*

11:00 am – 11:45 am & 3:10 pm – 3:50 pm

COMPANION REGISTRATION includes the Sunday Evening Welcome Mixer, Monday Exhibit Hall Opening Reception, and Wednesday Night at the Oscars Gala Event. Cost is \$75 and companions may be added at registration.

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

Welcome Mixer and SAS Sponsored Student Poster Session

Sunday, 7:15 pm, Primrose Foyer

Exhibit Opening and Reception

Monday, 5:30 pm, Exhibit Hall (Oasis)

A Night at the Oscars Gala Event

Wednesday, 6:30 pm, Primrose Foyer

Come dressed to impress!

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



Manage your schedule
Download the free app

Scan the QR codes or enter the URL in your device's browser to download










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etvchairs.com

EVENTS OF INTEREST TO STUDENTS

SUNDAY

- Welcome Mixer and SAS Sponsored Poster Session, 7:15 - 9:15 pm, *Primrose Foyer*
Student Award presentations by SAS, FACSS, Coblenz, and AES

MONDAY through FRIDAY

- FACSS Student Poster Awards will be announced daily at 7:50 am before each Plenary Session in Primrose A

MONDAY

- Coblenz Speed Mentoring, 11:45 am - 1:30 pm (seating is limited), *San Jacinto*

MONDAY through THURSDAY

- Job Board, *Registration Area, Mesquite G-H*

JOB BOARD

There is a job board located in Mesquite G-H in the registration area.

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.

CONFERENCE REGULATIONS AND CODE OF CONDUCT

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

General:

1. There is no smoking in any conference areas.
2. An official name badge is required at all times.
3. No advertising may be placed in the conference areas.
4. Only official exhibitors may display in the Exhibit Hall.
5. No demonstration of instrumentation or distribution of any type of literature is allowed outside the Exhibit Hall.

While in Sessions:

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

Expected Behavior throughout the Conference:

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

Unacceptable Behavior:

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

JOIN US WEDNESDAY NIGHT AT OUR SPECIAL EVENT FOR ALL SciX ATTENDEES



The SciX 2019 GALA

A NIGHT AT THE OSCARS

WEDNESDAY AT 6:30 PM

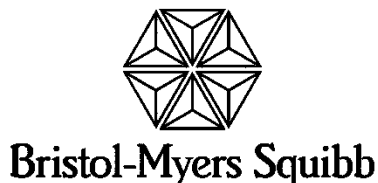
Food, Fun, Libations, and Networking!

This exciting event is included with your SciX registration
Dress in your best Hollywood chic or
come as your favorite celebrity

ADMIT ONE

TICKET NO. 2019

PLATINUM SPONSORS



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FOUNDATION**

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Kaiser Optical Systems, Inc.
Necsel IP
Lumibird, Inc.
Wasatch Photonics

AES

ACS Division of Analytical Chemistry
Royal Society of Chemistry

ATOMIC SPECTROSCOPY

Advion
Agilent Technologies, Inc.
Analytik Jena US LLC
Applied Spectra, Inc.
Elemental Scientific
HORIBA Scientific
Innovative Solutions in Chemistry, S.L.
JAAS
LECO Corporation
Nu Instruments
SciAps, Inc
Thermo Fisher Scientific

AWARDS

Royal Society of Chemistry
Thermo Fisher Scientific

CHEMOMETRICS

Center for Intelligent Chemical Instrumentation
Eigenvector Research, Inc.
GERSTEL Inc.
HORIBA Scientific
JEOL USA, Inc
Society for Applied Spectroscopy

CONTEMPORARY ISSUES

Society for Applied Spectroscopy

FORENSICS

Agilent Technologies, Inc.
JASCO
Metrohm USA
Pace Analytical Services, LLC

IR/MOLECULAR SPECTROSCOPY

Bruker
neaspec GmbH
Photothermal Spectroscopy Corp

LIBS

Applied Spectra, Inc.
Avantes
LTB Lasertechnik Berlin GmbH
OptoSigma
RPMC Laser
SciAps, Inc

MASS SPECTROMETRY

Agilent Technologies, Inc.
Bruker Daltonics
Omata Labs LLC
Phenomenex

NANO

MSE Supplies

PHARMACEUTICAL

Amgen Inc.
Bristol-Myers Squibb
Kaiser Optical Systems, Inc.
MarqMetrix Inc.
Metrohm USA
Thermo Fisher Scientific

PROCESS ANALYTICAL TECHNOLOGY

Biogen
CPACT
Hellma USA
Metrohm USA

RAMAN

Agilent Technologies, Inc.
Metrohm USA
Ondax, now a Coherent company

SPECIAL SESSIONS

Elsevier
Far Western Anthropological Research Group
Meinhard-Elemental Scientific
SciAps, Inc
The Society for Archaeological Sciences

SPSJ

Japan Council for Near Infrared Spectroscopy

STUDENT SPONSORS

Mary and Mike Carrabba
Society for Applied Spectroscopy

SOCIETY and COMMITTEE MEETINGS

FACSS/SciX

Sunday, October 13

- 1:00 pm - 3:00 pm SciX Long Range Planning Meeting (Conference), *Agua Caliente B*
3:00 pm - 5:00 pm FACSS Long Range Planning Meeting (Federation), *Agua Caliente B*

Monday, October 14

- 12:30 pm - 1:30 pm SciX 2021 Providence: General Meeting, *Agua Caliente B*

Tuesday, October 15

- 12:15 pm - 1:15 pm SciX 2020 Sparks, Nevada: Program Meeting, *Agua Caliente B*

Wednesday, October 16

- 12:15 pm - 1:15 pm SciX 2020 Sparks, Nevada: Budget and Planning, *Agua Caliente B*
3:00 pm - 4:00 pm FACSS Budget and Finance Committee, *Agua Caliente B*

Thursday, October 17

- 12:00 pm - 2:00 pm Executive Committee Meeting (*for the Executive Committee only*)
6:00 pm - 9:00 pm Governing Board Meeting (light dinner will be provided), *Catalina*
9:00 pm Governing Board Chair Reception (delegates and invitees)

COBLENTZ SOCIETY

Monday, October 14

- 7:00 am - 9:00 am Coblentz Annual Member Meeting and Breakfast, *San Jacinto*
11:45 am - 1:30 pm Coblentz Speed Mentoring Session, *San Jacinto*.
The Coblentz Society is hosting a Speed Mentoring Event. Prospective mentors and mentees will interact in a fun, fast-paced one-on-one setting to meet other scientists, expand professional networks, and potentially form a mentoring relationship. Registration is free and lunch will be provided.

SOCIETY FOR APPLIED SPECTROSCOPY

Sunday, October 13

- 8:00 am - 12:00 pm SAS Executive Committee, *Andreas*
7:15 pm - 9:15 pm SAS Student Poster Session, *Primrose*

Monday, October 14

- 9:00 am - 11:00 am SAS Membership/Marketing Committee, *Agua Caliente*
12:00 pm - 2:00 pm SAS Governing Board Meeting, *Andreas*

Tuesday, October 15

- 9:00 am - 11:00 am AMSAS Publications Committee, *Andreas*
12:00 pm - 2:00 pm SAS Editorial Board Meeting, *Andreas*
7:00 pm - 8:00 pm SAS Award Presentations, *Catalina*
8:00 pm SAS Members' Wine and Cheese Reception, *Santa Rosa and San Jacinto*

NASLIBS

Monday, October 14

- 5:30 pm - 7:30 pm NASLIBS Board Meeting, *Agua Caliente B*

AES ELECTROPHORESIS SOCIETY

Sunday, October 13

- 4:00 pm - 8:00 pm AES Board Meeting, *Santa Rosa*

Monday, October 14

- 12:00 pm - 1:00 pm AES Lunch with Leaders, *Santa Rosa*

Tuesday, October 15

- 11:45 am - 1:00 pm AES Business Meeting, *Ventura*

SciX EXHIBITS KEY

Check out the mobile app for the interactive exhibit floor plan and exhibitor descriptions!

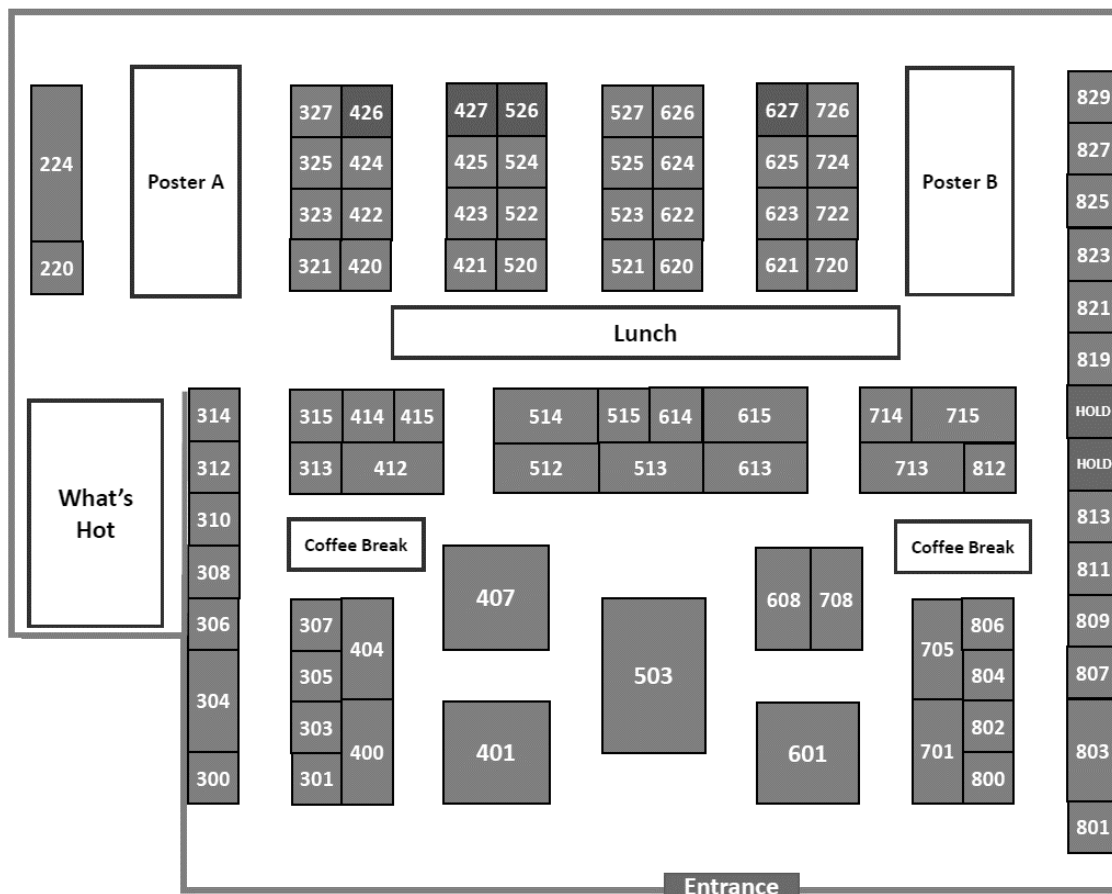


ABB Measurement & Analytics.....	515	Eigenvector Research, Inc.	321	Photon Systems.....	714
ACS Division of Analytical Chemistry.....	424	EmVision LLC.	305	Photothermal Spectroscopy Corp	608
Advion.....	527	FACSS / SciX.....	827	PIKE Technologies.....	301
AES Electrophoresis Society.....	425	Fette Compacting.....	825	Pittcon 2020.....	422
Agilent Technologies, Inc.	613	FiberTech Optica, Inc.	520	Princeton Infrared Technologies, Inc.	415
Alluxa.....	809	Hamamatsu Corporation.....	807	R Specialty Optical Fibers	622
Andor Technology.....	315	Harrick Scientific.....	811	Renishaw, Inc.	400
Anton Paar USA.....	806	Hellma USA	522	Royal Society of Chemistry	525
Applied Spectra, Inc.	404	HORIBA Scientific	503	RPMC Lasers, Inc.....	314
Armadillo SIA.....	802	Ibsen Photonics.....	300	SCIEX	623
art photonics GmbH	220	ICP Information Newsletter, Inc.....	625	Sentronic GmbH.....	819
Avantes.....	420	Innovative Photonic Solutions.....	407	Shimadzu Scientific Instruments, Inc.	312
B&W Tek.....	421	JASCO.....	303	Society for Applied Spectroscopy	224
Barnett Technical Services	514	Kaiser Optical Systems, Inc.....	401	Society for Archaeological Sciences . 523TT	
BaySpec, Inc.....	624	Keit Spectrometers	307	Specac, Inc.....	310
Beijing RealLight Technology Co., Ltd	414	Lumibird (formerly Quantel Laser)	423	Spectral Systems LLC	821
Biophotonics, a Photonics		Malvern Panalytical.....	724	Spectroscopy Magazine /	
Media Publication.....	626	Metrohm USA	512	LCGC Magazine.....	304
Bio-Rad Laboratories,		MONTFORT Laser GmbH.....	621	Spring SciX	524
Informatics Division.....	812	Mott Cororation	306	Teledyne Princeton Instruments	715
Broadcom.....	521	Neaspec GmbH.....	823	Thermo Fisher Scientific	615
Bruker Corporation.....	803	Necsel IP	513	Timegate Instruments Ltd.....	708
California State Polytechnic University		NKT Photonics.....	800	Tornado Spectral System.....	701
Pomona.....	325	Ocean Insight.....	601	TSI ChemLogix Inc	614
CloudMinds Technology, Inc	813	Ondax, now a Coherent company.....	705	Wasatch Photonics.....	713
Coblentz Society	327	OPCO Laboratory.....	720	WITec Instruments Corp.	313
Cobolt by HUBNER Photonics	722	Optigrate Corp.....	412		
Czitek	726	OptoSigma.....	308		
DRS Daylight Solutions	801	Pendar Technologies.....	620		
Edinburgh Instruments.....	804	PerkinElmer	323		

SciX EXHIBITS AND EXHIBIT HALL ACTIVITIES

The exhibit hall is a focal point of the SciX Conference. Exhibits are the realization of the research presented during the scientific symposia and displays include innovative instrumentation, software, and supplies. View technologies and products and connect with a wide-ranging mix of representatives with sales, scientific, and engineering expertise.

Sunday, October 13

4:20 pm - 6:00 pm What's Hot Exhibitor Presentations, *Primrose A*

Monday, October 14

5:30 pm - 7:30 pm Exhibit Hall Opening Reception, *Exhibit Hall (Oasis Ballroom)*

5:30 pm - 6:30 pm Drop raffle ticket at HORIBA Scientific booth or Ocean Insight booth for a chance to win an iPad

6:30 pm Be present at the HORIBA booth to win

7:15 pm Be present at the Ocean Insight booth to win

Tuesday, October 15 and Wednesday, October 16, *Exhibit Hall (Oasis Ballroom)*

11:00 am - 12:00 pm Poster session and break

11:40 am - 1:10 pm What's Hot Exhibitor Presentations (11:50 am on Wednesday)

12:00 pm - 12:30 pm Complimentary lunch for all attendees, *ticket required*

1:30 pm - 3:40 pm Drop raffle ticket each day at booth printed on ticket for a chance to win an iPad (Tues-Kaiser; Wed-IPS)

3:10 pm - 3:50 pm Poster session and break

3:40 pm Be present at the designated booth to win

EXHIBITOR DIRECTORY

ABB Measurement & Analytics.....Booth 515

3400, Rue Pierre-Ardouin
Quebec, Canada
new.abb.com

ACS Division of Analytical ChemistryBooth 424

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

AdvionBooth 527

61 Brown Rd. Ste 100
Ithaca, New York 14850
advion.com

AES Electrophoresis Society.....Booth 425

1202 Ann St
Madison, WI 53713
aesociety.org

Agilent Technologies, Inc.Booth 613

2850 Centerville Road
Wilmington, DE 19808
agilent.com

AlluxaBooth 809

3600 N. Laughlin Rd.
Santa Rose, CA 95403
alluxa.com

Andor TechnologyBooth 315

300 Baker Avenue
Concord, CT 01742
andor.com

Anton Paar USABooth 806

10215 Timber Ridge Drive
Ashland, VA 23005
anton-paar.com

Applied Spectra, Inc.Booth 404

46665 Fremont Blvd
Fremont, CA 94538
appliedspectra.com

Armadillo SIA.....Booth 802

1111 Elko Dr. Suite D
Sunnyvale, CA
armadillosia.com

art photonics GmbHBooth 220

Rudower Chaussee 46
Berlin 12489, Germany
artphotonics.com

Avantes.....Booth 420

500 S Arthur Ave, #500
Louisville, CO 80027
avantes.com

B&W Tek.....Booth 421

19 Shea Way, ste 301
Newark, DE 19713
bwtek.com

Barnett Technical ServicesBooth 514

5050 Laguna Blvd., Suite 112-620
Elk Grove, CA 95758
Barnett-Technical.com

BaySpec, Inc.Booth 624

1101 McKay Drive
San Jose, CA 95131
bayspec.com

Beijing RealLight Technology Co., Ltd.....Booth 414

139 Jinghai 3rd Road, Room 501, Building F
Beijing, 100176 China
http://real-light.com

Biophotonics, a Photonics Media PublicationBooth 626

100 West Street, 2nd floor
Pittsfield, Massachusetts 01201
photonics.com

Bio-Rad Laboratories, Informatics Division.....Booth 812

2000 Market Street, Suite 1460
Philadelphia, PA 19103
knowitall.com

Broadcom.....Booth 521

WernerwerkstaBe 2
Regensburg, Bayern 93049
wwwbroadcom.com

Bruker CorporationBooth 803

40 Manning Rd
Billerica, MA 01821
bruker.com/optics

California State Polytechnic University PomonaBooth 325
3801 W. Temple Ave
Pomona, California 91768
cpp.edu

CloudMinds Technology, Inc......Booth 813
4500 Great America Parkway, Suite 230
Santa Clara, CA 95054
cloudminds.com

Coblentz SocietyBooth 327
955 Drew Lane
Ashland, OR 97520
coblentz.org

Cobolt by HUBNER Photonics.....Booth 722
Vretenvagen 13
Solna 17154, Sweden
cobolt.se

Czitek.....Booth 726
6 Finance Dr
Danbury, CT 06810
czitek.com

DRS Daylight Solutions.....Booth 801
15378 Avenue of Science, Suite 200
San Diego, CA 92128
daylightsolutions.com

Edinburgh Instruments.....Booth 804
2 Bain Sq
Kirkton Campus
Livingston, Scotland EH54 7DQ
edinst.com

Eigenvector Research, Inc.Booth 321
196 Hyacinth Rd
Manson, WA 98831
eigenvector.com

EmVision LLC.....Booth 305
1471 F Road
Loxahatchee, FL33470
emvisionllc.com

FACSS / SciXBooth 827
19 Mantua Rd
Mt. Royal, NJ 08061
facss.org / scixconference.org

Fette Compacting.Booth 825
400 Forge Way
Rockaway, New Jersey 07866
fette-compacting.com

FiberTech Optica, Inc.Booth 520
330 Gage Avenue, Ste 1
Kitchener, ON, N2M 5C6 Canada
fibertech-optica.com

Hamamatsu Corporation.....Booth 807
360 Foothill Road
Bridgewater, NJ 08807
hamamatsu.com

Harrick ScientificBooth 811
141 Tompkins Ave, Box 277
Pleasantville, NY 10570
harricksci.com

Hellma USABooth 522
80 Skyline Drive
Plainview, NY 11704
hellmausa.com

HORIBA Scientific.....Booth 503
3880 Park Avenue
Edison, NJ 08820
horiba.com/scientific

Ibsen Photonics.....Booth 300
Ryttermarken 15-21
Farum, Denmark DK-3520
ibsen.com

ICP Information Newsletter, Inc.Booth 625
PO Box 666
Hadley, MA 01035-0666
http://icpinformation.org

Innovative Photonic Solutions.....Booth 407
4250 U. S. Highway 1, Ste 1
Monmouth Junction, NJ 08852
innovativephotonics.com

JASCOBooth 303
28600 Marys Court
Easton, MD 21601
jascoinc.com

Kaiser Optical Systems, Inc.Booth 401
371 Parkland Plaza
Ann Arbor, MI 48103
kosi.com

Keit Spectrometers.....Booth 307
Rutherford Appleton Lab, R71, Harwell Campus
Didcot, OX11 0QX UK
keit.co.uk

Lumibird Inc.Booth 423
49 Willow Peak Dr
Bozeman, MT 59718
quantel-laser.com

Malvern Panalytical.....Booth 724
117 Flanders Rd.
Westborough, Massachusetts 01581
malvernpanalytical.com

Metrohm USABooth 512
6555 Pelican Creek Circle
Riverview, FL 33578
metrohmusa.com

MONTFORT Laser GmbH.....Booth 621
Im Holderlob 6A
Goetzix, VA 6840, Austria
montfortlaser.com

Mott Corporation.....Booth 306
84 Spring Lane
Farmington, CT
mottcorp.com

Neaspec GmbH.....Booth 823
Bunsenstrasse 5
Martinsried, 82152 Germany
neaspec.com

Necsel IPBooth 513
30-B Pennington-Hopewell Road
Pennington, NJ 08534
pd-ld.com

NKT PhotonicsBooth 800
3514 N. Vancouver Ave Suite 310
Portland, OR 97227
nktphotonics.com

Ocean Insight.....Booth 601
830 Douglas Avenue
Dunedin, FL 34698
oceanoptics.com

Ondax, now a Coherent companyBooth 705
850 E. Duarte Road
Monrovia, CA 91016
ondax.com

OPCO LaboratoryBooth 720
704 River St.
Fitchburg, MA 01420
opcolab.com

Optigrate CorpBooth 412
562 S Econ Circle
Oviedo, FL 32765
optigrate.com

OptoSigmaBooth 308
3210 S. Croddy Way
Santa Ana, CA 92704
america.optosigma.com

Pendar TechnologiesBooth 620
30 Spineli Place
Cambridge, MA 02138
pendartechnologies.com

PerkinElmerBooth 323
940 Winter St.
Waltham, MA 02451
perkinelmer.com

Photon SystemsBooth 714
1512 Industrial Park Street
Covina, CA 91722-3417
photonsystems.com

Photothermal Spectroscopy CorpBooth 608
325 Chapala Street
Santa Barbara, CA 93101
photothermal.com

PIKE TechnologiesBooth 301
6125 Cottonwood Drive
Madison, WI 53719
piketech.com

Pittcon 2020Booth 422
300 Penn Center Blvd #332
Pittsburgh, PA 15235
pittcon.org

Princeton Infrared Technologies, Inc.Booth 415
9 Deerpark Dr, Ste J5
Monmouth Junction, NJ 08852
princetonirtech.com

R Specialty Optical FibersBooth 622
5248 Olde Town Road Suite 13
Williamsburg, VA 23188
rsfibers.com

Renishaw, Inc.Booth 400
5277 Trillium Blvd.
Hoffman Estates, IL 60192
renishaw.com

Royal Society of ChemistryBooth 525
Thomas Graham House, Science Park, Milton Road
Cambridge, UK CB4 0WF
rsc.org

RPMC Lasers, Inc.Booth 314
203 Joseph Street
Ofallon, MO 63366
rpmclasers.com

SCIEXBooth 623
71 Four Valley Dr.
Concord, ON L4K4V8 Canada
sciex.com

Sentronic GmbHBooth 819
sentronic.de

Shimadzu Scientific Instruments, incBooth 312
7102 Riverwood Dr.
Columbia, MD 21046
ssi.shimadzu.com

Society for Applied SpectroscopyBooth 224
168 West Main Street #300
New Market, MD 21774
s-a-s.org

Society for Archaeological SciencesBooth 523TT
PO Box 3003
Lancaster, PA 17604
socarchsci.org

Specac, Inc.Booth 310
414 Commerce Dr, Suite 175
Fort Washington, PA 19034
specac.com

Spectral Systems LLCBooth 821
35 Corporate Park Drive
Hopewell Junction, NY 12533
spectral-systems.com

Spectroscopy Magazine / LCGC MagazineBooth 304
485F US Highway 1 South, Ste 100
Iselin, NJ 08830
spectroscopyonline.com

Spring SciXBooth 524
springscix.org

Teledyne Princeton Instruments, Inc.Booth 715
3660 Quakerbridge Road
Trenton, NJ 01720
princetoninstruments.com

Thermo Fisher ScientificBooth 615
2 Radcliff Road
Tewksbury, MA 01876
thermoscientific.com/portableid

Timegate Instruments LtdBooth 708
Tutkijantie 7
90590 Oulu, Finland
timegate.com

Tornado Spectral SystemBooth 701
555 Richmond Street West, Suite 402
Toronto, ON M5V 3B1 Canada
tornado-spectral.com

TSI ChemLogix Inc.Booth 614
500 Cardigan Road
St. Paul, MN 55126
tsi.com

Wasatch PhotonicsBooth 713
4022 Stirrup Creek Drive, Ste 311
Durham, NC 27703
wasatchphotonics.com

WITec Instruments Corp.Booth 313
130G Market Place Blvd
Knoxville, TN 37922
WITec-Instruments.com

FACSS THOMAS HIRSCHFELD AWARD

*The FACSS Thomas Hirschfeld recognizes outstanding contributions by a Ph.D. or M.Sc. candidate.
There are two recipients in 2019.*

Presented at 7:15 pm Sunday at the Welcome Mixer, Primrose A



Shachi Mittal

University of Illinois Urbana-Champaign

Shachi Mittal is a Beckman Postdoctoral Fellow in University of Illinois at Urbana Champaign. She completed her dissertation work in June 2019 supervised by Prof. Rohit Bhargava in the Department of Bioengineering, University of Illinois at Urbana Champaign. Prior to joining graduate school, Shachi earned both her bachelor's and master's degree in Biochemical Engineering and Biotechnology from the Indian Institute of Technology, Delhi in 2014. She was then selected as an Illinois Distinguished Fellow for her graduate study. Her work focused on developing efficient and robust computational models using spectroscopy data for early cancer detection and prognostic assessment, particularly breast cancer. Her research work has resulted in 13 peer reviewed publications, 10 oral/poster presentations and several awards including Baxter Young Investigator award, invited speaker and first prize winner at Annual Engineering PhD Summit in EPFL, Lausanne, Eastern Analytical Symposium Graduate Student Research award, Nadine Barrie Smith fellowship, Beckman Institute Graduate Fellow and Big Data Summer fellowship.

She has mentored 8 students (high school and undergraduate) to promote research awareness and skill development. Her recent work on building digital tools for identifying different disease states and microenvironment analysis using infrared spectroscopic imaging and machine learning can provide more detailed diagnoses for precise treatment planning. Risk stratification of early stage patients has been a challenge as there are no clinical factors, histopathologic features, or molecular markers that permit reliable assessment of recurrence risk. Consequently, many more women are over diagnosed, resulting in potential short term and long-term morbidities as well as healthcare costs. Therefore, precise diagnosis of in-situ cancer and predictive models for their progression is indispensable for early detection and subsequently improved patient outcome. She has translated her models to discrete frequency measurements for rapid and efficient clinical translation. Her current plan is to combine patient information obtained from chemical imaging, genomics, proteomics, tissue and patient level disease information to identify multilevel statistical associations to drive improved diagnostics, treatment and management of cancer



Erika Portero

University of Maryland College Park

Erika Portero is a Ph.D. candidate in the Department of Chemistry & Biochemistry at the University of Maryland, College Park. Her current research under the supervision of Prof. Peter Nemes aims to develop next-generation mass spectrometry technologies to enable the analysis of small molecules in single cells. Erika is a first-generation college graduate who was born in Ecuador. She earned her B.S. in Chemistry from Drew University in New Jersey and participated in the International Research Experience for Undergraduates program by the National Science Foundation to conduct research at the Université Pierre-et-Marie-Curie in Paris, France. Erika received her M.S. in Chemistry from the George Washington University in Washington D.C. and was awarded a 2017 Graduate Scholar Award by the COSMOS Club Foundation to support financial costs of research during her first year of graduate studies. She also received a 2017 Helmsley Fellowship to attend a Cell and Developmental Biology course at the Cold Spring Harbor Laboratory. Erika is pursuing a Ph.D. in Analytical Chemistry, her research focuses on "Developing Single-cell Mass Spectrometry Tools to Investigate Cell Heterogeneity in the Developing Vertebrate Embryo" with the goal to extend bioanalytical tools for systems cell biology. Erika has disseminated her research via 6 peer-reviewed publications, followed by 2 manuscripts currently in preparation. She has presented at a number of national and international conferences, including the 2017 SciX. Most recently, Erika received a Nico Nibbering Travel Award by the International Mass Spectrometry Foundation to attend the 2018 International Mass Spectrometry Conference in Florence, Italy. During her graduate career, she has served as a mentor to several high school, undergraduate, and graduate students. Erika is committed to help underrepresented students join STEM careers. As such, she served as an ACS Chemistry Ambassador for Project SEED, which supports economically disadvantaged high school students to conduct research at the university level.



FACSS STUDENT AWARD

The prestigious FACSS Student Award recognizes outstanding contributions by a Ph.D. or M.Sc. candidate

Presented at 7:15 pm Sunday at the Welcome Mixer, Primrose A



Ewelina Mistek
SUNY Albany

Ewelina Mistek is a Ph.D. student in Chemistry at the University at Albany, State University of New York and a National Institute of Justice Graduate Research fellow. Ewelina is originally from Bukowno, a small village in Poland. She obtained an Academy Profession Degree in Chemical and Biotechnical Science from the Business Academy Aarhus, University of Applied Sciences in Denmark. During that program, she pursued a one-year internship in a forensic science laboratory with the Lednev Research Group at the University at Albany. After returning to Europe, Ewelina continued her undergraduate program in Forensic and Analytical Science at the Robert Gordon University, earning her Bachelor of Science with Distinction. In 2016, she returned to the University at Albany to pursue her doctorate degree under the mentorship of Professor Igor Lednev.

Ewelina's work involves the application of vibrational spectroscopy and statistical data analysis for the development of new forensic methods with a focus on the identification and characterization of body fluid traces. Her work has been recognized by a number of local, national, and international awards. Besides the prestigious National Institute of Justice Fellowship, Ewelina received the Coblentz Student Award in 2017, the Best Student Poster Award in her session at the 2019 ICAVS conference in Auckland, New Zealand, runner-up in the Three Minute Thesis Competition at the University at Albany, the Francis Dunstan Travel Award to present at the 2018 ICORS conference in Jeju, South Korea, the Ford Foundation Initiatives For Women in Science Fellowship at the University at Albany, the National Institute of Justice Travel Award to present at Pittcon 2018, the Chemistry Department Graduate Student Travel Award, a year membership in the AAAS/Science Program for Excellence in Science, and lastly, she was nominated for recognition at the first "Celebration of Scholarship" at the University at Albany. Just recently, she was also elected to the position of Student Representative of the Society for Applied Spectroscopy.

Ewelina has already published seven articles in peer-reviewed journals including five first-author papers, and one book chapter. Her 2016 Analytical Chemistry article was highlighted on the journal cover. She presented her research at 18 local, national, and international conferences. She was interviewed by the local TV stations, the University's podcast series, and her research was highlighted in the press on several different occasions. Ewelina's research continues to attract the attention of the forensic and spectroscopy societies, as she proceeds to disseminate her research around the world.

FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS CALL FOR 2020 APPLICATIONS

The Tomas Hirschfeld Scholar and the FACSS Student Awards recognize the most outstanding papers submitted to FACSS by a graduate student. Recipients receive financial support to help them attend the SciX conference. To have your presentation considered for one of these awards, students should submit abstracts through the SciX website and indicate during the submission process their interest in these awards.

Look for information online in January 2019 at scixconference.org. The submission process involves submitting an abstract and completing the online form, providing the following as one complete file.

- a) Application form
- b) Copy of abstract submitted to SciX
- c) Two letters of nomination, one of which should be written by the student's mentor. An explanation of the inventive contributions by the student to the work should be given. Creativity was a primary characteristic of Tomas Hirschfeld's work.
- d) Copy of the candidates resumé/CV
- e) Copy of the candidate's graduate transcript
- f) Copies of reprints and/or preprints of research accomplished



FACSS INNOVATION AWARD

The FACSS Innovation Award is given to the most innovative and outstanding new research advancements debuted at the SciX Conference. Only research findings presented for the first time in the public domain qualify for entry (work based on submitted papers not yet published electronically or in print at the time of abstract submission also qualify). Papers submitted for SciX will be considered for these awards – authors indicate during the submission process that they wish to be considered. Finalists present at the SciX conference in an exclusive plenary session on Thursday afternoon, with the award winner(s) selected and announced on Friday morning to conclude SciX 2019. The award includes a cash prize of \$1,000; a plaque; and publicity during and after SciX.

2019 FACSS INNOVATION AWARD SYMPOSIUM

Thursday | 3:50pm – 5:30pm | Primrose A

- 3:50 PM (644) **Accelerated Restricted Boltzmann Machines**
Peter B. Harrington¹, ¹*Center for Intelligent Chemical Instrumentation, OHIO University*
- 4:10 PM (645) **Molecular Basis for Chirality-regulated A β Self-assembly and Receptor Recognition Revealed by Ion Mobility-mass Spectrometry**
Gongyu Li¹, Lingjun Li²; ¹*University of Wisconsin-Madison*, ²*UW-Madison*
- 4:30 PM (646) **Chemical Approaches to Improve Nanopore Single-Molecule Sensing**
Jason R. Dwyer¹, James Hagan¹; ¹*University of Rhode Island*
- 4:50 PM (647) **Enhancing Enantioselective Absorption with Plasmonic and Dielectric Metasurfaces**
John M. Abendroth¹, Michelle Solomon¹, Jack Hu¹, Lisa Poulikakos¹, Amr Saleh¹, Yang Zhao², Jennifer Dionne¹; ¹*Stanford University*, ²*University of Illinois at Urbana-Champaign*

FACSS CHARLES MANN AWARD

For achievements in the field of Applied Raman Spectroscopy
Oral Presentation: 8:00 am | Tuesday | Primrose A
Development of SERS and SESORRS for Multiplexed Bioanalysis



Karen Faulds
University of Strathclyde

Karen Faulds is a Professor in the Department of Pure and Applied Chemistry at the University of Strathclyde and an expert in the development of Raman and surface enhanced Raman scattering (SERS) for novel analytical detection strategies and in particular multiplexed bioanalytical applications. Karen received her PhD from the University of Strathclyde under the supervision of Prof Ewen Smith in 2003 on the detection of drugs of abuse using SERS. She was appointed as a full-time lecturer at the University of Strathclyde in 2006 and promoted to Senior Lecturer in 2010, Reader in 2012 and full Professor in 2015 and she is currently the Head of Bionanotechnology and Analytical Chemistry.

She has published over 130 publications and 5 patents. She has been awarded over £2M in funding as principal investigator from EPSRC, BBSRC, charities, and industry and joint funding in the region of £20 M as a co-applicant. Her research groups' work has been recognized through award of the Nexxus Award (2009), the RSC Joseph Black Award (2013) and the Craver Award (2016). She was elected Fellow of the Royal Society of Chemistry (2012), Fellow of the Society of Applied Spectroscopy (2017) and Fellow of the Royal Society of Edinburgh (2018). She was named one of the Top 50 Women in Analytical Science (2016) and Top 10 Spectroscopist (2017) by The Analytical Scientist. She has given over 70 invited talks at national and international conferences including Thailand, Japan, China, Russia, India, Canada and the USA.

She was elected as the first female and youngest Chair of the Infrared and Raman Discussion Group (IRDG) in 2014 which is the oldest spectroscopic discussion society in the UK and a FACSS member society. She is a member of the FACSS Governing Board and has organized sessions in the Raman program at SciX since 2009. She was involved in organizing Spring SciX, Chaired by Duncan Graham, held in Glasgow, Scotland in April 2018 which was the first SciX meeting held outside of North America. She is also an appointed member of the Royal Society of Chemistry (RSC) Chemical Biology Interface Division and a member of the International Steering Committee of the International Conference on Raman Spectroscopy (ICORS) as well as sitting on several awards committees on behalf of the Coblenz Society and the SAS. She is the Strathclyde Director of the Centre for Doctoral Training in Optical Medical Imaging, serves on the editorial board of RSC Advances and the editorial advisory board for Analyst, Chemical Society Reviews and Analytical Chemistry.



SOCIETY FOR APPLIED SPECTROSCOPY DISTINGUISHED SERVICE AWARD

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

Presented at 7:00 pm Tuesday, Catalina



Michael W. Blades

Recognizing active participation in and longtime service to the Society for Applied Spectroscopy. During his tenure with SAS, Dr. Blades has been a dedicated volunteer, mentor, and leader. Most notably, he served as Applied Spectroscopy Editor-in-Chief and Editor leading the journal through key changes and upgrades. He has been a delegate to the SAS Governing Board and has served on numerous committees. Dr. Blades' willingness to serve SAS in any capacity defines his distinguished service.

Michael Blades received a BSc in Chemistry at St. Mary's University (Halifax, Nova Scotia) and a PhD at the University of Alberta in 1980 (under the supervision of Dr. Gary Horlick) working in the area of plasma spectrochemistry. He subsequently went to Indiana University to work as a postdoctoral fellow in the laboratory of Dr. Gary Hieftje (1980-81). He joined the Department of Chemistry at The University of British Columbia (UBC) in Vancouver 1981 and retired in 2018. Although Michael recently retired he is still engaged in research in a collaboration with several groups at UBC and continues as Editor for Applied Spectroscopy. Mike's current research interests are in the area Raman micro-spectroscopy for biophysical and bio-analytical measurements.

An active researcher and teacher, he and his colleagues have published over 160 papers in refereed journals, is a regular speaker at international symposia and has mentored dozens of undergraduate, MSc, and PhD students and several postdoctoral fellows. He has received a number of honors and awards including the 1987 Canadian Society for Chemistry McBryde Medal awarded annually to a young scientist "in recognition of a significant achievement in pure or applied analytical chemistry", a University of British Columbia Killam Research Prize (1988-89), and a Senior Killam Fellowship (1991-92), the Canadian Society for Chemistry 1994 Fisher Lecture Award, the 1995 Royal Society of Chemistry Analytical Spectroscopy Award, and was named a Fellow of the Society for Applied Spectroscopy in 2009. In 1999 he was the General Chair for the annual Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Meeting and in 2004 he served as the Governing Board Chair for FACSS. He has served on the editorial advisory board of *Analytical Chemistry* and *Spectrochimica Acta (B)* and has served as Editor (2009-2012, 2018-present) and Editor-in-Chief (2012-2018) for *Applied Spectroscopy*. During his tenure as Editor he spearheaded the successful transition to a new publisher (SAGE) for the journal.

His recent retirement has allowed Michael to spend more time doing the things that he loves – hanging out with his grandchildren, playing ice hockey, snowboarding, cycling and windsurfing.



Deborah Peru

Recognizing active participation in and longtime service to the Society for Applied Spectroscopy. During her tenure with SAS, Ms. Peru has been a dedicated volunteer, mentor, and leader. Most notably, she has faithfully served the New York SAS Regional Section for many years with multiple terms as Chair, Secretary, and Webmaster, sometimes filling multiple roles simultaneously. As Chair of the section, she ensured the section had a full schedule of activities and meetings and handled the Gold Medal Award and student awards given by the New York Section.

Deborah (Debbie) Peru is the Owner and President of DP Spectroscopy & Training, LLC. The company provides technical assistance in spectroscopy, data analysis, training development and facilitation. Ms. Peru has more than 35 years of experience working in research and development, manufacturing, and quality assurance environments in many industries including specialty chemicals, and consumer products. Much of her career focused on developing and implementing at-line and on-line spectroscopy methods for use in measuring oral care, personal care, home care and pet nutrition products. Ms. Peru developed numerous applications using Near Infrared, Mid Infrared, Raman, and Surface Enhanced Raman (SERS) spectroscopy for the purposes of quality assurance testing, problem solving, patent applications, and manufacturing cost savings programs.

At Colgate, Ms. Peru worked several years in Clinical Research where she managed development of hard and soft tissue clinical methodologies. Her research was dedicated to characterizing and optimizing clinical devices for use in testing products both in-vivo and in-vitro using instrumentation including white light imaging, and functional near infrared (FNIRS).

Ms. Peru received her B.S. in Nutritional Science and a B.A. in Chemistry from the University of Delaware and earned a Master's in Business Administration degree from the University of Phoenix. Ms. Peru is the current co-Chair, Webmaster, and Secretary of the New York Section of the Society for Applied Spectroscopy. In this role, she organizes monthly meetings, hosts executive officer meetings, and oversees the Website maintenance, Student Award and Gold Medal Award programs.

SOCIETY FOR APPLIED SPECTROSCOPY HONORARY MEMBERSHIP AWARD

Recognizing those individuals who have made exceptional contributions to spectroscopy.

Presented at 7:00 pm Tuesday, Catalina



John F. Jackovitz

Posthumously recognizing Dr. John F. Jackovitz for his active involvement and multiple roles in both SAS and Pittcon over more than 40 years, as well as for his spectroscopic research and student mentoring at the University of Pittsburgh. Dr. Jackovitz embodied the SAS mission of advancing and disseminating knowledge and information concerning the art and science of spectroscopy and other allied sciences, advancing the professional standing and growth of the Society and its members, coordinating cooperative endeavors of its individual members and sections, and promoting and maintaining a close bond among its members.

John F. Jackovitz (Jack) was born in Adamsburg, Pa. on Nov. 9, 1939. He earned his B.S. in Chemistry from St. Vincent College and his Ph.D. in Physical Chemistry at the University of Notre Dame under the guidance of Professors L.F. Pierce and J.L. Walter. It was there that he began study in Spectroscopy. After moving on to a Postdoctoral Fellowship and Visiting Scholar position working with D.F. Shriver at Northwestern University from 1966-67 he accepted a position at Westinghouse Research and Development in Pittsburgh. There he worked on nuclear reactor and battery design and analysis and was an inventor on 36 patents. His collaboration with Professors Sanford Asher and Alexander Star at the University of Pittsburgh focused on mentoring students in research. He played an integral role in bringing modern nanotechnology solutions to the sustainable energy challenges of the future. Jack had untiring dedication to both the Spectroscopy Society of Pittsburgh and the Society for Applied Spectroscopy of Pittsburgh by serving on countless committees. He became President of the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy in 1977, National President of the Society for Applied Spectroscopy in 1981 and SAS Governing Board Delegate from 1999-2016.

His many achievements include the Westinghouse Signature of Excellence and the Special Patent Awards, St. Vincent College Distinguished Alumnus Award, the SAS Distinguished Service Award and being named a SAS Fellow for outstanding contributions in the field of Spectroscopy.

Jack, a wonderful family man, is survived by Maryanne, his wife of 54 years, his brother, his three daughters and three grandchildren.



Isiah Warner

Recognizing Dr. Isiah Warner for his leading research using spectroscopy in applications ranging from chemical separations to nanomaterials and organized media. Most notably, he is recognized for his expertise in the area of fluorescence spectroscopy and is one of the world's experts in analytical spectroscopy.

Professor Isiah Warner is an analytical/materials chemist with more than 360 refereed publications and a dozen acquired or pending patents. He has particular expertise in the area of fluorescence spectroscopy, where his research has focused for more than 40 years. He is considered one of the world's experts in analytical spectroscopy. For example, from 1992 to 2016, he was the corresponding author in the highly cited biannual reviews on "Molecular Fluorescence, Phosphorescence, and Chemiluminescence Spectrometry", for the journal, *Analytical Chemistry*.

Over the past 20 years, he has also maintained a strong research effort in the areas of organized media, separation science, and more recently in the area of ionic liquid chemistry, particularly as applied to solid phase materials for applications in materials science and nanomaterials. He has also conducted educational research that focuses on mechanisms for maintaining and enhancing student education in science, technology, engineering, and mathematics (STEM), with a particular focus on encouraging under-represented students (women and minorities) to pursue terminal degrees in STEM.

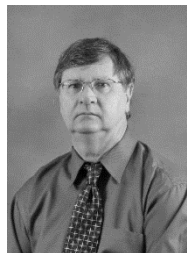
Dr. Warner was recently recognized as 2016 SEC Professor of the Year, member of the American Academy of Arts and Sciences (2016), Fellow of the National Academy of Inventors (2017), Fellow of the Royal Society of Chemistry (2017), and Nature Mentor of the Year (2019). He is Phillip W. West Professor of Chemistry, Howard Hughes Medical Institute Professor at LSU, and has achieved the highest professorial rank in the LSU system, i.e. Boyd Professor. He has chaired sixty-five doctoral theses and is currently supervising seven others. More than half of his doctoral students are women and more than a third are under-represented minorities.



SOCIETY FOR APPLIED SPECTROSCOPY LESTER W. STROCK AWARD

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

Presented at 7:00 pm Tuesday, Catalina



S. Michael Angel
University of South Carolina

Oral Presentation: 8:00 am | Wednesday | Primrose A

Remote LIBS, Raman and Hyperspectral Raman Imaging Using a Monolithic Spatial Heterodyne Spectrometer

Mike Angel is a Professor of Chemistry at the University of South Carolina where he has held the Fred M. Weissman Palmetto Chair in Chemical Ecology since 2005 and named a Carolina Trustee Professor in 2013. He received his PhD from North Carolina State University in 1985 and carried out Postdoctoral work with Tomas Hirschfeld at Lawrence Livermore National Laboratory. Angel's research group works mainly in the areas of remote and in-situ laser spectroscopy with a focus on deep-ocean, planetary, and homeland security applications of Raman and LIBS. Recent work includes developing the spatial heterodyne Raman spectrometer (SHRS), and exploring miniature SHS spectrometers for deep UV Raman, remote Raman and LIBS, underwater LIBS, and for use on future planetary landers and SmallSats.

Angel is an elected Fellow of AAAS and a SAS Fellow and became a member of the Mars 2020 SuperCam science team in 2014. He has been a SAS Tour speaker, an A-Page Advisory Panel member for Analytical Chemistry and editorial advisory board member of Talanta and the International Journal of Spectroscopy, and a member of the scientific committee of NASLIBS and the International LIBS conference. Other honors include the 2015 Southern Chemist Award, 2012 and 2018 Society of Applied Spectroscopy William F. Meggers Award, 2012 ACS South Carolina Chemist of the Year Award, 2011 Federation of Analytical Chemistry & Spectroscopy Societies (FACSS) Innovation Technology Award, and 2006 Lawrence Livermore National Laboratory Physics and Advanced Technologies Directorate Award.

SOCIETY FOR APPLIED SPECTROSCOPY ELLIS R. LIPPINCOTT AWARD

This award is given to honor the memory of Ellis R. Lippincott. The award is sponsored jointly by the Society for Applied Spectroscopy, the Coblenz Society, and the Optical Society of America.

The recipient of the award shall have made significant contributions to vibrational spectroscopy.

Presented at 7:00 pm Tuesday, Catalina



Ji-Xin Cheng
Boston University

Recognizing outstanding contributions in inventing and developing a broad spectrum of vibrational spectroscopic imaging technologies with ground-breaking discoveries and clinical applications.

Oral Presentation: 8:00 am | Monday | Primrose A

From Bond-selective Chemistry to Bond-selective Imaging: My 30 Years' Path to Tackle Missions Impossible

Ji-Xin Cheng attended University of Science and Technology of China (USTC) from 1989 to 1994. From 1994 to 1998, he carried out his PhD study on bond-selective chemistry at USTC. As a graduate student, he worked as a research assistant at Universite Paris-sud (France) on vibrational spectroscopy and the Hong Kong University of Science and Technology (HKUST) on quantum dynamics theory. After postdoctoral training on ultrafast spectroscopy at HKUST, he joined Sunney Xie's group at Harvard University as a postdoc, where he and others developed CARS microscopy that allows high-speed vibrational imaging of cells and tissues. Cheng joined Purdue University in 2003 as Assistant Professor in Weldon School of Biomedical Engineering and Department of Chemistry, promoted to Associate Professor in 2009 and Full Professor in 2013. He joined Boston University as the Inaugural Moustakas Chair Professor in Photonics and Optoelectronics in summer 2017. Cheng received the Craver Award from Coblenz Society in 2015. Cheng and his team has been constantly at the most forefront of the rising field of chemical imaging in innovation, discovery, and clinical translation. Cheng is authored in over 230 peer-reviewed articles with an h-index of 72 (Google Scholar). His research has been supported by over 25 million (\$) fund from federal agencies and private foundations including the Keck Foundation. In 2014 He co-founded Vibronix Inc which has the mission of saving lives through medical device innovations. Cheng is a Fellow of Optical Society of America and a Fellow of American Institute of Medicine and Biological Engineering.



SOCIETY FOR APPLIED SPECTROSCOPY BARBARA STULL GRADUATE STUDENT AWARDS

*Recognizing a graduate student(s) for outstanding research in spectroscopy and presented in honor and memory of our longtime
SAS staff member and colleague Barbara L. Stull*

Presented at 7:00 pm Tuesday, Catalina



Santosh Paidi
Johns Hopkins University

Recognizing outstanding research efforts in the application of Raman spectroscopy and multivariate data analysis to develop novel quantitative approaches for addressing unmet needs in the molecular study of cancers.

Santosh Paidi is a doctoral student in the Department of Mechanical Engineering at Johns Hopkins University. His current research efforts in Dr. Ishan Barman's lab are directed towards application of Raman spectroscopy and multivariate data analysis to develop novel quantitative approaches for addressing unmet needs in the molecular study of cancers. His recent work in this area has resulted in the creation of a new landscape for spectroscopic monitoring of stromal adaptations in the lungs of animals bearing breast tumor xenografts, prior to the arrival of metastatic cancer cells. He demonstrated this by exploiting the unique Raman markers stemming from the stromal modifications (induced by factors secreted from the primary tumor) to develop a decision algorithm for accurate differentiation of premetastatic lungs in mice bearing high metastatic tumor xenografts from those in mice with low metastatic tumor xenografts and normal controls.

In addition to applications in cancer, a major focus of Santosh's graduate study is the development of a detection framework based on label-free plasmon-enhanced Raman spectroscopy for rapid identification of closely related human and murine antibody drugs during their manufacturing, with the ultimate goal of translation to fill-finish sites. Prior to commencing doctoral study at Johns Hopkins, Santosh graduated from Indian Institute of Technology Bombay in 2014 with a B.Tech. in Mechanical Engineering and a minor in Aerospace Engineering. Overall, his research efforts have resulted in 13 peer-reviewed publications in journals such as Cancer Research, Analytical Chemistry and Scientific Reports. He has been awarded the Tomas A. Hirschfeld Scholar Award, Tony B. Academic Travel Award, Whiting School Doctoral Fellowship, Molecular Medicine Tri-Conference Student Fellowship and Undergraduate Research Award by IIT Bombay in recognition of his work. In roles such as GRO Advocacy Chair and WSE Representative on the Homewood Graduate Board, Santosh strove for enriching graduate student experience at Johns Hopkins University. Outside Hopkins, he volunteers for outreach programs aimed at encouraging involvement and enthusiasm of school students in STEM fields. Santosh currently serves as an associate editor for the Journal of Emerging Investigators, which publishes original research conducted by middle and high school students.



Saumya Tiwari
University of Illinois at Urbana Champagne

Recognizing outstanding research on the development and application of spectroscopic imaging to determine patient outcome in colon cancer which adds independently to the current clinical information provided by stage and grade.

Saumya Tiwari earned her B.Tech in Biotechnology from the Indian Institute of Technology, Roorkee, India in 2013. She did her PhD in Bioengineering, with a focus on applied spectroscopic imaging and computational analysis under Professor Rohit Bhargava at University of Illinois at Urbana Champaign. Her thesis focused on development and application of spectroscopic imaging to determine patient outcome in colon cancer which adds independently to the current clinical information provided by stage and grade. In addition to this, she has also worked on integrating genomic information with spectroscopic data to improve and automate outcome in surgical resections and on developing applied computational models to analyze spectroscopic imaging data.

In 2017, she was one of the four graduate students awarded by the Eastern Analytical Symposium for her exemplary research. She has also received the Nadine Barrie Smith Memorial Fellowship, the Beckman Graduate Fellowship, the Biomedical Engineering Society's Graduate Speaker Exchange award, and the award for Best poster presentation at the BMES-FDA Frontiers in Medical Devices Conference. With three first author publications, several secondary author publications as well as three upcoming first author papers under her belt, she continues to work on applying spectroscopic and spectroscopic data to improve patient health and disease outcomes.

**SOCIETY FOR APPLIED SPECTROSCOPY
WILLIAM J. POEHLMAN AWARD**

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

Presented at 7:00 pm Tuesday, Catalina

SAS New York-New Jersey Regional Section

The SAS New York-New Jersey Section is being recognized as this year's outstanding section for maintaining a consistently high level of activity throughout the year and completing many projects which furthered the mission and goals of SAS.

**SAS / NASLIBS AWARD
FOR THE BEST PAPER PUBLISHED IN APPLIED SPECTROSCOPY in 2019
ON LASER INDUCED BREAKDOWN SPECTROSCOPY**

Presented to

Ammon Williams and Supathorn Phongikaroon

for

“Laser-Induced Breakdown Spectroscopy (LIBS) Measurement of Uranium in Molten Salt”

Applied Spectroscopy, Vol. 72, 7

Presented at 7:00 pm Tuesday, Catalina

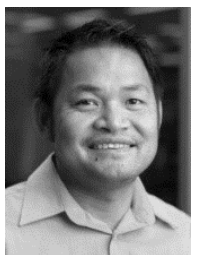


Ammon N. Williams

Idaho National Laboratory

Dr. Ammon Williams received a BS degree in Mechanical Engineering in 2009 from Brigham Young University – Idaho. He then studied Chemical Engineering and earned a MS degree in 2012 from the University of Idaho. Finally, Dr. Williams received his PhD in Nuclear and Mechanical Engineering from the Virginia Commonwealth University in 2016 for his dissertation titled, “Measurement of Rare Earth and Uranium Elements using Laser-Induced Breakdown Spectroscopy (LIBS) in an Aerosol System for Nuclear Safeguards Applications.” Since graduation, he has worked as a research scientist at the Idaho National Laboratory. Dr.

Williams’s current research interest are nuclear safeguards and nonproliferation, specifically, analytical techniques and approaches to monitor special nuclear materials (uranium and plutonium) in harsh and remote environments. Dr. Williams has made significant contributions in the area of molten salt LIBS as well as other measurement approaches such as electroanalytical and bubble level measurement techniques.



Supathorn Phongikaroon

Virginia Commonwealth University

Dr. Phongikaroon is currently an Associate Professor and the Director of Nuclear Engineering Program at the Virginia Commonwealth University (VCU)’s Department of Mechanical and Nuclear Engineering. He earned his PhD and BS degrees in chemical engineering and nuclear engineering from University of Maryland, College Park in 2001 and 1997, respectively. Prior joining VCU in January 2014, he held academic and research positions at University of Idaho in Idaho Falls, ID; Idaho National Laboratory in Idaho Falls, ID; and Naval Research Laboratory, Washington, D.C. During his research career, Dr. Phongikaroon has established chemical and electrochemical separation of used nuclear fuel through pyroprocessing technology and extended his expertise toward reactor physics and material detection and accountability for safeguarding applications using laser spectroscopy techniques. Dr. Phongikaroon’s work has been published in over 40 papers in peer-reviewed journals and presented at over 100 international and national conferences and workshops. Dr. Phongikaroon has been able to maintain continuous diverse research support from international and national programs through Department of Energy, national laboratories, and other universities.

NAS LIBS



SOCIETY FOR APPLIED SPECTROSCOPY WILLIAM F. MEGGERS AWARD

*Recognizing the authors of an outstanding paper appearing in Applied Spectroscopy
Presented at 7:00 pm Tuesday, Catalina*

Presented to

**Timothy J. Johnson, Tanya L. Myers, Russell G. Tonkyn, Tyler O. Danby, Matthew S. Taubman,
Bruce E. Bernacki, Jerome C. Birnbaum, and Steven W. Sharpe**

for

**“Accurate Measurement of the Optical Constants n and k for a Series of 57 Inorganic and
Organic Liquids for Optical Modeling and Detection”**

Applied Spectroscopy 2018, Volume 72

Oral Presentation: 8:00 am | Thursday | Primrose A



Tim J. Johnson is a *cum laude* graduate of Carleton College and received his Ph.D. in Chemical Physics from Washington State University in 1987 where he studied crystallographic effects on the Raman and infrared spectra of solids. This was followed by a Max Planck Postdoc in Germany using diode laser spectroscopy for trace gas detection. Dr. Johnson also

worked in atmospheric trace gas detection using lasers and FTIRs at York University in Toronto, as well as a tenure as applications scientist at Bruker Optics FTIR. Since coming to PNNL in 2000, Dr. Johnson has had experience with spectroscopic signatures, including key contributions to the PNNL gas-phase database. He has also been (co-)PI for other high fidelity spectroscopic signature efforts including for solids and liquids, leading efforts for better quantitation of using both infrared and Raman methods. He also developed novel methods using infrared and visible reflectance spectroscopies for identification of target chemicals via derivation of the n and k optical constants. He is the inventor on two U.S. patents, co-author of one book, as well as the author of over 75 refereed publications.



Dr. Tanya Myers is a Senior Research Scientist at Pacific Northwest National Laboratory. She has over 25 years of extensive experience with laser-based experiments in chemical physics, including high resolution infrared (IR) spectroscopy. She received a Ph.D. and M.S. in chemistry from the University of Chicago and a B.S. degree in chemistry

with honors and distinction from the University of North Carolina at Chapel Hill. Before joining PNNL in 2000, she was a National Research Council Postdoctoral Fellow with NIST at JILA at the University of Colorado in Boulder where she investigated vibrationally-mediated photolysis of size- and quantum state-selected clusters via laser-induced fluorescence. She has extensive experience with cavity enhanced techniques (e.g., cavity ring-down, multi-pass absorption spectroscopy) for trace gas detection using diode and quantum cascade lasers. Her current research includes quantitative measurement of optical constants for solid and liquid materials. She is the author of over 40 refereed publications.



Russell G. Tonkyn received a BA in chemistry from Reed College and a PhD in physical chemistry from the University of Wisconsin at Madison. He received his PhD for work on ion-molecule reaction in the gas phase in 1988, followed by post-doctoral work at Brookhaven National Lab where he studied the pulsed field ionization of extremely high Rydberg states prepared by

single photon absorption. He has been at PNNL since 1992 and has worked on many diverse projects over the years, including various gas, liquid and solid databases using FTIR and Raman spectroscopy.



Tyler O. Danby earned dual bachelor's degrees in biological science and general history from Washington State University in 2015. From 2016 to 2018 he worked at Pacific Northwest National Laboratory as a post-bachelor's research associate in the spectroscopic signatures group. Mr. Danby contributed to several scientific projects during this time, including the accurate measurement of optical constants n and k for liquids.



Dr. Matt Taubman holds a PhD in physics from The Australian National University, Canberra, Australia. He specializes in sensor and detection system design and integration with particular focuses on analog electronics, especially low-noise, high-voltage, precision design. His deep skill set involves servo control

and feedback systems, such as laser locking and stabilization. Systems that Dr. Taubman has developed or helped refine since joining Pacific Northwest National Laboratory in 2000 include ultra-sensitive laser-based instruments such as quantum cascade laser-based chemical sensors, ultra-sensitive unattended sensors and radiation detection systems, and acoustic excitation systems. Dr. Taubman also serves as a Technical Team Lead for the Sensors and Measurement Systems Team within the Advanced Electronic Systems Group at PNNL.





Dr. Bruce Bernacki earned a Ph.D in Optical Sciences from the University of Arizona. Prior to working at Pacific Northwest National Laboratory, he spent nearly five years as Vice President of New Product Development and CTO at LightPath Technologies, in Orlando, Florida. He is now a senior research scientist (2005 – present) in the National

Security Directorate at PNNL. An optics professional with 30 years of experience in optical design, modeling, optical data storage and optical component manufacturing, Dr. Bernacki has worked in both the government and the private sector on basic research and product development. He is the inventor or co-inventor of 12 U.S. patents and the author or co-author of 35 peer-reviewed publications, 46 conference publications and one book chapter. In 2017, he was an R&D 100 Award winner with IRsweep, the sole inventor of the IRcell, and shared a Federal Lab Consortium award with IRsweep in 2019 for excellence in technology transfer. In 2014, he received the Federal Lab Consortium award for technology transfer, as well as an R&D 100 as co-inventor of the Glyph, an immersive head mounted display commercialized by Avegant Corporation. He is a member of the Optical Society of America and a Life Member of IEEE.



Dr. Jerome Birnbaum received a BS in chemistry and math from the College of St. Scholastica in 1979. He worked as an analytical chemist for an EPA accredited water quality laboratory for seven years (he was lab manager for three years) and taught chemistry and math courses part-time at Western Wyoming College. He received a Ph.D. from the University of

Colorado in 1990 for his work in synthetic organometallic chemistry studying the catalytic capabilities of molybdenum hydro-sulfido complexes. He was an assistant professor at Western Wyoming College for eight years before accepting a research position at Pacific Northwest National Lab, where he worked for twenty years. At PNNL, he was a project manager on several programs and authored over 60 refereed publications, over 40 internal DOE reports, and obtained seven patents. He is now working as a research scientist for Ideal Innovations in the Washington, DC area.



Dr. Steven Sharpe obtained a bachelor's degree in chemistry from the University of Bridgeport and a Ph.D. from The State University of New York. He worked as a postdoctoral fellow at the University of Southern California before his 25-year career at the Pacific Northwest National Laboratory, primarily practicing infrared spectroscopy of clusters

and gases. He was the Principal Investigator and lead scientist on the PNNL IR gas-phase database project. He is now retired and living happily ever after.



The Society for Applied Spectroscopy cordially invites
all SAS members to join us at our
annual awards presentation

Tuesday October 15, 2019 at 7:00 p.m.
Catalina Ballroom

Followed by a members only reception at 8:00 pm
San Jacinto and Santa Rosa



Doors will open to non-members at 9
pm with limited refreshments.

To become a member, please go to
www.s-a-s.org or visit SAS booth 224.

SOCIETY FOR APPLIED SPECTROSCOPY SAS FELLOWS AWARDS

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

Presented at 7:00 pm Tuesday, Catalina



Prof. Young Mee Jung was received her B.S., M.S. as well as Ph.D in Chemistry from Kyungpook National University, Korea. During her Ph.D. thesis, she investigated the surface-enhanced Raman scattering (SERS). She studied at Prof. Yukihiro Ozaki group in Kwansei Gakuin University, Japan as a postdoctoral fellow in 1998-2000. She

was a visiting professor in University of California Santa Barbara, USA in 2014-2015.

Her research interest is in the area of spectroscopy, especially 2D correlation spectroscopy (2D-COS) and SERS. She was awarded the Young Physical Chemistry Scientist Award of Korean Chemical Society (KCS) in 2007 and the KCS/Sigma-Aldrich Excellent Chemist Award in KCS in 2014. She was also awarded the Award of Ministry of Science and ICT of Korea in 2019. She has published many papers including book chapters on 2D-COS, SERS and vibrational spectroscopy.

In 2013, she chaired the 7th International Symposium on Two-Dimensional Correlation Spectroscopy (2DCOS-7) in Seoul, Korea. She also chaired the 26th International Conference on Raman Spectroscopy (ICORS 2018) in 2018 Jeju Island, Korea. She is currently an international steering committee of ICORS conferences, a program committee of ICAVS-8, ICAVS-9 and ICAVS-10 (International Conference on Advanced Vibrational Spectroscopy) and an organizing committee of 2DCOS-8, 2DCOS-9 and 2DCOS-10 conferences. She also organized 2D-COS sessions in SciX meeting in 2012 and 2018. She is currently an Associate Editor of Applied Spectroscopy and an Editorial Board of Vibrational Spectroscopy.

Currently she is a professor of Department of Chemistry, Kangwon National University, Korea and well recognized in 2D-COS filed.



Prof. Boris Mizaikoff joined the faculty at the University of Ulm, Germany, as a Chaired Professor and Director at the Institute of Analytical and Bioanalytical Chemistry in 2007 with prior appointments at the Vienna University of Technology (Austria), and at the Georgia Institute of Technology (USA). His

research interests focus on optical chem/bio sensors, tailored (bio)molecular recognition interfaces, molecularly imprinted materials, system miniaturization and integration, and multifunctional (nano)analytical techniques with applications in environmental analysis, process monitoring, and biomedical diagnostics. He is author/co-author of 320+ peer-reviewed publications, 16 patents, and numerous invited contributions at scientific conferences.



David L. McCurdy earned an A.S. degree from Iowa Western Community College in 1977 and a BS degree in chemistry from Northwest Missouri State University in 1979. After graduation, he worked at Streck Laboratories, Inc. in product development and quality assurance. He left the position to attend graduate school in chemistry at Kansas State University in

1983. David earned his Ph.D. in analytical chemistry in 1987 under the direction of Professor Robert C Fry. The same year he began a position as an Assistant Professor of Chemistry at Truman State University. He was appointed Professor of Chemistry in 2000, serving as the Chair of the Department of Chemistry for 3½ years prior to his retirement in 2016. He is presently employed as a Lecturer in Chemistry at the University of Iowa.

David's graduate training was in atomic spectroscopy. In 1999, he served as a visiting research faculty member at Texas A&M University in the lab of Professor David Russell. He has co-authored 15 publications, a book chapter, and more than 75 scientific presentations, most including undergraduate coauthors. David worked with more than 150 students in undergraduate research, with more than 35 of these students continuing at the graduate level to earn a Ph.D. degree in chemistry.

David is a 35-year member of SAS. He was a local section officer of the St. Louis Professional Section for more than 24 years, organized sessions of presentations for the FACSS conference, and served as the Employment Bureau Chairman in 1994. He helped form a student chapter of the SAS at Truman State and served as faculty advisor. More recently, he served on the SAS Awards Committee and Publications Committee as a volunteer and chair. David is also a member of the American Chemical Society, served as a Contributing Editor for the Analytical Sciences Digital Library project (2000-2005) and was the Associate Editor for the Council on Undergraduate Research Quarterly (1996-2000).





Diane B. Parry earned her B.S. in Biology from the University of Cincinnati in 1982. She initially worked at the University of Cincinnati's College of Medicine making monoclonal antibodies, and worked her way up to run a research Fluorescence-Activated Cell Sorter to support a wide range of projects, from

brain cancer to graft-versus-host disease research. Her work to computerize the laser instrumentation came to the attention of a Raman group at the Procter & Gamble Company, and Diane was hired by P&G in 1984.

With P&G, she had a chance to learn about resonance Raman from Professor Sanford Asher, waveguide spectroscopy from Professor Paul Bohn, and met Professors Jeanne Pemberton and Geraldine Richmond in consultation on SERS work. With her employer's support, Diane left P&G to attend graduate school in Physical and Analytical Chemistry at the University of Utah in 1986, under the direction of Professor Joel Harris. After obtaining her PhD in 1989, Diane moved to California to complete post-doctoral work in theoretical chemistry and optical surface science with Professor Michael R. Philpott, at IBM's Almaden Research Center. Diane was re-hired by Procter & Gamble in 1991. Within P&G, she became a manager, leading international teams responsible for analytical measurements, formula design, process design and modeling and simulation. She retired from P&G as an Associate Director, after 28 years, in 2017.

Diane holds over a dozen international patents, has 22 peer reviewed publications and has written two book chapters. Diane received a Distinguished Alumnus Award from The University of Utah Department of Chemistry in 2015. Her science-related volunteer work has included teaching an annual short course "Analytical Chemists in Industry," which was co-sponsored by FACSS and P&G and was free for science students from 1995-2014. Diane also organized special conference sessions to celebrate "Analytical Chemists Easing World Poverty," (ACEWP), which has been a regular part of SciX Programs, since 2011, and was part of PittCon in 2013. Rebecca Airmet took over organizing ACEWP sessions in 2015, and Diane has organized a related session for SciX 2019. Diane and Rebecca co-authored a chapter on ACEWP, published in the 2017 ACS Book "Mobilizing Chemistry Expertise to Solve Humanitarian Problems" edited by Ronda Grosse (Chemists Without Borders). Diane has served on the FACSS/SciX Governing Board and Long Range Planning for many years, and was the FACSS Governing Board Chair in 2006. Diane was the FACSS Distinguished Service Award recipient in 2017. Diane has also served SAS for many years, and was SAS President in 2015. She received an SAS Distinguished Service Award in 2018. Diane is currently the SAS Treasurer and an R&D-related industry consultant.



Shiv K. Sharma is a Professor at the University of Hawaii at the Hawaii Institute of Geophysics and Planetology in the School of Ocean Earth Science and Technology. He is on the Graduate Faculty of the Departments of Earth Sciences and Electrical Engineering. He received his PhD (Physics) in 1973 from the Indian Institute of Technology, Delhi, India. In

1974 he joined as a Research Associate in Professor David Adams' Group in the Department of Chemistry at the University of Leicester, England. From 1977 - 1980 he worked as a Post-Doctoral Fellow at the Geophysical Laboratory of Carnegie Institution of Washington. Since 1980, Sharma's group at the University of Hawaii has been working mainly in the area of in situ and remote laser spectroscopy with focus on Earth, ocean and planetary science, biomedical applications, and homeland security.

Recent work includes development of combined Raman and LIBS technique, standoff underwater Raman and time-resolved spatial heterodyne Raman spectrometer (SHRS), and exploring use of these techniques for future planetary landers and rovers. Sharma is a member of the Mars 2020 SuperCam team. He is serving as a member and Chair Elect for the SAS Lester Strock Award Committee. He is a fellow of the Mineralogical Society of America, National Academy of Sciences - India, and a Senior Member of the Optical Society of America and SPIE. He was awarded by FACSS Innovation Award (2011) and shared the William F. Meggers Award (2012) with Michael Angel for the paper on SHRS.



SAS ATOMIC TECHNICAL SECTION STUDENT AWARD

Recognizing outstanding student research in the area of Atomic Spectroscopy

Presented at 7:00 pm Tuesday, Catalina



Oral Presentation: 3:50 pm | Tuesday

Dr. Carlos Abad is currently a postdoctoral associate at the Federal Institute for Material Research and Testing (BAM) in Germany. Dr. Abad earned his B.S. in Chemistry at the Universidad Central de Venezuela in Caracas, Venezuela, and its German

equivalency at the Georg-August-Universität in Göttingen, Germany. He attended the Graduate School of Analytical Sciences Adlershof (SALSA) and received in spring 2019 his Ph.D. in analytical sciences with honors at the Humboldt-Universität zu Berlin. Dr. Abad was a visiting scientist at the Leibniz-Institute for Analytical Science (ISAS) in Berlin, Germany between 2015-2018 and the Lawrence Berkeley National Laboratory (LBNL) in 2018. During his Ph.D., under the supervision of Dr. Norbert Jakubowski and Prof. Dr. Ulrich Panne, he developed a great passion for spectrochemical analysis by using optical and mass spectrometry. His research interests focus on the development and application of optical spectrometry of transient diatomic molecules for trace analysis of non-metals and stable isotope analysis. Besides lab's work, Dr. Abad is an active science communicator and a member of the Society for Applied Spectroscopy since 2017.



Oral Presentation: 4:50 pm | Wednesday

Htoo Paing is a current 4th year graduate student in analytical chemistry under the mentorship of Dr. Kenneth Marcus at Clemson University. Htoo works to develop the Liquid Sampling Atmospheric Pressure Glow Discharge Plasma (LS-APGD) as a miniature ionization/

excitation source for various applications from nuclear security to pharmaceutical analysis. His research hopes to deconvolute some of mechanisms and processes occurring in the LS-APGD as well as developing methods to improve the analytical performance of the LS-APGD. For his work with ambient desorption LS-APGD, Htoo has most recently been awarded the "Innovations in Nuclear Technology R&D Award" from the Department of Energy. After graduation, Htoo wishes to pursue a career in academia. Htoo spends his time away from the lab playing soccer, playing boardgames sometimes unironically about doing research, and fish keeping.



Oral Presentation: 9:55 am | Wednesday

Joseph E. Lesniewski is a PhD student at Georgetown University, where he works under the guidance of Dr. Kaveh Jorabchi. Prior to his work at Georgetown, he was twice awarded a Summer Undergraduate Research Fellowship (SURF), which supported his research at the National

Institute of Technology (NIST) headquarters in Gaithersburg, MD. While at the NIST Center for Neutron Research (NCNR) his work applied Bayesian statistics to automation of data analysis of neutron and x-ray diffraction data. At Georgetown University, Joseph's work has focused on addressing high-sensitivity elemental quantification of non-metals, such as chlorine and fluorine, for facile quantification of analytes without compound-specific standards. Such analyses are challenging using the current state-of-the-art elemental MS technique, ICP-MS, because of low ionization efficiency of Cl and F in the ICP and occurrence of isobaric polyatomic interferences. Joseph's work has addressed these problems through the development of a new elemental ionization approach where an ICP is used to convert analytes into element-specific neutrals followed by chemical ionization in the atmospheric-pressure afterglow. This method, termed plasma assisted reaction chemical ionization (PARCI), offers improved ionization efficiency and reduced isobaric interferences for F and Cl, while facilitating high-sensitivity elemental analysis using widely available molecular mass spectrometers. Joseph has demonstrated the application of this technique in quantification of infant formula fluoride content. He hopes to further improve sensitivity of non-metal elemental analyses through exploring new ionization chemistries, and to expand the applications of elemental quantification in environmental and pharmaceutical investigations.



Oral Presentation: 9:35 am | Thursday

Ingo Streng is currently a final year Ph.D. candidate in Chemistry at the University of Siegen, Germany under the guidance of Prof. Carsten Engelhard. Prior to his graduate studies, he earned a B.S. and a M.S. degree in Chemistry from the University of Muenster, Germany. Ingo's research focuses on

improving methods and instrumentation for the detection and characterization of single nanoparticles (NPs) using inductively coupled plasma mass spectrometry (ICP-MS). He developed novel data acquisition and processing concepts to overcome current limitations of ICP-MS platforms such as insufficient time-resolution, finite measurement duration, low duty cycle, and other measurement artifacts known to occur in the realm of single-particle ICP-MS (spICP-MS). The benefits of this approach are significant and summarized in his key publication, which was also featured as one of the "Top 30 Most Accessed JAAS Articles in 2016". His advances in spICP-MS could be merged into concurrent studies within the group and resulted in the publication of three additional peer-reviewed papers. Eventually, it enabled the analysis of NPs by means of on-line fractionation/separation, providing an additional layer of information while allowing for a thorough characterization of NPs at environmentally relevant concentration levels. Ingo presented his work at national and international conferences in Europe and the US with several poster and oral talks. Currently he works at the National Institute of Standards and Technology (Gaithersburg, MD), where he continues his research but also helps to establish, evaluate, and improve microsecond time resolved spICP-MS within their laboratories.



SAS UNDERGRADUATE STUDENT AWARD

Given to up to 5 junior or senior undergraduate students in recognition of outstanding research in the area of spectroscopy.
Presented at 7:15 pm Sunday at the Welcome Mixer, Primrose A



Melissa Fernandez

Recognizing work in the development of portable and near-real time analytical technology for carcinogen detection, STEM education among the public, and statistical analysis using Chemometrics.

Melissa is an undergraduate Biomedical Engineering student at South Dakota School of Mines pursuing a medical career in Oncology. Through two years of experience working on this project, she has learned many valuable scientific techniques that will help her become a better physician.



Jessica Hellinger

Recognizing a project to simultaneously obtain elemental and small molecule information with a novel plasma source, the Solution Cathode Glow Discharge (SCGD), via optical emission spectroscopy and mass spectrometry.

Jessica Hellinger was born in Flushing, NY in 1998. She graduated from Nonnewaug High School in Woodbury, CT in 2016 and went on to study chemistry at Rensselaer Polytechnic Institute in Troy, NY. In her free time, she likes to get far too invested in new hobbies like knitting, baking, book binding, and anything else that catches her interest. She also enjoys reading fantasy and sci-fi novels, though she doesn't get too as much as she would hope. Jessica is involved in the chemistry department at her university as the president of the Rensselaer Chemistry Society and a chemistry mentor to incoming freshmen taking Chem I. She finds both rewarding and has made many friends through both groups. During the summer of 2018 she got the Research in Science and Engineering (RISE) internship under DAAD. There she worked in Professor Carsten Engelhard's lab in Siegen, Germany analyzing silver nanoparticles in fish using inductively coupled plasma mass spectrometry (ICP-MS). As her first time out the country she also used this opportunity to travel around Europe and immerse herself in the culture. For the past three years she has been a part of Professor Jacob Shelley's lab working to pair mass spectrometry and optical emission spectroscopy using a solution cathode glow discharge (SCGD) ionization source. Thanks to these opportunities she has been able to present her work at her universities and local ACS meetings undergraduate research symposiums, and the Northeast regional ACS meeting (NERM). She is now in the last year of her bachelor's degree and plans to start applying to graduate school, though the direction of her future is still open.



COBLENTZ SOCIETY CLARA CRAVER AWARD

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



Xiaoyun "Shawn" Chen

The Dow Chemical Company

Oral Presentation: 8:00 | Thursday | Primrose A

Have Fun & Impact with in Situ Spectroscopy in the Chemical Industry

Shawn (Xiaoyun) Chen is currently a senior research scientist working at Core R&D Analytical Sciences, the Dow Chemical Company, where he applies all types of optical spectroscopy tools for problem-solving in both Research & Development and Manufacturing and Engineering projects. Shawn has been leading Dow's global optical spectroscopy technology network since 2013 and also the molecular structure capability since 2016. Shawn has mentored many junior spectroscopists and introduced many non-spectroscopist users such as process engineers and synthetic chemists to the wonderful world of in situ spectroscopy for reaction and process monitoring, and in-field deployment. Shawn's current work involves the collaboration with many world-class experts in their own fields such as organic synthesis, catalyst discovery and development, reaction scale-up and optimization, and process analytical, and accelerate and improve their R&D processes by optical spectroscopy. Shawn has successfully introduced and implemented in situ spectroscopy to more than ten Dow sites globally, which has won him multiple awards within Dow.

Prior to joining Dow, Shawn obtained his PhD at University of Michigan 2002-2007, under the guidance of Professor Zhan Chen. His research focused on the development of sum frequency generation vibrational spectroscopy as a powerful tool to investigate biointerfaces. His thesis research won him multiple prestigious awards such as the 2007 Kasimir Fajans Award, nomination for 2008 National Distinguished Dissertation Award, and 2007 Distinguished Dissertation Awards. Shawn received his B.S. from Tsinghua University, Beijing, China, studying polymeric materials and their applications in tissue engineering.



Shawn has been a member of Society of Applied Spectroscopy and the Coblenz Society since 2013, and is currently serving on the Board of managers for the Coblenz Society, and as the Newsletter Editor for the Society of Applied Spectroscopy. Shawn has been chairing a session on industrial applications of vibrational spectroscopy at SciX every year since 2015.



SPEED MENTORING

JOIN US MONDAY AT 11:45 AM
[LUNCH FOR THOSE
PRE-REGISTERED]
SAN JACINTO ROOM
RENAISSANCE HOTEL

Students • Post Docs • Young Professionals
Get your questions answered about working in
industry, academia, and national labs
in a one-on-one setting with experienced professionals.
Sign up at <https://members.coblenz.org/event-3355333>



COBLENTZ SOCIETY WILLIAM G. FATELEY STUDENT AWARD

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



Presented at 7:15 pm Sunday at the Welcome Mixer, Primrose A



Shachi Mittal

University of Illinois at Urbana Champaign

Shachi Mittal is currently a final year graduate student in the Department of Bioengineering at University of Illinois at Urbana Champaign. Her current research in Prof. Rohit Bhargava's lab focuses on developing efficient and robust computational models using spectroscopy data for early cancer detection and prognostic assessment, particularly breast cancer. Risk stratification of early stage patients has been a challenge as there are no clinical factors, histopathologic features, or molecular markers that permit reliable assessment of recurrence risk. Consequently, many more women are over diagnosed, resulting in potential short term and long term morbidities as well as healthcare costs. Therefore, precise diagnosis of in-situ cancer and predictive models for their progression is indispensable for early detection and subsequently improved patient outcome. Her recent work on building digital tools for identifying different disease states and microenvironment analysis using infrared spectroscopic imaging and machine learning can provide more detailed diagnoses for precise treatment planning. She has translated her models to discrete frequency measurements for rapid and efficient clinical translation. Her future goal is to combine patient information obtained from chemical imaging, genomics, proteomics, tissue and patient level disease information to identify multilevel statistical associations to drive improved diagnostics, treatment and management of cancer.

Prior to graduate school, Shachi earned Bachelor's and Master's degrees in Biochemical Engineering and Biotechnology from the Indian Institute of Technology, Delhi in 2014. She's had 13 peer reviewed publications and awards including Baxter Young Investigator award, invited speaker at Annual Engineering PhD Summit in EPFL, Lausanne, Eastern Analytical Symposium Graduate Student Research award, Nadine Barrie Smith fellowship, Beckman Institute Graduate Fellow, Big Data Summer fellowship and Illinois Distinguished Fellowship.

COBLENTZ SOCIETY STUDENT AWARD

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.

Presented at 7:15 pm Sunday at the Welcome Mixer, Primrose A



Nicole Ralbovsky

University of Albany, SUNY

Nicole Ralbovsky is a third-year doctoral candidate in Dr. Igor K. Lednev's laboratory at the University at Albany, SUNY. Her research focuses on developing a novel method for medical diagnostics which uses Raman hyperspectroscopy in combination with advanced statistical analysis. Nicole has had great success in developing the technique and has published an article in Biophotonics magazine describing the methodology. Specifically, Nicole was able to apply the method for diagnosing Alzheimer's disease through investigation of saliva, achieving over 99% accuracy. Nicole has extended her research efforts toward diagnosing Celiac disease, muscular dystrophy, diabetes, and Lyme disease. Nicole has three first-author manuscripts published and has recently submitted two additional manuscripts, with several others in progress. The advantage of her developed methodology resides in the ability to definitively, quickly, and accurately make a diagnosis in a cost-effective and non-invasive manner – thus providing a significant advantage over current diagnostic procedures. Nicole received a grant from the State University of New York Technology Accelerator Fund and an NIH-funded RNA fellowship awarded by SUNY Albany to pursue this research.

In addition to the progress she has made regarding her research, Nicole has also maintained an overall 4.0 GPA and was the two-time recipient of SUNY Albany's Harry L. Frisch Memorial scholarship in Chemistry as a result of her academic achievements. Nicole was an invited speaker at Pittcon 2019, was the recipient of the Ford Foundation Initiatives for Women in Science Fellowship, and has been the recipient of multiple travel awards, including five awards presented to her by SUNY Albany, an ACS Women Chemists Committee/Eli Lilly and Company co-sponsored award, and an award sponsored by SCIEX to attend the 2019 International Symposium on Microscale Separations and Bioanalysis. What's more, Nicole has demonstrated her ability to successfully balance her academic career with community outreach and volunteerism; she spends time participating in SUNY Albany's Graduate Student Club for Chemistry, where she is the secretary, is involved in SUNY Albany's Graduate Student Association, volunteers with the Alzheimer's Association, and spends many weekends throughout the year at her local church, volunteering with various projects and fundraisers.





Ishan Barman
Johns Hopkins University

Oral Presentation: 8:00 am | Monday | Primrose A

Decoding the Molecular Pathology of Cancer with Vibrational Spectroscopy

Ishan Barman is an Assistant Professor in the Department of Mechanical Engineering at the Johns Hopkins University with joint appointments in the Departments of Oncology, and Radiology and Radiological Science. He is also a senior investigator of the National Institutes of Health (NIH)-funded Laser Biomedical Research Center. He graduated from Indian Institute of Technology, Kharagpur, and then moved to Massachusetts Institute of Technology (MIT) for his Ph.D., where he investigated transcutaneous blood analyte detection using Raman spectroscopy. His doctoral research established many of the experimental and computational methods that are now common to in vivo spectroscopic investigations, notably tissue turbidity correction, integration of nonimaging optical elements, and non-linear chemometric analysis. Following a postdoctoral stint at the G. R. Harrison Spectroscopy Laboratory at MIT, Dr. Barman established his independent group at the Johns Hopkins University in 2014.

His laboratory's research is focused on the development of cutting-edge and transformative biophotonics technologies with the goal of disease detection at early, manageable stages, monitoring therapeutic effects and treatment outcomes, and guiding interventions. Specifically, his work features spectroscopic imaging, which combines the molecular basis of spectroscopy with the imaging capabilities of microscopy and bridges the chemical and morphologic domains. The optical tools generated from these investigations have been successfully adopted in diverse biomedical environments including in automated recognition of biopsy specimen, real-time diagnosis of middle ear pathology, and as a customized monoclonal antibody identification platform. More recently, Dr. Barman's group has leveraged the molecular specificity and multiplexing capability of nanostructured plasmonic probes to develop serum assays for asymptomatic surveillance of cancer survivors and speedy assessment of treatment benefit.

His work has been extensively published in journals such as Proceedings of National Academy of Sciences, Cancer Research, Angewandte Chemie, Chemical Science, Analytical Chemistry, and Accounts of Chemical Research, and has also been prominently featured in leading scientific (Technology Review, Physics Today, Physics World, C&E News) and popular media (Wall St. Journal, CNN Newsroom with Ali Velshi) outlets. He has received numerous awards for his research contributions, notably the NIH Director's New Innovator Award, Maryland Outstanding Young Engineer Award, American Society for Lasers in Surgery and Medicine (ASLMS) Dr. Horace Furumoto Innovations Young Investigator Award, and the Tomas Hirschfeld Award by the Federation of Analytical Chemistry and Spectroscopy Societies.



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.



Robert Kennedy
University of Michigan

Oral Presentation: 8:00 am | Tuesday | Primrose A

Droplet Microfluidics with Mass Spectrometry for High-throughput Chemistry, Screening, and Sensing

Robert Kennedy developed an interest in analytical chemistry and chemical separations while earning his BS degree in chemistry at the University of Florida. He became fascinated with the ability of GC to separate subtly different molecules while he was performing undergraduate research in organic chemistry. His analytical classes taught by Prof. John Dorsey further enhanced this interest. He went on to earn a PhD with James Jorgenson at University of North Carolina where his work focused on using open tubular LC to analyze single cells. After a post-doc with Mark Wightman he started his own research program at University of Florida before moving to University of Michigan as the Hobart H. Willard Professor of Chemistry in 2002. His research has combined his lifelong interest in biology with chemical analysis and separations. A theme of his group has been development of miniaturized, high-speed separations for sensing, detection of non-covalent complexes, and screening. His group has developed capillary separation methods for monitoring neurotransmitters in vivo. These methods have been used for studying changes in neurotransmitter concentrations associated with behavior and diseases. His group has also developed microfluidic electrophoresis devices for monitoring insulin secretion from pancreatic cells. These methods are coupled with LC-MS metabolomics to understand the biochemical mechanism of insulin secretion and perturbations associated with diabetes. His group is also researching use of rapid electrophoretic and mass spectrometric assays for high-throughput screening. His work has been recognized by several awards including ACS Award in Chromatography, McKnight Award for Technical Innovations in Neuroscience, EAS Separation Science Award, Golay Award for Achievements in Chromatography, The Ralph Adams Award in Bioanalytical Chemistry and several teaching awards. He has held several service posts and is presently Associate Editor of Analytical Chemistry and Chair of the Chemistry Department at University of Michigan.



ROYAL SOCIETY OF CHEMISTRY THEOPHILUS REDWOOD AWARD



Christy Haynes

University of Minnesota

Oral Presentation: 8:00 am | Monday | Primrose A

Polymer-enabled Plasmonic Sensing

Christy Haynes is the Elmore H. Northey Professor of Chemistry at the University of Minnesota where she leads the Haynes Research Group, a lab dedicated to applying analytical and nanomaterials chemistry in the context of biomedicine, ecology, and toxicology.

Professor Haynes completed her undergraduate work at Macalester College in 1998 and earned a Ph.D in chemistry at Northwestern University in 2003 under the direction of Richard P. Van Duyne. Before joining the faculty at the University of Minnesota in 2005, Haynes performed postdoctoral research in the laboratory of R. Mark Wightman at the University of North Carolina, Chapel Hill.

Among many honors, she has been recognized as an Alfred P. Sloan Fellow, a Searle Scholar, a Dreyfus Teacher-Scholar, a National Institutes of Health “New Innovator,” and a 2018 Guggenheim Fellow. In addition to wide recognition for her research contributions, including over 250 peer-reviewed publications, she has been recognized by her university as an Outstanding Postdoctoral Mentor and the Sara Evans Faculty Woman Scholar/Leader Award. Professor Haynes is currently the Associate Head of the University of Minnesota, Department of Chemistry, the Associate Director of the National Science Foundation-funded Center for Sustainable Nanotechnology, and an Associate Editor for the journal Analytical Chemistry. In addition, Prof. Haynes is a champion for diversity in STEM fields and dialogue between scientists and the public.



IRDG CHALMERS AND DENT AWARD

The Chalmers and Dent Student Travel Award was 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. The award is named after two previous chairs of the IRDG, John Chalmers and Geoff Dent, in recognition of their continuing support for the IRDG and in particular for their support of students and early career researchers. John and Geoff have been active in the development and promotion of the vibrational spectroscopists of the future in both academia and industry through mentoring and inspiration.

Presented at 7:15 pm Sunday at the Welcome Mixer, Primrose A



Elizabeth Legge

National Physical Laboratory (NPL)

Elizabeth graduated with a BEng in Electronic Engineering from the University Of Surrey in 2016, which included a placement year at Buhler Sortex, working in the research and development hardware team. In July 2016 Elizabeth started her PhD in Electronic Engineering from the University of Surrey and National Physical Laboratory (NPL). The PhD is under the supervision of Prof S. Ravi P. Silva (Surrey), Dr Vlad Stolojan (Surrey) and Dr Andrew J. Pollard (NPL), with a focus on investigating larger area graphene and other 2D materials for real world applications. Now in her third year of her PhD, Elizabeth has published a paper on the characterisation of reduced graphene oxide for conductive thin films and contributed to the graphene good practice guide published by NPL. Her most recent work includes using tip-enhanced Raman spectroscopy (TERS) to determine the location of defects on commercial graphene samples. During her PhD, Elizabeth has been a postgraduate institute (PGI) ambassador and member of the Juno team at NPL. During her role as an ambassador she has helped to organise two student conferences. She has been awarded grants from the Graphene Flagship to attend Women in Graphene (March 2018 and February 2019). Elizabeth is a member of the Institute of Engineering and Technology (IET) and the Infrared and Raman Discussion Group (IRDG).



AES LIFETIME ACHIEVEMENT AWARD



Hsueh Chia Chang
University of Notre Dame

Oral Presentation: 1:30 pm | Wednesday | Mesquite D
AES Lifetime Achievement Award Session Honoring Hsueh-Chia Chang
Isolation, Fractionation, and Analysis of Exosomes

Professor Hsueh-Chia (Chia) Chang is the Bayer Corporation Chair of Chemical and Biomolecular Engineering at Notre Dame. He was born to a diaspora Chinese family and grew up in Taiwan, Singapore, Malaysia and California. His early career included two moves (UC Santa Barbara and U of Houston) to be with his mathematician wife and a stint as the Department Chair at Notre Dame (at 35).

His original research was on the mathematical theories of nonlinear reaction dynamics, reactant transport and interfacial fluid dynamics. Building on this diverse background, he reoriented his research in 2002 towards the development of diagnostic biochips based on electrokinetics. With collaborators/students from backgrounds in fabrication, manufacturing, medicine and chemistry, he parlayed his fluid mechanics and electrokinetics knowledge into integrated commercializable devices. These devices often involve new technologies based on fundamental insights into the underlying physics and intricate systemic integration of different modules. His lab has brought to the field several key electrokinetic technologies for flow and pressure actuation, dielectrophoretic cell sorting and molecule concentration, electrophoretic exosome isolation and purification, acoustic cell and vesicle lysing, droplet molecular quantification and cell encapsulation, molecular sensing and fractionation etc. Eleven of these technologies have been patented, with 5 more pending. Five have been licensed to startups.

He served as the Chief Scientific Advisor of F Cubed LLC (now Cubed Laboratories) for 4 years. He believes that robust multiplexed point-of-care (POC) diagnostic devices will transform health care within the next decade. Professor Chang founded a new journal, *Biomicrofluidics* of the American Institute of Physics, to serve this community. Since 2003, more than 15 PhD and post-doc students from his laboratory have embarked on academic careers in electrokinetics as tenure-track professors in all engineering and science disciplines over 5 continents. Professor Chang received the Frenkiel Award from the American Physical Society for his interfacial dynamics work. With Leslie Yeo, he coauthored the book “Electrokinetically Driven Microfluidics and Nanofluidics” by Cambridge University Press. He was recognized with a commercialization award from the First-Source Bank of South Bend. He has delivered several named and keynote lectures on electrokinetics and integrated diagnostic technologies.

AES MID-CAREER AWARD

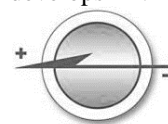
Recognizes exceptional contributions to the field of electrophoresis, microfluidics, and related areas by an individual who is currently in the middle of their career.



Christopher Easley
Auburn University

Oral Presentation: 8:00 am | Wednesday | Primrose A
Digitizing Endocrine Tissue Secretions into Nanoliter Droplets for Analysis of Hormones and Metabolites at High Temporal Resolution

Christopher J. Easley is currently the C. Harry Knowles Professor of Chemistry and Biochemistry at Auburn University. He received his B.S. degree in chemistry at Mississippi State University in 2002 and his Ph.D. in bioanalytical chemistry from the University of Virginia in 2006, under training from Prof. James P. Landers. His postdoctoral training was provided by Prof. David W. Piston at the Vanderbilt University Medical Center in the Department of Molecular Physiology and Biophysics, from 2006-2008. He began his independent career at Auburn in 2008 and was recently promoted to full professor in 2018. He teaches chemistry from the fundamental undergraduate level up to the special topics graduate level in bioanalytical techniques. Prof. Easley is currently a member of the International Advisory Board of Analytical and Bioanalytical Chemistry (2016-present) and is an associate editor at *Analytical Methods* (2017-present). He is also a co-founder of Proximity Biosciences, Inc. and holds several U.S. patents based on biosensing and microfluidics. In work funded mostly by the National Institutes of Health, his bioanalytical research laboratory develops droplet-based microfluidic methods to study dynamic function of small numbers of cells in intact, primary tissue from mouse models of disease. To accommodate bioanalysis at the microscale, the team also develops DNA-driven assays for highly sensitive protein quantification in nanoliter volumes using both fluorescence and electrochemistry, work primarily funded by the National Science Foundation. The Easley laboratory has focused their customized analytical tools on improving the understanding of dynamic function of adipose and pancreatic endocrine tissues, which are of paramount importance in diabetes, obesity, and metabolic syndrome.



AES BLUE FINGERS STUDENT AWARD

Recognizes the most outstanding student paper submitted for the AES Annual Conference by a graduate student.



Anna Nielsen
Brigham Young University

Oral Presentation: 10:35 am | Wednesday | Mesquite D

3D Printed Integrated Microfluidic Devices for Extraction, Fluorescence Labeling, and Separation of Preterm Birth Biomarkers

Anna is a Chemistry Ph.D. student at Brigham Young University studying microfluidics and 3D printing with Dr. Adam Woolley. She was born in Utah and received a Bachelor's degree in Chemistry from Brigham Young University-Idaho. Anna is currently preparing to defend her dissertation and is currently starting up a business called Acrea 3D, which will market high resolution 3D printers for rapid prototyping and development of microfluidic devices. In her free time, Anna enjoys hiking, reading, and playing tennis.



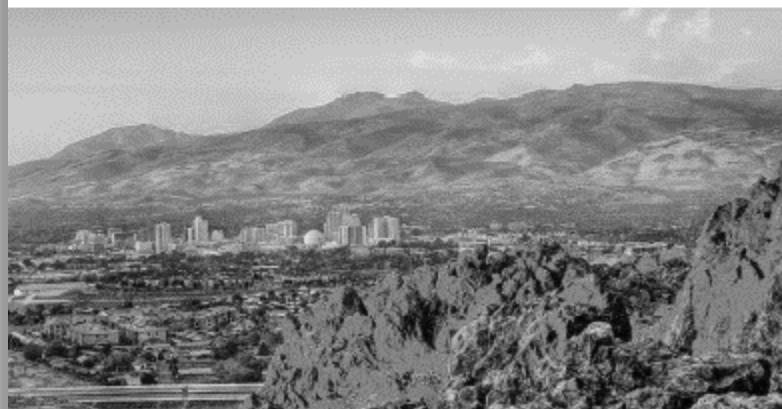
FACSS PRESENTS

SCIX2020

The Great **Sci**entific **eX**change

October 9 - 16
Nugget Casino Resort
Sparks, NV

Setting Our Sights on Sparks



PREVIOUS FACSS BOARD AND MEETING CHAIRS

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

PREVIOUS FACSS BOARD AND MEETING CHAIRS

1996 - Kansas City

Rachael Barbour	Governing Board Chair
O. Karmie Galle	General
William Fateley	Program
Scott McGeorge	Exhibit

1997 - Providence

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

1998 - Austin

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

1999 - Vancouver

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

2000 - Nashville

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

2001 - Detroit

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

2002 - Providence

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

2003 - Fort Lauderdale

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

2004 - Portland

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

2005 - Quebec City, Canada

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

2006 - Orlando

Diane Parry	Governing Board Chair
Christine Wehlburg	General
S. Douglas Gilman	Program
Scott McGeorge	Exhibit

2007 - Memphis

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

2008 - Reno

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

2009 - Louisville

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

2010 - Raleigh

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

2011 - Reno

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

2012 - Kansas City

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

2013 - Milwaukee

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

2014 - Reno

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

2015 - Providence

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

2016 - Minneapolis

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

2017 - Reno

Steven Ray	Governing Board Chair
Becky Dittmar	SciX General
Matthieu Baudalet	SciX Program
Mike Carrabba	SciX Exhibit

2018 - Atlanta

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

PROGRAM AT-A-GLANCE

SUNDAY, OCTOBER 13

- 9:00 am – 4:00 pm Workshops/Short Courses, *Pueblo A&B*
- 4:20 pm – 7:15 pm Opening Sessions, *Primrose A*
- 4:20 pm What's Hot Exhibitor Presentations
- 6:15 pm **Keynote Lecture: The Convergence of Measurement and Data Sciences: A Great Exchange**
Rohit Bhargava, University of Illinois
- 7:15 pm – 9:15 pm Welcome Mixer and SAS Sponsored Student Poster Session, *Primrose Foyer*

MONDAY, OCTOBER 14

- 7:00 am – 9:00 am Coblenz Members Meeting/Breakfast, *San Jacinto*
- 7:30 am Coffee, *Primrose Foyer*
- 7:45 am – 9:30 am Awards and Plenary Session, *Primrose A*
- 7:45 am Welcome and Award Presentations
- 8:00 am **RSC Theophilus Redwood Award; Christy L. Haynes, University of Minnesota**
- 8:30 am **SAS Ellis R. Lippincott Award; Ji-Xin Cheng, Boston University**
- 9:00 am **Spectroscopy's Emerging Leader in Molecular Spectroscopy Award;**
Ishan Barman, Johns Hopkins University
- 9:00 am – 4:00 pm Workshops/Short Courses, *Pueblo A&B*
- 9:45 am – 10:45 am Poster Session (pg 83) and Break, *Primrose Foyer*
- 10:50 am – 12:30 pm Oral Symposia (pg. 38)
- 11:45 am – 1:30 pm Coblenz Society Speed Mentoring
- 12:30 pm – 1:30 pm Lunch on own
- 1:30 pm – 3:10 pm Oral Symposia (pg 42)
- 3:10 pm – 3:50 pm Poster Session (pg 83) and Break, *Primrose Foyer*
- 3:50 pm – 5:30 pm Oral Symposia (pg 45)
- 5:30 pm – 7:30 pm Exhibit Hall Opening Reception (Bring your iPad raffle and drink tickets), *Oasis*



Download the mobile app to search, filter by topic, and build your own agenda! Scan a QR code at registration!

TUESDAY, OCTOBER 15

- 7:30 am Coffee, *Primrose Foyer*
- 7:45 am – 9:00 am Awards and Plenary Session, *Primrose A*
- 7:45 am Award Presentations
- 8:00 am Charles Mann Award for Raman Spectroscopy; Karen Faulds, University of Strathclyde**
- 8:30 am ANACHEM Award; Robert Kennedy, University of Michigan**
- 9:00 am – 4:00 pm Workshops/Short Courses, *Pueblo A&B*
- 9:15 am – 10:55 am Oral Symposia (pg. 50)
- 10:00 am – 4:30 pm Exhibit Hall Open, *Oasis*
- 11:00 am – 11:45 am Poster Session (pg 85) and Break, *Oasis*
- 11:40 am – 1:10 pm What's Hot Exhibitor Presentations, *Oasis*
- 12:00 pm – 12:30 pm Lunch in Exhibit Hall (ticket required), *Oasis*
- 1:30 pm – 3:10 pm Oral Symposia (pg. 54)
- 3:10 pm – 3:50 pm Poster Session (pg 85) and Break with iPad drawing, *Oasis*
- 3:50 pm – 5:30 pm Oral Symposia (pg. 58)
- 7:00 pm – 8:00 pm SAS Award Presentations, *Catalina*
- 8:00 pm SAS Members' Wine and Cheese Reception, *Santa Rosa and San Jacinto*

PROGRAM AT-A-GLANCE

WEDNESDAY, OCTOBER 16

7:30 am	Coffee, <i>Primrose Foyer</i>
7:45 am – 9:00 am	Awards and Plenary Session, <i>Primrose A</i>
7:45 am	Award Presentations
8:00 am	SAS Lester W. Strock Award; S. Michael Angel, University of South Carolina
8:30 am	AES Electrophoresis Mid-Career Award; Christopher J. Easley, Auburn University
9:00 am – 4:00 pm	Workshops/Short Courses, <i>Pueblo A&B</i>
9:15 am – 10:55 am	Oral Symposia (pg. 62)
10:00 am – 4:00 pm	Exhibit Hall Open, <i>Oasis</i>
11:00 am – 11:45 am	Poster Session (pg 88) and Break, <i>Oasis</i>
11:50 am – 1:00 pm	What's Hot Exhibitor Presentations, <i>Oasis</i>
12:00 pm – 12:30 pm	Lunch in Exhibit Hall (ticket required), <i>Oasis</i>
1:30 pm – 3:10 pm	Oral Symposia (pg. 66)
3:10 pm – 3:50 pm	Poster Session (pg 88) and Break with iPad drawing, <i>Oasis</i>
3:50 pm – 5:30 pm	Oral Symposia (pg. 70)
6:30 pm	SciX 2019 A Night at the Oscars Gala (badge and ticket required), <i>Primrose Foyer</i>

THURSDAY, OCTOBER 17

7:30 am	Coffee, <i>Primrose Foyer</i>
7:45 am – 9:00 am	Awards and Plenary Session, <i>Primrose A</i>
7:45 am	Award Presentations
8:00 am	SAS and Applied Spectroscopy William F. Meggers Award; Tim J. Johnson, Pacific Northwest National Laboratory
8:30 am	Coblentz Society Clara Craver Award; Xiaoyun "Shawn" Chen, Dow Chemical Company
9:15 am – 10:55 am	Oral Symposia (pg. 74)
11:00 am – 11:45 am	Poster Session (pg 90) and Break, <i>Primrose Foyer</i>
12:00 pm – 12:30 pm	Lunch on Own
1:30 pm – 3:10 pm	Oral Symposia (pg. 78)
3:10 pm – 3:50 pm	Poster Session (pg 90) and Break, <i>Primrose Foyer</i>
3:50 pm – 5:30 pm	FACSS Innovation Award Finalists Plenary Session, <i>Primrose A</i> (pg. 82)

FRIDAY, OCTOBER 18

7:30 am	Continental Breakfast, <i>Sierra-Ventura Foyer</i>
7:45 am – 10:00 am	Awards and Closing Plenary Session, <i>Sierra-Ventura</i>
7:45 am	Announcement of 2019 FACSS Innovation Award Winner
	Closing Plenary Presentations: Data Science Meets Measurement Science
8:00 am	Phase Engineering for Targeted Super-Resolution Applications, Christy Landes
8:30 am	Multiplexing Spatial and Hyperspectral Imaging with Dynamically Structured Illumination; Randy Bartels
9:00 am	Spectral Deep Learning for Prediction and Prospective Validation of Functional Groups for Autonomous Instrumentation; Gaurav Chopra
9:30 am	Setting Our Sights on SciX 2020

SHORT COURSES / WORKSHOPS

**These half- or full-day workshops are available for a separate registration fee.
Visit the registration desk to sign up. Space is limited and some courses may sell out.**

Half day conferee: \$225

Half day student: \$25

Full day conferee: \$450

Full day student: \$50

SUNDAY, OCTOBER 13

Basic Chemometrics, Pueblo B

Instructor: Neal Gallagher, *Eigenvector*

9:00 am - 4:00 pm

A Practical Introduction to Infrared, Raman, and Near Infrared Spectroscopy, Pueblo A

Instructor: James A. de Haseth, *University of Georgia*

9:00 am - 12:00 pm

Searching Infrared and Raman Spectra, Pueblo A

Instructor: James A. de Haseth, *University of Georgia*

1:00 pm - 4:00 pm

MONDAY, OCTOBER 14

Intro to Raman with Imaging Applications Instructor: David Tuschel, *HORIBA Scientific, Pueblo B*

9:00 am - 12:00 pm

Introduction to Hyperspectral/Multivariate Image Analysis, Pueblo A

Instructor: Robert T. Roginski, *Eigenvector*

9:00 am - 12:00 pm

Non-Linear Methods for Regression and Classification, Pueblo A

Instructor: Donal O'Sullivan, *Eigenvector*

1:00 - 4:00 pm

Problems with FT-IR Spectra and How to Avoid Them, Pueblo B

Instructors: Ellen Miseo, *TeakOrigin*; Jenni Briggs, *Pike Technologies*; Gloria Story, *Procter & Gamble*

1:00 - 4:00 pm

TUESDAY, OCTOBER 15

Laser Fundamentals for Spectroscopy, Pueblo A

Instructor: Robert Chimenti, *RVC Photonics/Rowan University*

9:00 am - 12:00 pm

Electrokinetic Microfluidics: Theory and Hands-on Simulations, Pueblo B

Instructor: Cornelius (Neil) Ivory, *Washington State University*

9:00 am - 12:00 pm

Advance Applications of LA-ICP-OES, LA-ICP-MS and LIBS, Pueblo B

Instructor: Jhanis Gonzalez, *Applied Spectra / Lawrence Berkeley National Laboratory*

1:00 pm - 4:00 pm

WEDNESDAY, OCTOBER 16

Process Analytical Technology: Out of the Lab and into the Line, Pueblo B

Instructor: Jim Rydzak, *Specere Consulting*

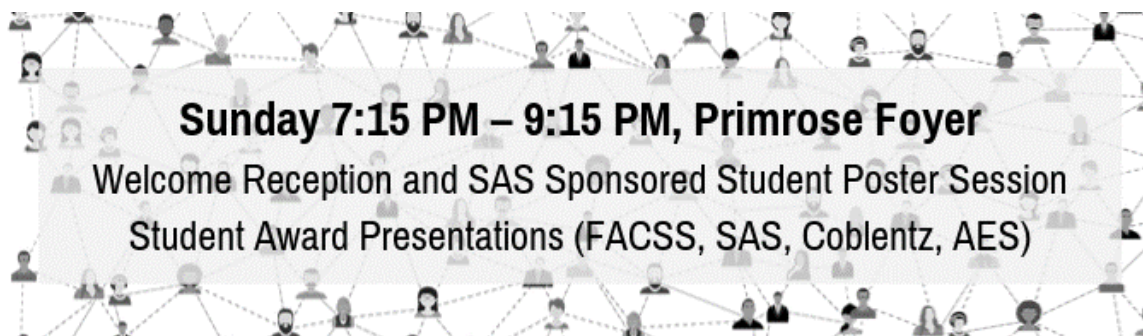
9:00 am - 4:00 pm

TECHNICAL PROGRAM – SUNDAY
WHAT'S HOT EXHIBITOR PRESENTATIONS 4:20 PM – 6:00 PM
Chair: Brian Dable
Primrose A

- 4:20 PM Faster, Smaller and Beyond for Next Generation Spectroscopy
Ibsen Photonics: Heidi Olson
- 4:30 PM Shortwave Infrared Imaging For the 21st Century from Princeton Infrared Technologies, Inc.
Princeton Infrared Technologies, Inc.: Robert Struthers
- 4:40 PM Robust Lasers for Raman
Cobolt by HUBNER Photonics Inc.: Andreas Naeslund
- 4:50 PM High-speed and High-density Multi-channel Raman Spectroscopy using a Back-illuminated sCMOS based Spectrometer
Andor Technology: Justin T. Cooper
- 5:00 PM Introducing New PAT Solutions for BioProcess Analytics: Mid-IR Quantum Cascade Laser Molecular Sensing Instruments
DRS Daylight Solutions: Craig Magee
- 5:10 PM Using Smart Filters and Standards to Make Diode-Array Based NIR Analyzers Robust and Reliable in a Process Environment
Sentronic GmbH: Owen Rehrauer
- 5:20 PM Elemental Analysis of Various Matrices: Choosing the Best Technique
Shimadzu Scientific Instruments, Inc.: Jon Peters
- 5:30 PM Diamonds are a Process Spectroscopist's Best Friend
Keit Spectrometers: Dan Wood
- 5:40 PM A Novel Cloud AI Enabled Raman with MEMS Scanning Mirror
CloudMinds: Lynn Chandler
- 5:50 PM The AvaSpec-ULS2048X64TEC-EVO: High Performance Raman Spectrometer
Avantes: Damon Lenski

TECHNICAL PROGRAM – SUNDAY
WELCOME AND KEYNOTE LECTURE 6:15 PM – 7:15 PM
Chair: Garth Simpson, Program Chair
Primrose A

- 6:15 PM (1) **The Convergence of Measurement and Data Sciences: A Great Exchange**; Rohit Bhargava¹; ¹University of Illinois at Urbana-Champaign



TECHNICAL PROGRAM - MONDAY
AWARDS AND PLENARY LECTURES 7:45 AM – 9:30 AM
 Chair: Mary Kate Donais
Primrose A

- 7:45 AM Award Presentations
- 8:00 AM (2) **RSC Theophilus Redwood Award / 2018 Coblenz Society Craver Award; Polymer-enabled Plasmonic Sensing;** Christy Haynes¹; ¹*University of Minnesota Twin-Cities*
- 8:30 AM (3) **SAS Ellis R. Lippincott Award; From Bond-selective Chemistry to Bond-selective Imaging: My 30 Years' Path to Tackle Missions Impossible;** Ji-Xin Cheng¹; ¹*Boston University*
- 9:00 AM (4) **Spectroscopy's Emerging Leader in Molecular Spectroscopy Award; Decoding the Molecular Pathology of Cancer with Vibrational Spectroscopy;** Ishan Barman¹; ¹*Johns Hopkins University*

TECHNICAL PROGRAM - MONDAY
POSTER SESSION 9:45 AM – 10:45 AM
Primrose Foyer

See page 83 for Monday posters by category. Posters will be displayed all day and attended again in the afternoon.

TECHNICAL PROGRAM - MONDAY
ORAL SYMPOSIA 10:50 AM – 12:30 PM

19AES01: Electrokinetic Fundamentals *Mesquite D*

Chairs: Aliaksei Boika, Karina Torres Castro

- 10:50 AM (5) **Gigantic Dielectrophoresis of Proteins in Solution;** Dmitry Matyushov¹; ¹*Arizona State University*
- 11:10 AM (6) **Exploiting Dielectrophoresis to Separate Single Walled Carbon Nanotubes;** Alexandra Ros¹, Mahammad Rabbani², Christoph Schmidt³; ¹*Arizona State University / The Biodesign Institute*, ²*Arizona State University*, ³*Duke University*
- 11:30 AM (7) **AC Electrokinetic Phenomena in Electroanalysis;** Aliaksei Boika¹; ¹*The University of Akron*
- 11:50 AM (8) **Strategies for Dynamic Particle Manipulation and Assessment Employing Insulator-based Dielectrophoresis;** Blanca H. Lapizco-Encinas¹; ¹*Rochester Institute of Technology*
- 12:10 PM (9) **A Parallelized in Flow Electrorotation Platform with Individual Control on the Trapping and Release of Single Cells;** Kevin Keim¹, Mohamed z Rashed¹, Carlotta Guiducci¹; ¹*École Polytechnique Fédérale de Lausanne*

- 10:50 AM (10) **Tunable Chiroptical Properties in Metamaterials and Nanocrystals;** Vivian Ferry¹; ¹*University of Minnesota*

- 11:10 AM (11) **Studies of Biomolecules with Multiphoton Microspectroscopy;** Janina Kneipp¹; ¹*Humboldt-Universität zu Berlin*

- 11:30 AM (12) **Plasmon-enhanced Single-molecule Fluorescence in Living Bacterial Cells;** Julie S. Biteen¹; ¹*University of Michigan*

- 11:50 AM (13) **Nanoscale Battery Materials Induce DNA Damage in Bacteria;** Tian (Autumn) Qiu¹, Valeria Guidolin², Khoi Nguyen L. Hoang³, Thomas Pho³, Andrea Carra², Peter W. Villalta², Silvia Balbo², Z. Vivian Feng³, Christy Haynes²; ¹*University of Illinois, Urbana-Champaign*, ²*University of Minnesota*, ³*Augsburg University*

- 12:10 PM (14) **Breakdown of Plastics in the Environment: The Impact of Weathering on the Fate and Transformation of Aquatic Plastic Debris;** Melissa Maurer-Jones¹, Thomas Mundhenke¹, Taylor Hebner¹, Faith Murphy¹, Victoria Fringer¹, Daniel Zoltek¹; ¹*University of Minnesota Duluth*

19AWD01: RSC Theophilus Redwood Award Honoring Christy Haynes *Mojave*

Chair: Christy Haynes

19BIM01: Biomedical Spectroscopy and Imaging for Cancer *Catalina*

Chair: Michael Schmitt

- 10:50 AM (15) **Fluorescence Lifetime Spectroscopy and Imaging in Clinical Applications;** Laura Marcu¹; ¹*University of California Davis*

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 10:50 AM – 12:30 PM

- 11:10 AM (16) **Hyperspectral SRS Imaging for Label-free Molecular Subtyping of Glioblastomas;** Zhiwei Huang¹; ¹National University of Singapore
- 11:30 AM (17) **Multiplex SRS Imaging Cytometry Reveals Novel Metabolic Signatures in Drug-resistant Cancer Cells;** Ji-Xin Cheng¹, Ji-Xin Cheng¹; ¹Boston University
- 11:50 AM (18) **Exploring Raman Spectroscopy for the Identification of Vulval Squamous Cell Carcinoma and Vulval Intraepithelial Neoplasia;** Nick Stone¹, Jonathan Frost, Linmarie Ludeman, Kathryn Hillaby, Catherine Kendall, Gavin Lloyd, Rob Gornall, Angela Shore, Nick Stone¹; ¹University of Exeter
- 12:10 PM (19) **Nonlinear Multimodal Imaging for Intraoperative Tumor Diagnosis;** Michael Schmitt¹, Juergen Popp²; ¹Friedrich-Schiller University Jena, Germany, ²Leibniz Institute of Photonic Technology e.V. Jena, Germany

19FORENS01: Nuclear Forensics *Smoketree A*

Chairs: Dallas Reilly, Greg Klunder, Robert Lascola

- 10:50 AM (20) **Infrared Spectroscopic Method for Uranium Isotopic Analysis;** Alicia Strange Fessler¹, Patrick O'Rourke¹, Nicholas DeRoller¹, Steven Serkiz², Darrell Simmons³, Leigh Martin³; ¹Savannah River National Laboratory, ²Savannah River National Laboratory (retired), ³Oak Ridge National Laboratory
- 11:10 AM (21) **Inferring Nuclear Fireball Properties from Experimental Data;** Batikan Koroglu¹, Jonathan Crowhurst¹, Mike Armstrong¹, Zurong Dai¹, Scott Wagon¹, David Weisz¹, Joseph Zaug¹, Harry Radousky¹, Kim Knight¹, Tim Rose¹; ¹Lawrence Livermore National Laboratory
- 11:30 AM (22) **Resonance Ionization Mass Spectrometry for Actinide Isotope Analysis;** Brett H. Isselhardt¹, Michael Savina², Reto Trappitsch²; ¹Lawrence Livermore National Laboratory, ²LLNL
- 11:50 AM (23) **Elemental and Isotope-ratio Mass Spectrometry with a Solution-cathode Glow Discharge Ionization Source;** Garett M. MacLean¹, Malina Helling², Asaf Harel¹, George Chan³, Jacob Shelley¹; ¹Rensselaer Polytechnic Institute, ²University of Münster, ³Lawrence Berkeley National Laboratory
- 12:10 PM (24) **Laser-induced Spectrochemical Assay for Uranium Enrichment;** George Chan¹, Zhenli Zhu², Rick Russo¹; ¹Lawrence Berkeley National Laboratory, ²China University of Geosciences(Wuhan)

19IR02: Nanoscale IR Spectroscopy I: Recent Advances *Smoketree D*

Chair: Andrea Centrone

- 10:50 AM (25) **Unlocking the Potential of Photothermal Infrared Microscopy on Spatial Resolution, Sensitivity, and Richness of Information;** Xiaoji Xu¹, Xiaoji Xu¹; ¹Lehigh University
- 11:10 AM (26) **Tapping-mode PTIR: A Versatile IR Nanoscopy Method for Challenging Samples;** Georg Ramer¹, Karin Wieland², Andrea Centrone³, Bernhard Lendl¹; ¹TU Wien, ²TU Munich, ³NIST, Gaithersburg, MD
- 11:30 AM (27) **Tapping Mode AFMIR: A Versatile Tool to Characterize Drug-loaded Polymeric Nanoparticles;** Ariane Deniset-Besseau¹, Alexandre Dazzi², Jérémie Mathurin², Ruxandra Greff³, Elisabetta Pancani³, Seray Merve Ural³; ¹Faculty of science, Paris-Sud University, ²Laboratoire de Chimie Physique, CNRS, Université Paris Sud, Université Paris-Saclay, ³ISMO, UMR 8214 CNRS, Université Paris Sud, Université Paris Saclay
- 11:50 AM (28) **Correlative Nanoscopy for Organic, Inorganic and Hybrid Material Analysis;** Tobias Gokus¹, Stefan Mastel¹, Andreas Huber¹; ¹neaspec GmbH
- 12:10 PM (29) **Nanoscale Spectroscopy and Imaging (s-SNOM and AFM-IR) Using a Femtosecond Difference Frequency Generation Laser Source;** Qichi Hu¹, Honghua Yang¹, Omar Khatib²; ¹Bruker Nano Surfaces, ²University of Colorado

19IR12: Forefront of Molecular Spectroscopy *Smoketree E*

Chair: Isao Noda

- 10:50 AM (30) **Understanding of Biodegradable Polymer Blend Thin Films Using 2D Correlation Analysis and Chemical Images;** Young Mee Jung¹, Yeonju Park¹, Isao Noda²; ¹Kangwon National University, ²University of Delaware
- 11:10 AM (31) **Effective Use of Spectral Database Software with Two-dimensional Correlation Spectroscopy (2D-COS);** Isao Noda¹, Michelle D'Souza², Gregory Banik²; ¹University of Delaware, ²Bio-Rad Laboratories, Inc.
- 11:30 AM (32) **Application of NIR Spectroscopy to Physical Chemistry;** Yukihiro Ozaki¹; ¹Kwansei Gakuin University
- 11:50 AM (33) **Raman Hyperspectroscopy for Forensic Purposes and Medical Diagnostics;** Igor K. Lednev¹; ¹University at Albany, SUNY

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 10:50 AM – 12:30 PM

12:10 PM (34) **Advances in Balanced Detection Interferometric Cavity Assisted Photothermal Spectroscopy**; Bernhard Lendl¹; ¹*Technische Universität Wien*

19LIBS01: Fundamentals Smoketree C

Chair: Alessandro Digiacomo

10:50 AM (35) **Time-resolved Characterization of Laser Induced Plasmas with Dual-comb Spectroscopy**; Jason Jones¹, Yu Zhang¹, Caroline Lecaplain¹, Reagan Weeks¹, Jeremy Yeak², Sivanandan Harilal³, Mark Phillips¹; ¹*University of Arizona*, ²*Opticslab*, ³*Pacific Northwest National Laboratory*

11:10 AM (36) **Modeling Equilibrium Chemistry in Laser Induced Plasmas and Plasma Chemical Reactors**; Igor Gornushkin¹, Sergei Shabanov², Petr Sennikov³; ¹*BAM Federal Institute for Materials Research and Testing*, ²*University of Florida*, ³*G.G. Devyatikh Institute of Chemistry of High-Purity Substances of RAS*

11:30 AM (37) **What Are We Looking At? An Atypical View of the LIP**; Jonathan A. Merten¹; ¹*Arkansas State University*

11:50 AM (38) **Probe Volume and Energy Balance in Laser-induced Breakdown Spectroscopy**; Jörg Hermann¹, Jörg Hermann², Catalin D. Constantinescu², Aya Taleb³, Frédéric Pelascini⁴; ¹*French National Centre for Scientific Research (CNRS)*, ²*French National Center for Scientific Research (CNRS)*, ³*Aix-Marseille University and Cetim Grand Est*, ⁴*Cetim Grand Est*

12:10 PM (39) **On the Plasma Phase Immediately After the Laser Matter Interaction**; Alessandro De Giacomo¹, Marcella Dell'Aglio², Vincent Gardette¹; ¹*University of Bari*, ²*CNR-NANOTEC*

19NANO01: Carbon-based Nanomaterials: Synthesis, Properties, and Applications Mesquite E

Chair: Wei Zhao

10:50 AM (40) **Resolving Carbon Nanotube Structures by DNA**; Ming Zheng¹; ¹*NIST*

11:10 AM (41) **Magnetic Brightening of Hidden Fine Structures in Carbon Nanotube Quantum Defects**; HAN Htoon¹, Yonghee Kim¹, Sergei Goupalov², Xiaowei He³, Avishek Saha¹, Brendan Giffort¹, Mijin Kim⁴, Geyou Ao⁴, YuHuang Wang⁴, Ming Zheng⁵, Sergei Tretiak¹, Stephen Doorn¹; ¹*LOS ALAMOS NATL LAB*, ²*Jackson State University*, ³*Steven's institute*, ⁴*University of Maryland*, ⁵*National Institute of Standards and Technology*

11:30 AM (42) **Carbon-based Functional Nanomaterials for Electrochemical Energy Technologies**; Shaowei Chen¹; ¹*University of California Santa Cruz*

11:50 AM (43) **Carbon Nanomaterials in Energy Storage: From 1D to 3D**; Jie Liu¹, Jie Liu¹; ¹*Duke University*

12:10 PM (44) **Tip-enhanced Raman Spectroscopy Investigation of Transition Complex Immobilization on 2D Carbon Nanosheet**; Marie Richard-Lacroix¹, Maria Kuellmer², Elisabeth Hofmeister³, Max von delius³, Turchanin Andrey⁴, Volker Deckert¹; ¹*Leibniz Institute of Photonic Technology Jena*, ²*Friedrich-Schiller University Jena Institute of Physical Chemistry*, ³*Ulm university*, ⁴*Friedrich-Schiller University Jena, Institute of Physical Chemistry*

19PMA03: Biopharmaceutical Raw Material Characterization Madera

Chair: John Bobiak

10:50 AM (45) **Determination of Amino Acid Glycation and Vitamin Degradation in Chemically Defined Media Powders by HPLC**; Lisa Bareford¹, Lisa Bareford¹, David Kolwyck¹; ¹*Biogen*

11:10 AM (46) **Evaluation of Cell Culture Media Using Absorption and Transmission Fluorescence Excitation Emission Matrix (A-TEEM) Spectroscopy**; Adam M. Gilmore¹, Karoly Csatorday², Adam Gilmore², Alvin Togonon²; ¹*HORIBA*, ²*Horiba Scientific*

11:30 AM (47) **Digital Image Processing for Quantitative Analysis**; Kevin Cantrell¹, Sarah Bunger¹, David Campbell¹, Lauren Naatz¹, Miguel M. Erenas², Luis Fermin Capitan-Vallvey²; ¹*University of Portland*, ²*University of Granada*

11:50 AM (48) **Protein Mobility Evaluated by Fourier-transform Fluorescence Recovery After Photobleaching (FT-FRAP)**; Andreas C. Geiger¹, James Ulcickas¹, Garth Simpson¹; ¹*Purdue University*

12:10 PM (49) **Warehouse Verification of Incoming Materials in Pharma with Mobile Raman**; Keith Carron¹, Corbin Haugen¹; ¹*Metrohm Raman*

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 10:50 AM – 12:30 PM

19RAM11: Food Security *Sierra*

Chair: Roy Goodacre

- 10:50 AM (50) **Detection of Multiple Food Bacteria by SERS**; Karen Faulds¹, Duncan Graham¹, Roy Goodacre², Hayleigh Kearns¹; ¹*University of Strathclyde*, ²*University of Liverpool*
- 11:10 AM (51) **Confirmatory, Non-invasive and Non-destructive Raman-based Diagnostics of Biotic and Abiotic Stresses on Plants**; Dmitry Kurouski¹, Dmitry Kurouski¹; ¹*Texas A&M University*
- 11:30 AM (52) **Emerging Approaches for Representative Food Analysis Using Raman Spectroscopy**; Nils Kristian Afseth¹, Sileshi Wubshet², Petter Vejle Andersen², Ulrike Böcker², Katinka Dankel², Carl Emil Eskildsen², Pavel Matousek³, Jens Petter Wold²; ¹*Nofima*, ²*Nofima*, ³*Central Laser Facility, STFC Rutherford Appleton Laboratory*
- 11:50 AM (53) **Raman Spectroscopic Measurements of Salmon Meat Composition Using 1000 nm Excitation**; Mary Lewis¹, Ulrike Bocker², Karen A. Esmonde-White¹; ¹*Kaiser Optical Systems, Inc.*, ²*Nofima*
- 12:10 PM (54) **Vibrational Spectroscopy with Chemometrics: A Rapid Screening Tool to Determine Authenticity of Extra Virgin Olive Oil**; Didem P. Aykas¹, Ayse Karaman², Burcu Keser², Luis Rodriguez-Saona¹; ¹*The Ohio State University*, ²*Adnan Menderes University*

19SPECIAL03: Society for Archaeological Sciences Session on Chemistry in Art and Archaeology I *Chino AB*

Chairs: Mary Kate Donais, Andrew Zipkin

- 10:50 AM (55) **Spectroscopic Mapping of the Vinland Map and Related Manuscripts: New Analytical Tools Offer New Evidence**; Richard R. Hark¹, Anikó Bezur², Marie-France Lemay³, Pablo Londero², Paula Zyats³; ¹*Institute for the Preservation of Cultural Heritage, Yale University*, ²*Yale University, Institute for the Preservation of Cultural Heritage*, ³*Yale University Library, Conservation & Exhibition Services*

- 11:30 AM (56) **When Heritage Meets Science - Integrated Approaches and International Cooperation**; Antonio Candeias¹, Jose Mirão²; ¹*University of Evora*, ²*HERCULES Laboratory, Evora University*
- 11:50 AM (57) **Novel Biotechnological Approaches for Cultural Heritage: Challenges and Perspectives**; Ana Teresa Caldeira¹; ¹*University of Evora / HERCULES Laboratory*
- 12:10 PM (58) **Spectroscopic Characterization of Historic Fabrics from a Turn of the Century New England Mill**; Mary Kate Donais¹, Giovanna Beaulieu¹, Madaleine Hunt², Fred Morris³; ¹*Saint Anselm College*, ²*Bucknell University*, ³*Bruker*

19SPSJ01: VUV/FUV/DUV I *Smoketree B*

Chairs: Yukihiro Ozaki, Yusuke Morisawa

- 10:50 AM (59) **Standoff Deep UV Raman Imaging Spectrometer for Trace Explosives: Photonic Crystal Narrow Wavelength Devices**; Sandy A. Asher¹, Sergei Bykov¹, Kyle Hufziger¹, Dipak Rout¹, Ivan Pallares¹, Thomas Deering¹, Sandy Asher¹; ¹*University of Pittsburgh*
- 11:10 AM (60) **DUV Raman Spectroscopy for Probing Protein Aggregates: Spontaneous Refolding of Amyloid Fibrils**; Igor K. Lednev¹; ¹*University at Albany, SUNY*
- 11:30 AM (61) **UV Photochemistry and Photophysics of Tryptophan in Azurin**; Judy Kim¹, Joel Rivera¹, Justine Liang¹; ¹*UC San Diego*
- 11:50 AM (62) **Synchrotron-based UV Resonance Raman Investigation of DNA Structure and Interactions**; Barbara Rossi¹, Cettina Bottari¹, Alessandro Gessini¹, Claudio Masciovecchio¹; ¹*Elettra Sincrotrone Trieste*
- 12:10 PM (63) **Spectroscopic Characterization of Individual Wide-gap Semiconductor Nanoparticles**; Yuika Saito¹, Takahiro KONDO², Kenta HIROSE², Mahiro Hanazawa²; ¹*Department of Chemistry, Gakushuin University*, ²*Gakushuin University*

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 1:30 PM - 3:10 PM

19AES02: Electrokinetic Applications *Mesquite D*

Chairs: Jeffrey Moran, Anna Nielsen

- 1:30 PM (64) **Breaking the Diagnostic Barrier for Hemoglobinopathies in Low-resource Settings with Electrophoresis;** Umut Gurkan¹, ¹*Case Western Reserve University*
- 1:50 PM (65) **Self-electrophoretic Microswimmers for Wastewater Treatment and Remediation;** Jeffrey L. Moran¹, David Warsinger²; ¹*George Mason University*, ²*Purdue University*
- 2:10 PM (66) **Electrophysiology of Biosorbent: Cupriavidus Necator;** Anthony T. Giduthuri¹, Soumya K. Srivastava¹; ¹*University of Idaho*
- 2:30 PM (67) **Electrokinetic Determination of Solution Phase Kinetic Properties at Microfluidic Liquid Interfaces;** Md Nazibul Islam¹, Zachary Gagnon¹; ¹*Texas A&M University*
- 2:50 PM (68) **Perspectives on Selected Dielectrophoresis Platforms for Particle Separations;** Rodrigo Martinez-Duarte¹, Rucha Natu¹, Devin Keck¹; ¹*Clemson University*

19ATOM01: Low Pressure Glow Discharge Spectroscopies *Pasadena*

Chair: Jorge Pisonero

- 1:30 PM (69) **Selection of Analytical Lines in Glow Discharge Optical Emission - New Opportunities with a State-of-the-art Spectrometer;** Arne Bengtson¹, David Malmström¹; ¹*SWERIM AB*
- 1:50 PM (70) **A Critical Review of the Analytical Potential of Pulsed Radiofrequency Glow Discharge Time-of-flight Mass Spectrometry;** Nerea Bordel¹, Jonatan Fandino¹, Cristina Gonzalez-Gago¹, Alfredo Sanz-Medel¹, Jorge Pisonero¹; ¹*University of Oviedo*
- 2:10 PM (71) **Glow Discharge Optical Emission Spectroscopy with Compressed Sensing Encoding in the Spectral Dimension;** Gerardo Gamez¹, Yue She², Kevin Finch²; ¹*Texas Tech University*, ²*Texas Tech University Department of Chemistry and Biochemistry*
- 2:30 PM (72) **Elemental analysis of multi-layered structures using GD-OES and Micro-XRF;** Matthieu F. Chausseau¹, Patrick Chapon², Jocelyne Marciano², Sofia Gaiaschi²; ¹*HORIBA Scientifc*, ²*HORIBA France*

- 2:50 PM (73) **The Continued Development of a New DC/RF/Pulsed-RF Glow Discharge Lamp and Supply;** Kim Marshall¹, Kim Marshall²; ¹*Leco Corp.*, ²*LECO Corporation*

19AWD13: SAS Ellis R. Lippincott Award Symposium Honoring Ji-Xin Cheng *Mojave*

Chair: Ji-Xin Cheng

- 1:30 PM (74) **Stimulated Raman Imaging with Chemical Tags;** Wei Lu¹; ¹*California Institute of Technology*
- 1:50 PM (75) **Retinal Oximetry by Visible Light Optical Coherence Tomography;** Ji Yi¹; ¹*Boston University*
- 2:10 PM (76) **High-resolution spectroscopic imaging for understanding myelofibrosis;** Rohith Reddy¹, Licheng Zhang¹, Chalapathi Gajjala¹, Shihao Ran¹, Rupali Mankar¹, David Mayerich¹, Rohith Reddy¹; ¹*University of Houston*
- 2:30 PM (77) **Revealing Subcellular Structures with Live-cell and 3D Fluorescence Nanoscopy;** Fang Huang¹; ¹*Purdue University*
- 2:50 PM (78) **Dispersion-based Spectroscopic Imaging: Principles and Applications in Biomedicine;** Francisco E. Robles¹; ¹*Georgia Tech and Emory University BME*

19BIM02: Spectroscopic Approaches to Tackle Infectious Diseases *Catalina*

Chair: Jürgen Popp

- 1:30 PM (79) **Finally, a Slam Dunk SERS Application: Metabolic Responses for Fast Antibiotic Susceptibility Testing;** Lawrence Ziegler¹, Lawrence Ziegler¹; ¹*Boston University*
- 1:50 PM (80) **Plasmonic Nanostructures for Pathogen Fingerprinting and Killing;** Wei-Chuan Shih¹, Wei-Chuan Shih¹; ¹*University of Houston*
- 2:10 PM (81) **Raman Spectroscopic Characterization of Leukocyte in Scenario of Infection and Inflammation;** Anuradha Ramoji¹, Anuradha Ramoji¹, Daniel Thomas-Rüddel², Oleg Ryabchykov³, Natalie Töpfer¹, Iwan Schie¹, Thomas Bocklitz³, Michael Bauer¹, Ute Neugebauer¹, Juergen Popp¹; ¹*Leibniz Institute of Photonic Technology*, ²*Jena University Hospital*, ³*Institute of Physical Chemistry and Abbe Center of Photonics*

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 1:30 PM - 3:10 PM

2:30 PM (82) **Phosphorescent Liquid Bandages for the Identification of Inflammatory Bacterial Infections;** Haley Marks¹, Haley Marks², Conor Evans²; ¹Wellman Center for Photomedicine, ²MGH

2:50 PM (83) **Raman Spectroscopic Phenotyping - Identification of the Infection Causing Bacteria and Quantification of the Antibiotic Susceptibility;** Jürgen Popp¹; ¹Leibniz Institute of Photonic Technology

19IR03: Nanoscale IR Spectroscopy II: Fundamentals and Applications *Smoketree E*

Chairs: Andrea Centrone, Georg Ramer

1:30 PM (84) **Thermal Effects in Photo-induced Force Microscopy (PiFM);** Eric O. Potma¹; ¹University of California, Irvine

1:50 PM (85) **Exploration of the Origin of Photo-induced Force in Tapping Mode Nanoscale Infrared Microscopy;** Xiaoji Xu¹, Le Wang¹; ¹Lehigh University

2:10 PM (86) **Novel Concepts in Infrared Nano-Imaging – Competing, Confusing, Controversial, or Complementary?;** Markus B. Raschke¹; ¹University of Colorado

2:30 PM (87) **Characterization 2D Materials and Heterostructures with Infrared Nanospectroscopy (PTIR);** Andrea Centrone¹; ¹National Institute of Standard and Technology

2:50 PM (88) **Nanoscale Materials Analysis Using AFM-IR;** Liang Gong¹; ¹3M Company

19LIBS03: Biomedical and Pharmaceutical Applications *Smoketree C*

Chair: Nouredine Melikechi

1:30 PM (89) **Laser-induced Breakdown Spectroscopy (LIBS) for the Diagnosis of Neurodegenerative Diseases;** Rosalba Gaudioso¹, Weiming Xia², Xinzi Sun¹, Benyuan Liu¹, Nouredine Melikechi¹; ¹University of Massachusetts Lowell, ²Boston University - Edith Nourse Rogers Memorial Veterans Hospital

1:50 PM (90) **Diagnosis of Human Malignancies Using Blood Sample Laser-induced Breakdown Spectroscopy in Combination with Chemometric Methods;** Xiaohui Li¹, Xue Chen², Sibao Yang³, Yao Zhang³, Aichun Liu², Xin Yu³; ¹Harbin Institute of Technology, ²Department of

Hematology, Harbin Medical University, ³Institute of Opto-Electronics, Harbin Institute of Technology

2:10 PM (91) **Bacterial Limit of Detection Reduction Utilizing a Novel Sample Preparation Protocol;** Steven J. Rehse¹, Jeremy Marvin², Alexandra Paulick², Emma Blanchette², Sydney Sleiman²; ¹University of Windsor, Department of Physics, ²University of Windsor

2:30 PM (92) **In Situ Analytical Characterization and Chemical Imaging of Tablet Coatings Using Laser Induced Breakdown Spectroscopy;** Lanfeng Zou¹, Brittany Kassim², Joseph Smith², James Ormes², Xiaodong Bu²; ¹Biogen, ²Merck

2:50 PM (93) **From Bench to Bedside: LIBS Imaging Is Entering the Clinic as a New Diagnostic Tool for Respiratory Diseases;** Motto-Ros Vincent¹, Benoit Busser², Vincent Motto-Ros¹; ¹ILM, ²IAB / CHUGA

19MASS04: Forensic Applications of Mass Spectrometry *Smoketree B*

Chair: Glen Jackson

1:30 PM (94) **Sourcing of Latent Print Chemical Residue Using 2D-GC-MS;** Candice Bridge¹, Candice Bridge², Jessica Kindell³; ¹University of Central Florida & National Center for Forensic Science, ²UCF/NCFS, ³UCF

1:50 PM (95) **GC-MS and Product Ion MS-MS Studies on Substituted Cathinone Designer Drugs;** Randall Clark¹, Jack DeRuiter¹, Younis Abiedalla¹; ¹Auburn University HSOP

2:10 PM (96) **Barking up the Wrong Tree: Combating Illegal Trade in Endangered Wood Species with Mass Spectrometry;** Rabi A. Musah¹, Meghan Fogerty², Samira Beyramysoltan²; ¹University at Albany, State University of New York, ²University at Albany-SUNY

2:30 PM (97) **Statistical Comparison of Mass Spectra for Seized Drug Identification;** Ruth Smith¹, Emma Stuhmer¹, Victoria McGuffin¹; ¹Michigan State University

2:50 PM (98) **Integrated SERS-PSI-MS Platform Using Gold Nanoparticle-embedded Paper for Trace Detection of Illegal Drugs;** Jeremy D. Driskell¹, Christopher Mulligan², Jun-Hyun Kim², William Fatigante¹, Daniel Burr¹, Jemima Lartey¹; ¹Illinois State University, ²Illinois State University

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 1:30 PM - 3:10 PM

19NANO02: Nano-Facilitated Sensing *Mesquite E*

Chair: David Thompson

- 1:30 PM (99) **Imaging Nano Particles with X-ray Excited Optical Luminescence;** Jeffrey N. Anker¹, Unaiza Uzair¹, Meena Ranasinghe¹, Gretchen Schober¹, Matt Case¹, Md. Arifuzzaman¹, Sriparna Bhattacharya¹, Apparao Rao¹; ¹*Clemson University*
- 1:50 PM (100) **Investigating Antibody-gold Nanoparticle Adsorption Dynamics to Optimize Conjugates for Biosensing;** Jeremy D. Driskell¹, Kiran Tripathi¹, Guadalupe Ruiz¹, Samuel Okyem¹, Olatunde Awotunde¹; ¹*Illinois State University*
- 2:10 PM (101) **Prospects for Detection of a Wide Variety of Analytes with SERS;** Erik Emmons¹, Erik Emmons²; ¹*US Army CCDC Chemical Biological Center*, ²*US Army CCDC CBC*
- 2:30 PM (102) **Sensor Surface Temperature and Headspace-sampled SERS Signals;** David E. Thompson¹, Reece Thompson¹, Md Nure Alam¹, Waruni Senanayake¹, C. James McMurray¹, David E. Thompson¹; ¹*Sam Houston State University*

19PMA01: Solving Industrial Problems using Vibrational Spectroscopy *Madera*

Chair: Andrew Marriott

- 1:30 PM (103) **Drug-amino Acid Co-amorphous Formulation Analysis by FTIR Spectroscopy;** Mohammed Alsalhi¹, Ka Lung Andrew Chan¹; ¹*KINGS COLLEGE LONDON*
- 1:50 PM (104) **Use of FT-IR Modelling to Determine Isotopic Impurities in the Deuterated Reagent d3-methylamine Hydrochloride;** Andrew Marriott¹, Alistair Boyd¹, Emma Quirk¹; ¹*Bristol-Myers Squibb*
- 2:10 PM (105) **ATR-FTIR Imaging to Study the Aggregation of Biopharmaceuticals Through Secondary Structure Analysis;** Hannah Tiernan¹, Patrick Wray², Bernadette Byrne¹, Sergei Kazarian¹; ¹*Imperial College London*, ²*Bristol-Myers Squibb*
- 2:30 PM (106) **In-column ATR-FTIR spectroscopy for analysis of monoclonal antibody purification;** Sergei Kazarian¹, Sergei Kazarian¹, Bernadette Byrne¹, Christian Bortolini¹, James Beattie¹; ¹*Imperial College London*
- 2:50 PM (107) **Enantioselective Raman Spectroscopy – a Novel Tool for Enantiomeric Discrimination;** Claudia C. Rullich¹, Johannes Kiefer¹; ¹*University of Bremen*

19RAM09: IRDG *Sierra*

Chair: Karen Faulds

- 1:30 PM (108) **What Can We Learn from SERS of Bacteria and Their Metabolites;** Bell Steven¹, Steven Bell², Jessica Kelly¹, Danielle Allen¹, Michael Tunney¹; ¹*Queen's University*, ²*Queen's University*
- 1:50 PM (109) **Elucidation of Two-photon Properties via Surface-enhanced Hyper-raman Scattering of Rhodamine-like Dyes;** Jacob Olson¹, Jon Camden¹, Lasse Jensen², Michael Detty³; ¹*University of Notre Dame*, ²*Pennsylvania State University*, ³*University of Buffalo*
- 2:10 PM (110) **SERS Probes to Monitor Communicable and Non-communicable Diseases;** Laura Fabris¹, Hao Wang¹, Manjari Bhamidipati¹, Kholud Dardir¹; ¹*Rutgers University*
- 2:30 PM (111) **Single-molecule and Single-particle Surface-enhanced Raman Scattering (SERS) in Analytical Chemistry;** Alexandre Brolo¹; ¹*University of Victoria*
- 2:50 PM (112) **Determining the Level and Location of Functional Groups on Commercial Graphene Using Tip-enhanced Raman Spectroscopy;** Elizabeth J. Legge^{1,2}, Keith R. Paton¹, Magdalena Wywijas¹, Greg McMahon¹, Rory Pemberton¹, Naresh Kumar¹, Arun Prakash Aranga Raju³, Craig P. Dawson³, Andrew J. Strudwick³, James W. Bradley⁴, Vlad Stolojan², S. Ravi P. Silva², Stephen Hodge⁵, Barry Brennan¹, Andrew J. Pollard¹; ¹*National Physical Laboratory, Hampton Road, Teddington, Middlesex, UK*; ²*Advanced Technology Institute, University of Surrey, Guildford, UK*; ³*Graphene Engineering Innovation Centre (GEIC), University of Manchester, Manchester, UK*; ⁴*Department of Electrical Engineering and Electronics, University of Liverpool, Liverpool, UK*; ⁵*Versarien Plc., Cheltenham, UK*

19SPECIAL04: Society for Archaeological Sciences Session on Chemistry in Art and Archaeology II *Chino AB*

Chairs: Mary Kate Donais, Andrew Zipkin

- 1:30 PM (113) **From Coast to Karoo: A Radiogenic Bioavailable Strontium Isoscape in South Africa for Provenience Studies;** Andrew M. Zipkin¹, Erich Fisher¹, Gwyneth Gordon¹, Hayley Cawthra², Kelly Knudson¹, Curtis Marean¹; ¹*Arizona State University*, ²*Nelson Mandela University*

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 1:30 PM - 3:10 PM

1:50 PM (114) **Micro- to Nanoscale IR in Heritage Science: the Distribution of Metal Carboxylates in Oil Paint;** XIAO Ma¹, Xiao Ma², Victoria Beltran³, Georg Ramer⁴, Georges Pavlidis⁴, Dilworth Parkinson⁵, Mathieu Thoury⁶, Tyler Meldrum⁷, Andrea Centrone⁴, Barbara Berrie²; ¹Scientific Research Department, National Gallery of Art, ²National Gallery of Art, ³University of Antwerp, ⁴National Institute of Standards and Technology, ⁵Lawrence Berkeley National Laboratory, ⁶IPANEMA, CNRS, ⁷The College of William & Mary

2:10 PM (115) **Trace Element Analysis of Archaeological Human Enamel and Bone Apatite: Implications for Documenting Biological Sex and Health Status;** Beth K. Scaffidi¹, Beth Scaffidi¹, Gwyneth Gordon¹, Kelly Knudson¹; ¹Arizona State University

2:30 PM (116) **Strengths and Limitations of Fecal Stanols as a Population Proxy for Cahokia, Illinois and the Jordanian Desert;** AJ White¹, Varenka Lorenzi², Lisa Maher¹, Lora Stevens²; ¹University of California, Berkeley, ²California State University, Long Beach

2:50 PM (117) **Food, Networks, Power: Exploring Ancient Cypriot Foodways Through Organic Residue Analysis;** Rebecca Gerdes¹, Sturt Manning¹; ¹Cornell University

19SPR01: Nanostructure Implications on Plasmonics
Smoketree A

Chair: Amanda Haes

1:30 PM (118) **Aluminum Plasmonic Antennas for Surface-enhanced Infrared Absorption Spectroscopy;** Jennifer S. Shumaker-Parry¹, Caitlin Coplan¹, Mark Swartz¹; ¹University of Utah

1:50 PM (119) **Plasmonic Properties of Non-precious Metal Cu-based Nanostructures;** Jingyi Chen¹; ¹University of Arkansas

2:30 PM (120) **Observation of Hot-Carrier Driven Chemical Reaction by TERS;** Dmitry Kurouski¹, Dmitry Kurouski¹; ¹Texas A&M University

2:50 PM (121) **Plasmonic Properties of Multimetal Layers Nanodisk Array;** Benjamin Charron¹, Jean-Francois Masson²; ¹University of Montreal, ²Universite de Montreal

TECHNICAL PROGRAM - MONDAY

POSTER SESSION 3:10 PM – 3:50 PM

Primrose Foyer

See page 83 for a listing of Monday posters by category. Student poster award winners will be announced the following morning during the plenary session.

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19AES03: ACS ANYL-AES Joint Session: Micro/Nano Scale Analytics Driven by Electric Fields *Mesquite D*

Chairs: Mark Hayes, Lane Baker

3:50 PM (122) **Thread-based Sensors and Fuel Cells;** Frank Gomez¹, Kathryn Uchida¹, Ricardo Ortiz¹, Lauren Duenas¹, Kevin Diego-Perez¹, Jessica Vazquez¹, Michelle Gaines¹, Mariajose Gonzalez¹; ¹California State University, Los Angeles

4:10 PM (123) **Multi-detector approaches for improved resolution in capillary electrophoresis;** Christopher A. Baker¹; ¹University of Tennessee

4:30 PM (124) **DNA Sequence-specific Enrichment Using Isotachophoresis;** Juan G. Santiago¹, Ashwin

Ramachandran¹, Futai Nobuyuki², Catherine Hogan¹, Niaz Banaei¹; ¹Stanford University, ²Shibaura Institute of Technology

4:50 PM (125) **Single-particle Analysis of Virus Capsid Assembly by Resistive-pulse Sensing;** Stephen C. Jacobson¹, Panagiotis Kondylis, Mi Zhang, Jinsheng Zhou, Christopher Schlicksup, Adam Zlotnick; ¹Indiana University

5:10 PM (126) **Electrokinetic Assessment of Bacteriophage Virus;** Adriana Coll De Peña¹, Nurul Humaira Mohd Redzuan¹, Milky Abajorga¹, Julie A. Thomas¹, Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19ATOM02: Laser Ablation Based Spectroscopies

Pasadena

Chair: Jorge Pisonero

- 3:50 PM (127) **Laser ionization mass spectrometry for direct atomic analysis of solids;** Jose Miguel Vadillo¹, J. Javier Laserna²; ¹Universidad de Málaga, UMALASERLAB, ²Universidad de Málaga, UMALASERLAB, Málaga, España-Spain
- 4:10 PM (128) **Fast and High Resolved Elemental Analysis Using ns/fs-LA;** Jorge Pisonero¹, Cristina Méndez¹, Ana Méndez¹, Miguel Iglesias¹, Nerea Bordel¹; ¹University of Oviedo
- 4:30 PM (129) **Novel Reference Materials for LA-ICP-MS Analysis on Hair;** Mauro Martinez¹, Matthieu Baudelet², Terra Brown²; ¹National Center of Forensic Science, ²University of Central Florida
- 4:50 PM (130) **Exploring the Potential of Fast Washout LA with Quasi-simultaneous Multi-isotope Detection for Single Cell Elemental Imaging Using LA-ICP-ToF-MS;** Kharmen Billimoria¹, Gonzalo Huelga Suarez¹, David A. Ramsay¹, Stanislav Strekopytov¹, David N. Douglas³, Leif Summerfield³, Heidi Goenaga-Infante⁴; ¹LGC, ²LGC and University of Warwick, ³ESL, ⁴LGC Ltd., UK
- 5:10 PM (131) **Direct Detection of Single Particles with SIMS and ICP-MS: On Recent Advances and Remaining Challenges;** Carsten Engelhard¹, Birgit Hagenhoff², Darya Mozhayeva¹, Annika Schardt¹, Ingo Streng³, Lothar Veith⁴; ¹University of Siegen, ²Tascon GmbH, ³University of Siegen / NIST, ⁴Max Planck Institute for Polymer Research

19AWD06: Spectroscopy's Emerging Leader in Molecular Spectroscopy Award Symposium Honoring Ishan Barman

Mojave

Chair: Ishan Barman

- 3:50 PM (132) **Developing Surface Enhanced Deep Raman Spectroscopy for Clinical Applications;** Nick Stone¹, Ben Gardner¹, Priyanka Dey¹, Sara Mosca², Adrian Ghita¹, Martha Vardaki¹, Pavel Matousek²; ¹University of Exeter, ²STFC Rutherford Appleton Laboratory
- 4:10 PM (133) **Raman Microscopy for High-throughput Molecular Analysis;** Katsumasa Fujita¹; ¹Osaka University
- 4:30 PM (134) **Label-free Morphomolecular Microscopic Investigation of Live Leukemic Cells;** Rishikesh Pandey¹; ¹CytoVeris Inc.

- 4:50 PM (135) **Nanoengineered Interfaces for Optical Sensing of Chemicals and Biochemicals;** Steve Semancik¹; ¹National Institute of Standards and Technology

- 5:10 PM (136) **Quantitative Confocal Raman Microscopy Detection of a Hybrid Phospholipid Bilayer-Based Sandwich Immunoassay within Individual Chromatographic Silica Particles;** Jay P. Kitt¹, David A. Bryce¹, Joel M. Harris¹; ¹University of Utah

19CTP01: Commercialization of Analytical Technologies

Chino AB

Chairs: Karen Esmonde-White, Scott Rudder

- 3:50 PM (137) **Tips 4 Successful Entrepreneurship: Jump Don't Step!;** Scott Rudder¹; ¹Innovative Photonic Solutions
- 4:10 PM (138) **Moving Disruptive Innovation to Market;** Isao Noda¹, Jennifer Moe², Michael Satkowski², Pedr Rodriguez³; ¹University of Delaware, ²Procter & Gamble Company, ³P&G, retired
- 4:30 PM (139) **Growing a Company on Customer Specifications;** Cheryl Provost¹; ¹FiberTech Optica, Inc
- 4:50 PM (140) **Navigating a Successful Pathway to Exit: Strategies for Building Value and Finding the Right Partner;** Randy Heyler¹; ¹Ondax, Now a Coherent Company.
- 5:10 PM (141) **Speaker Roundtable;** Scott Rudder¹, Isao Noda², Cheryl Provost³, Randy Heyler⁴; ¹Innovative Photonic Solutions, ²University of Delaware, ³FiberTech Optica, Inc, ⁴Ondax, Now a Coherent Company

19IR04: Advances in Molecular Spectroscopy Smoketree D

Chair: William Wang

- 3:50 PM (142) **A Novel Analytical Technique of Chemical Reaction in a Ultra-thin Film Using pMAIRS;** Takeshi Hasegawa¹, Ryoji Fujiwara¹, Kazutaka Tomita¹, Nobutaka Shioya¹, Takafumi Shimoaka¹; ¹ICR, Kyoto University
- 4:10 PM (143) **Variations in Bone Composition at Sub-micron Resolution;** Nancy Pleshko¹, William Querido¹, Jay Anderson², Curtis Marcott³, Frank Weston²; ¹Temple University, ²Photothermal Spectroscopy Corp, ³Light Light Solutions

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

4:30 PM (144) **Polarized Infrared Light Reveals Order and Disorder in 2-, 4- and 8-week Post-infarct Rat Heart;** Kathleen M. Gough¹, Nebojsa Oravec², Negar Atefi², Sunil Rattan², Eoghan Dillon³, Mustafa Kansiz³, Ian Dixon²; ¹Department of Chemistry, University of Manitoba, ²University of Manitoba, ³Photothermal Spectroscopy Corp

4:50 PM (145) **Submicron Simultaneous IR and Raman Spectroscopy (IR-Raman): Breakthrough Developments in Optical Photothermal IR (O-PTIR) Combined with Raman Provide New Capabilities;** Mustafa Kansiz¹, Curtis Marcott²; ¹Photothermal Spectroscopy Corp, ²Light Light Solutions

5:10 PM (146) **Identification of Unknown Samples Through Simultaneous IR and Raman Measurement and Database Searching: Exploiting Synergies for Complementary and Confirmatory Analysis;** Gregory M. Banik¹, Michelle D'Souza², Mustafa Kansiz³, Roshan Shetty³, Ty Abshear²; ¹Bio-Rad Laboratories, Inc., ²Bio-Rad Laboratories, Informatics Division, ³Photothermal Spectroscopy Corp

19IR11: Nanoscale IR Spectroscopy III: Bio-Applications Smoketree E

Chairs: Andrea Centrone, Liang Gong

3:50 PM (147) **Understanding the Recorded Signal in Atomic Force Microscopy-infrared Spectroscopy (AFM-IR) Measurements;** Rohit Bhargava¹, Seth Kenkel¹; ¹University of Illinois Urbana-Champaign,

4:10 PM (148) **Nanoscale Chemical Analysis from Single Biomolecules to Living Organisms in Air and Native Liquid Environment;** Francesco Simone Ruggeri¹, ¹Department of Chemistry, University of Cambridge

4:30 PM (149) **Infrared Difference-nanospectroscopy to Probe the Light-induced Conformational Changes of Transmembrane Proteins in Individual Membrane Patches;** Valeria Giliberti¹, Raffaella Polito², Eglof Ritter³, Matthias Broser³, Peter Hegemann³, Ljiljana Puskar⁴, Ulrich Schade⁴, Laura Zanetti-Polzi⁵, Isabella Daidone⁵, Stefano Corni⁶, Francesco Rusconi⁷, Paolo Biagioni⁷, Leonetta Baldassarre², Michele Ortolani²; ¹Center for Life NanoScience - Istituto Italiano di Tecnologia, ²Department of Physics, Sapienza University of Rome Italy, ³Humboldt-Universität zu Berlin, Institut für Biologie, Berlin, Germany, ⁴Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, 12489

Germany, ⁵Department of Physical and Chemical Sciences, University of L'Aquila, L'Aquila, Italy, ⁶Department of Chemical Sciences, University of Padova, Padova, Italy, ⁷Dipartimento di Fisica, Politecnico di Milano, Milano, Italy

4:50 PM (150) **Structural Characterization of Plant Epicuticular Waxes Using AFM-IR;** Dmitry Kurouski¹; ¹Texas A&M University

5:10 PM (151) **Nanoscale Chemical Heterogeneity as a Function of Tissue Age for Wild Type Mice Femurs Measured by Photothermal Infrared Spectroscopy (PTIR);** Taeyong Ahn¹, Max Jueckstock¹, Kenneth Kozloff¹, Mark Banaszak-Holl²; ¹University of Michigan, ²Monash University

19LIBS09: Geology Smoketree C

Chair: Lütü Özcan

3:50 PM (152) **"LIBS and Geology," A Long and Nice Story: What It's Now Possible to Do and How to Do It Well;** Cécile Fabre¹; ¹Universite de Lorraine / GeoRessources

4:10 PM (153) **Ultrafast Analysis in Mining Industry for Noble Metals;** Lütü Özcan¹, Kheireddine Rifai¹, Francois R. Doucet¹, François Vidal², Félix Gervais³; ¹ELEMISSION INC., ²INRS, ³Polytechnic school of Montreal

4:30 PM (154) **Fast High-resolution Multi-elemental Mapping of Phosphate Pellets Using Laser Induced Breakdown Spectroscopy;** Nawfel Azami¹, Driss Lahlou Kitane², Laurent Deshayes³, Sara ElMrabet³, Abdeljabbar Lebbardi⁴, Lütü Özcan⁵, Francois R. Doucet⁶, Kheireddine Rifai⁵; ¹INPT-UM6P, ²Operations Research Center - Massachusetts Institute of Technology, ³UM6P, ⁴OCP Group, ⁵ELEMISSION INC., ⁶ELEMISSION inc.

4:50 PM (155) **In-situ Elemental Rock Testing (In-SERT) Probe: Development Feasibility of a LIBS and Raman Spectroscopy Based Characterization System;** Shane C. Lee¹, Prasoon K. Diwakar²; ¹South Dakota School of Mines & Technology, ²South Dakota School of Mines and Technology

5:10 PM (156) **Direct Determination of Soils Texture Using Laser-induced Breakdown Spectroscopy and Multivariate Linear Regressions;** Christian L. Goueguel¹; ¹Logiag Inc.

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19MASS02: Untargeted Metabolomics: Innovations and Applications *Mesquite E*

Chair: Amina Bouslimani

- 3:50 PM (157) **Unraveling Drug Metabolism Complexity via Untargeted Mass Spectrometry**; Alan Jarmusch¹, Alan Jarmusch¹, Mingxun Wang¹, Alison Vrbanc¹, Emmanuel Elijah¹, Fernando Vargas¹, Ricardo da Silva², Madeleine Ernst³, Rob Knight¹, Shirley Tsunoda¹, Pieter Dorrestein¹; ¹University of California, San Diego, ²University of São Paulo, Ribeirão Preto, ³Statens Serum Institut, Copenhagen
- 4:10 PM (158) **Contextualizing Host-parasite-microbiome Interactions Using Lc-ms/ms-based Metabolomics and Chemical Cartography**; Laura-Isobel McCall¹, Ekram Hossain¹, Chaoyi Wu¹, Sharmily Khanam¹, Danya Dean¹, Adwaita Parab¹, Shelley Kane¹, Karina Flores¹, Sharon Lostracco-Johnson², Diane Thomas², Danyang Li, Christine Woelfel-Monsivais¹, Michelle Katemauswa¹, Camil Gosmanov¹, Krithivasan Sankaranarayanan¹; ¹University of Oklahoma, ²University of California San Diego
- 4:30 PM (159) **Mass Spectrometry Based Machine Learning Approaches to Discover Nutrients That Can Revitalize the Modern Diet**; Gabriel Navarro¹, Jessie Ochoa¹, Sasha Marks¹, Chuan Wang¹, Jim flatt¹, Carol-Lynn Berseth¹, Meng Xu¹, Lee Chae¹; ¹Brightseed
- 4:50 PM (160) **Characterizing the Chemotypic Landscape of Polymicrobial Communities**; Vanessa Phelan¹, Vanessa Phelan¹; ¹University of Colorado - Anschutz Medical Campus
- 5:10 PM (161) **Scaling Molecular Networks to the Cloud Enables New Visualizations**; Mingxun Wang¹, Mingxun Wang¹; ¹Omata Labs LLC

19PAT07: Process Analytical in the Petroleum/Refineries Industry *Smoketree A*

Chair: Toni Miao

- 3:50 PM (162) **Process Analytics in the Petrochemical Industry: 30 Years Back and 10 Years Forward**; Charles E. Miller¹; ¹Camo Analytics
- 4:10 PM (163) **Chemometrics in Refinery applications - a new approach**; Michael Kleimann¹, Allan Rilling², Andreas Strauch²; ¹ABB Automation GmbH, ²ABB Inc.
- 4:30 PM (164) **Using Infrared Spectroscopy for Alkylation Process Monitoring**; Howard

Lacheen¹, Toni Miao², Huping Luo², Hye-Kyung Timken²; ¹Chevron Energy Technology Company, ²Chevron

- 4:50 PM (165) **The Benefits of High-throughput Raman for Process Analysis**; Mark S. Kemper¹, Mark Kemper¹, Bradford Behr¹, Charles Greenhalf¹, Shamus Driver¹; ¹Tornado Spectral Systems, Inc.
- 5:10 PM (166) **Evaluating the Capability of the Ultraportable, Ergonomic 4300 FTIR for Rapid Delineation of Hydrocarbons in Soil**; Natasha Sihota¹, Toni Miao¹; ¹Chevron

19PMA02: Biophysical Characteristics of Biotherapeutics: From Discovery to Development *Madera*

Chair: Deniz Temel

- 3:50 PM (167) **Raman Spectroscopy in Cancer Pathology Classification**; Sarah C. Shidler¹, Tim Prusnick¹, Gavin Lloyd², Neil Shepherd³, Manuel Rodriguez-Justo⁴, Hugh Barr³, Geraint Thomas⁵, Nick Stone⁶, Martin Isabelle⁷; ¹Renishaw Inc., ²Phenome Centre Birmingham, School of Biosciences, ³Gloucestershire Hospitals NHS Foundation Trust, ⁴University College London Hospitals NHS Foundation Trust, ⁵Cell & Developmental Biology, UCL, ⁶University of Exeter, ⁷Renishaw plc, Spectroscopy Products Division
- 4:10 PM (168) **Novel Method for Multidimensional Fluorescence Characterization of Protein Binding**; Karen E. Gall¹, Alex Siemiarczuk¹; ¹HORIBA Scientific
- 4:30 PM (169) **Scanning Electron Cryomicroscopy (CryoSEM)-Raman Spectroscopy for Analysis of Complex Drug Products**; Huzeyfe Yilmaz¹, Daniel Willett², Anna M. Wokovich¹, Jason D. Rodriguez¹, David A. Keire¹; ¹US Food and Drug Administration, ²U.S. Food and Drug Administration
- 4:50 PM (170) **An Integrated Data Analysis Approach for Analysis of Biotherapeutics by Native CE-MS**; Christopher D. Brown¹, Colin Gavin¹, Cody Griffith¹; ¹908 Devices
- 5:10 PM (171) **Monitoring and Control in Upstream and Downstream Bioprocessing Based on Process Raman Spectroscopy**; Karen A. Esmonde-White¹, Dave Strachan², Maryann Cuellar², Carsten Uerpmann³, Sean J. Gilliam⁴, Ian Lewis²; ¹Kaiser Optical Systems, Inc., ²Kaiser Optical Systems Inc., ³Kaiser Optical Systems SARL, ⁴Kaiser

TECHNICAL PROGRAM - MONDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19RAM06: SERS I Sierra

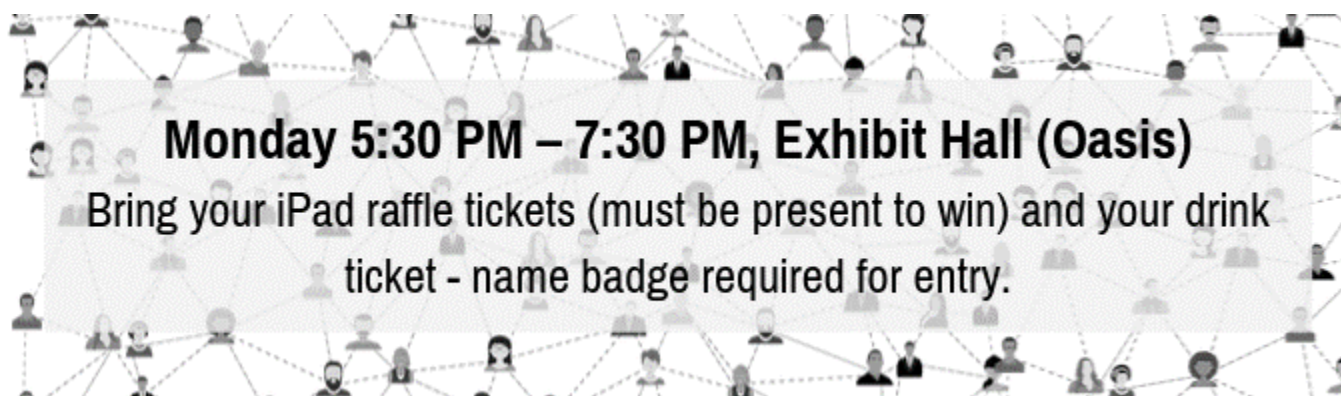
Chairs: Roy Goodacre, Colin Campbell, Duncan Graham

- 3:50 PM (172) **SERS in Tissue Models**; Colin Campbell¹, Holly Fleming¹, William Skinner¹, Ailsa Golightly¹, Hannah Johnston², Lauren Jamieson¹; ¹University of Edinburgh, ²Univeristy of Edinburgh
- 4:10 PM (173) **Multimodal Optical Biosensing Toward Point-of-care Diagnosis and Monitoring**; Gerard L. Cote¹, Dandan Tu¹, Sungyub Han¹; ¹Texas A&M University
- 4:30 PM (174) **Reproducible Immunoassay of Multiple Biomarkers Using SERS Mapping on Three-dimensional Nanopillar Arrays**; Jaebum Choo¹; ¹Chung-Ang University
- 4:50 PM (175) **Detection of MMP Activity Using Surface Enhanced Raman Scattering to Aid Cancer Detection**; Sian Sloan-Dennison¹, Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde
- 5:10 PM (176) **Surface-enhanced Raman Scattering Nanosensors for optophysiology: Exploring Neurochemistry in Near-real-time**; Gregory Q. Wallace¹, Benoît Delignat-Lavaud¹, Félix Lussier¹, Vincent Thibault¹, Xingjuan Zhao¹, Louis-Éric Trudeau¹, Jean-Francois Masson²; ¹Université de Montréal, ²Universite de Montreal

19SPSJ02: VUV/FUV/DUV II Smoketree B

Chair: Yukihiro Ozaki

- 3:50 PM (177) **Laser Cooling of (Anti)hydrogen Using Pulsed VUV Radiation**; Takamasa Momose¹; ¹The University of British Columbia
- 4:10 PM (178) **Taming DUV Raman Microscopy with Plasmonic Metals**; Atsushi Taguchi¹; ¹Hokkaido University
- 4:30 PM (179) **Investigation for Sigma Orbitals in the Liquids and Solids of Normal- and Cyclo-alkanes Using ATR-FUV**; Yusuke Morisawa¹, Yusuke Morisawa¹; ¹Kindai University
- 4:50 PM (180) **Electrochemical Attenuated Total Reflectance Spectroscopy in Far- and Deep-ultraviolet Regions**; Ichiro Tanabe¹, Ichiro Tanabe¹, Ken-ichi Fukui¹; ¹Osaka University
- 5:10 PM (181) **Attenuated Total Reflection FUV-DUV Spectroscopy of Graphene Nanostructures and Graphene-polymer Nanocomposites with Quantum Chemical Calculations**; Krzysztof B. Bec¹, ¹Institute of Analytical Chemistry and Radiochemistry, University of Innsbruck,



TECHNICAL PROGRAM - TUESDAY
AWARDS AND PLENARY LECTURES 7:45 AM – 9:00 AM
 Chair: Mary Kate Donais
Primrose A

7:45 AM Award Presentations

- 8:00 AM (182) **Charles Mann Award for Raman Spectroscopy; Development of SERS and SESORRS for Multiplexed Bioanalysis;** Karen Faulds¹; ¹*University of Strathclyde*
- 8:30 AM (183) **ANACHEM Award; Droplet Microfluidics with Mass Spectrometry for High-throughput Chemistry, Screening, and Sensing;** Robert Kennedy¹; ¹*University of Michigan*

TECHNICAL PROGRAM - TUESDAY
ORAL SYMPOSIA 9:15 AM – 10:55 AM

19AES04: 3D Printed Microfluidics: New Materials and New Applications *Mesquite D*

Chairs: R. Scott Martin, Ana Egatz-Gomez

- 9:15 AM (184) **Miniaturizing 3D Printed Microfluidics: Materials, Tools, and Trends;** Greg P. Nordin¹, Hua Gong¹, Adam Woolley¹; ¹*Brigham Young University*
- 9:35 AM (185) **Electron Microscopy Sample Preparation Systems Fabricated by 3D Printing;** Michael Roper¹, Julia Danyuk¹, Scott Staggs¹, Michael Roper²; ¹*Florida State University*, ²*Organization ...*
- 9:55 AM (186) **Realizing the Potential of Polyjet 3D Printing;** Andre Castiaux¹, R. Scott Martin¹; ¹*Saint Louis University*
- 10:15 AM (187) **3D Printed Analytical Tools for Quantitative Studies of Human Health;** Cody W. Pinger¹, Monica Jacobs¹, Dana Spence¹; ¹*Michigan State University*
- 10:35 AM (188) **3D Printed Microfluidic Devices for Immunoaffinity Extraction of Preterm Birth Risk Biomarkers;** Adam T. Woolley¹, Haifa Almughamsi¹, Taylor Fish¹, Karyna Howell¹, Anna V. Nielsen¹; ¹*Brigham Young University*

19AWD03: Charles Mann Award Symposium Honoring Karen Faulds *Mojave*

Chair: Karen Faulds

- 9:15 AM (189) **Mann versus Food;** Roy Goodacre¹, David Ellis², Howbeer Muhamadali¹, Yun Xu¹, Paul Richardson², Rebecca Eccles³, Ian Goodall³, Pavel Matousek⁴; ¹*University of Liverpool*, ²*University of Manchester*, ³*Scotish Whisky Research Institute*, ⁴*STFC Rutherford Appleton Laboratory*
- 9:35 AM (190) **SERS Optophysiology for Monitoring Chemical Gradients;** Jean-Francois Masson¹; ¹*Universite de Montreal*

- 9:55 AM (191) **Biosensing Devices for Consumer Focused Healthcare Applications;** Kristy S. McKeating¹; ¹*Fitbit, Inc.*

- 10:15 AM (192) **Electrochemically Modulated Liquid Chromatography (EMLC): An Approach to Manipulate Solute Retention and Quantify Fundamental Electrosorption Phenomena;** Marc D. Porter¹; ¹*University of Utah*

- 10:35 AM (193) **At Last, a Wo-Mann;** Duncan Graham¹, Karen Faulds¹; ¹*University of Strathclyde*

19BIM03: Liquid Biopsies for Biomedical Applications (CLIRSPEC) *Catalina*

Chair: Matthew Baker

- 9:15 AM (194) **The Role of Phospholipid Protein Balance in Neurodegenerative Disorders. Analysis of Human Blood Serum Using Raman Spectroscopy in Liquid Biopsies;** Joanna Depciuch¹; ¹*Institute of Nuclear Physics Polish Academy of Science*

- 9:35 AM (195) **Plasmonic Point of Care Sensors for the Detection of Disease Specific miRNA in Biofluids;** Samuel Mabbott¹, Duncan Graham², Karen Faulds², Charles Mace³, Syrena Fernandes³, Gerard Cote¹, Monika Schechinger¹; ¹*Texas A&M University*, ²*University of Strathclyde*, ³*Tufts University*

- 9:55 AM (196) **A Triage Blood Test for Brain Cancer: Development of High-throughput ATR-FTIR Technology for Rapid Spectroscopic Serum Diagnostics;** Holly J. Butler¹, Matthew Baker², Paul Brennan³, James Cameron², Duncan Finlayson², Mark Hegarty¹, Michael Jenkinson⁴, David Palmer², Benjamin Smith²; ¹*ClinSpec Diagnostics*, ²*University of Strathclyde*, ³*Translational Neurosurgery, Edinburgh*, ⁴*Institution of Translational Medicine, University of Liverpool and The Walton Centre NHS Foundation Trust*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

- 10:15 AM (197) **Raman Spectroscopy Reveals Distinct Metabolic Patterns in Blood of Crohn's Disease Subjects vs Healthy Controls;** Renzo Vanna¹, Carlo F. Morasso², Marta Truffi³, Sara Albasini², Luca Sorrentino³, Francesco Colombo⁴, Gianluca Sampietro⁴, Fabio Corsi¹; ¹*Istituti Clinici Scientifici Maugeri IRCCS*, ²*ICS Maugeri*, ³*Università degli Studi di Milano*, ⁴*ASST Fatebenefratelli Sacco - Ospedale "Luigi Sacco" Polo Universitario*
- 10:35 AM (198) **A Novel Screening Method for Diagnosing Alzheimer's Disease Based on Raman Hyperspectroscopy and Advanced Statistics;** Nicole M. Ralbovsky¹, Lenka Halámková¹, Igor K. Lednev¹; ¹*University at Albany, SUNY*

19CHEM01: New Frontiers in Chemometrics *Mesquite E*

Chair: Federico Marini

- 9:35 AM (199) **Chemometric Analysis of Mass and Infrared Hyperspectral Imaging Data in the Investigation of Biological Tissues Under Environmental Stressing Conditions;** Roma Tauler¹, Carmen Bedia², Joaquim Jaumot²; ¹*IDAEA CSIC*, ²*IDAEA-CSIC*
- 9:55 AM (200) **Spectral-Spatial Exploration of Hyperspectral Imaging Data Sets Using PCA and Wavelet Transform;** Ludovic Duponchel¹, Ludovic Duponchel¹; ¹*University of Lille*
- 10:15 AM (201) **Coupling Variable Selection and Multi-block Predictive Modeling Through the Socovsel Algorithm;** Federico Marini¹, Alessandra Biancolillo², Jean-Michel Roger³; ¹*University of Rome La Sapienza*, ²*University of Rome "La Sapienza"*, ³*ITAP, Irstea, Montpellier SupAgro, University of Montpellier*
- 10:35 AM (202) **Chemical Imaging measurements of the tumor microenvironment predict colorectal cancer outcome;** Saumya Tiwari¹, Andre Balla², Georgina Cheng³, Rohit Bhargava⁴; ¹*University Of California San Diego*, ²*University of Illinois at Chicago*, ³*Carle Foundation Hospital Champaign IL*, ⁴*University of Illinois Urbana-Champaign*

19FORENS02: Food Forensics *Smoketree A*

Chairs: Betsy Jean Yakes, Luis Rodriguez-Saona

- 9:15 AM (203) **Determination of the limit of detection of multiple pesticides utilizing gold nanoparticles and surface enhanced Raman spectroscopy (SERS);** Anne-Marie Dowgiallo¹, Derek Guenther²; ¹*Ocean Insight*, ²*Ocean Optics Inc.*

- 9:35 AM (204) **Determination of Seafood Decomposition by Large Volume Static Headpace Analysis and Chemometrics;** Zhengfang Wang¹, Susan Genualdi²; ¹*University of Maryland*, ²*U.S. FDA*
- 9:55 AM (205) **Miniature Instruments in the Hands of the Consumer: Are They Making the Right Measurement in the Right Place;** Ellen v. Miseo¹, Yagiz Sutcu¹; ¹*TeakOrigin*
- 10:15 AM (206) **Opportunities of Food Sensors for Field Applications: From Crop to Your Grocery Store;** Luis Rodriguez-Saona¹, Luis Rodriguez-Saona¹; ¹*The Ohio State University*
- 10:35 AM (207) **A SERS and Mobile Raman Platform for Combating Food Fraud;** Keith Carron¹, Wei Yu¹, Mark Harpster¹; ¹*Metrohm Raman*

19IR05: Quantum Cascade Lasers *Smoketree D*

Chair: Bernhard Lendl

- 9:35 AM (208) **Real-world Applications of Quartz-enhanced Photo Acoustic Gas Sensing;** Vincenzo Luigi Spagnolo¹, Pietro Patimisco¹, Angelo Sampaolo¹, Marilena Giglio¹, Hongpeng Wu², Lei Dong²; ¹*Politecnico di Bari*, ²*Shanxi University*
- 9:55 AM (209) **New Modalities in EC-QCL Spectroscopy for Liquid Sensing;** Bernhard Lendl¹; ¹*Technische Universität Wien*
- 10:15 AM (210) **A Qcl-based Photoacoustic Sensor for Online Monitoring of N2O Emissions of Wastewater Treatment Plants;** Christoph Haisch¹, Klemens Thaler², Christoph Berger², Reinhard Niessner²; ¹*TU Munich*, ²*Technical University of Munich*
- 10:35 AM (211) **Mid-infrared Quantum Cascade Laser Based Spectroscopic Ellipsometry;** Markus Brandstetter¹, Alexander Ebner¹, Robert Zimmerleiter¹, Christoph Cobet², Kurt Hingerl³, Christian Rankl¹, Jakob Kilgus¹; ¹*Research Center for Non Destructive Testing - RECENDT GmbH*, ²*Linz School of Education*, ³*Johannes Kepler University Linz*

19IR09: Recent Advances in Using Molecular Spectroscopy for PAT *Smoketree E*

Chair: Mike George

- 9:15 AM (212) **Deep Dive into a Telescope Reaction for the Synthesis of a Pharmaceutical;** John M. Wasyluk¹, Subha Mukherjee¹; ¹*Bristol-Myers Squibb Co.*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

- 9:35 AM (213) **A Robust NIR Quantitative Method Against Powder Stream Density for the Inline Monitoring of Drug Content in a Simulated Continuous Process;** Natasha L. Velez¹, Carl A. Anderson², James K. Drennen, III²; ¹*Graduate School of Pharmaceutical Sciences, Duquesne University*, ²*Duquesne University*
- 9:55 AM (214) **In Situ Monitoring of Heterogeneous Hydrosilylation Reactions by Infrared and Raman Spectroscopy;** Xiaoyun Chen¹; ¹*The Dow Chemical Company*
- 10:15 AM (215) **Lyophilization Process Understanding by In-line Raman Measurement;** Dongsheng Bu¹, Sudhir Chakravarthi¹; ¹*Bristol-Myers Squibb*
- 10:35 AM (216) **Chemdetect Mid-ir Analyzer for Online Monitoring of Bioreactor Growth Media and Waste Products;** Craig Magee¹, Jeremy Rowlette¹, Miles Weida¹; ¹*DRS Daylight Solutions*

19MASS03: Identification of Peptide Isomers with Mass Spectrometry *Smoketree C*

Chair: Ryan Julian

- 9:15 AM (217) **Lysosomal Degradation of Peptide Isomers and Epimers;** Ryan Julian¹; ¹*UC Riverside*
- 9:35 AM (218) **Single-cell Mass Spectrometry Enables Profiling of Anionic and Cationic Metabolites in the Live *Xenopus laevis* (Frog) Embryo;** Erika P. Portero¹, Peter Nemes¹; ¹*University of Maryland, College Park*
- 9:55 AM (219) **Developing New Approaches for the Better Characterization of Isomeric Peptides: Ion Mobility Separations Enabled by Structures for Lossless Ion Manipulations;** Gabe Nagy¹, Gabe Nagy¹, Isaac K. Attah¹, Sandilya V. B. Garimella¹, Vladislav A. Petyuk¹, Yehia M. Ibrahim¹, Richard D. Smith¹; ¹*Pacific Northwest National Laboratory*
- 10:15 AM (220) **Coupling Enzymatic and Mass Spectrometry Based Approaches for Non-targeted D-amino Acid Containing Peptide Discovery;** David Mast¹, James Checco², Jonathan Sweedler²; ¹*University of Illinois at Urbana-Champaign*, ²*University of Illinois at Urbana-Champaign*
- 10:35 AM (221) **Covalent Ion/Ion Reactions in an Ion Mobility Mass Spectrometer;** Ian K. Webb¹, Veronica Carvalho¹, Rebecca Cain¹; ¹*IUPUI*

19PMA07: Metabolic Screening and Small Molecule Detection *Madera*

Chair: Katherine Hollywood

- 9:15 AM (222) **High-throughput Chemical Reaction Screening and Correlative Metabolomics by MRM-profiling;** Christina Ferreira¹, David Logsdon¹, Zinia Jaman¹, Andy Koswara¹, Zhenwei Wei¹, Tiago Sobreira¹, Madison Edwards¹, Botond Szilagyi¹, David Thompson¹, Zoltan Nagy¹, Graham Cooks¹; ¹*Purdue University*
- 9:35 AM (223) **Using Mass Spectrometry to Discover New Bile Acids from the Gut Microbiome;** Emily Gentry¹, Emily Gentry¹, Pedro Belda-Ferre¹, Pieter Dorrestein¹; ¹*UC San Diego*
- 9:55 AM (224) **Online Monitoring of Volatile Organic Compounds by Proton Transfer Reaction Mass Spectrometry: Applications Within Synthetic Biology;** Katherine A. Hollywood¹, Katherine Hollywood¹, Feliz Lopez², Luca Cappellin², Adrian Jervis¹, Perdita Barran¹, Nigel Scrutton¹; ¹*University of Manchester*, ²*Tofwerk*
- 10:15 AM (225) **Development of Near Infrared Spectroscopy for On-line Monitoring of Biomass Quality Characteristics;** Timothy G. Rials¹, Nicolas Andre², Choo Hamilton², Nicole Labbe²; ¹*The University of Tennessee Institute of Agriculture*, ²*University of Tennessee Institute of Agriculture*
- 10:35 AM (226) **Ion Pair Chromatography versus HILIC: Comparison of the Two Separation Techniques for Highly Polar Compounds;** Ruchi P. Mehta¹; ¹*Pfizer Inc.*

19RAM03: Nano Raman *Ventura*

Chair: Andrew Whitley

- 9:15 AM (227) **Nanoscale Nonlinear Excitonic Photophysics in 2D Semiconductors;** Nicholas Borys¹, Nicholas Borys¹; ¹*Montana State University*
- 9:35 AM (228) **TERS Investigation of Combustion-generated Ultrafine Particulate Matter;** Marc Chaigneau¹, Jennifer Noble¹, Ophélie Lancry¹; ¹*HORIBA France*
- 9:55 AM (229) **Stokes and Anti-stokes in Tip-enhanced Raman Spectroscopy: Quantitative Insights into Plasmon Resonance, Near-field Temperature and Spatial Resolution;** Marie Richard-Lacroix¹, Volker Deckert¹; ¹*Leibniz Institute of Photonic Technology Jena*

TECHNICAL PROGRAM - TUESDAY
ORAL SYMPOSIA 9:15 AM – 10:55 AM

- 10:15 AM (230) **Recent TERS Adventures at the Solid-liquid Interface: Chemical and Chemical Reaction Imaging;** Ashish Bhattarai¹, Patrick El-Khoury; ¹*Pacific Northwest National Laboratory*
- 10:35 AM (231) **Forward and Reverse Chemical Nanoscopy at Solid-air and Solid-liquid Interfaces;** Patrick El Khoury¹, Patrick El-Khoury², Ashish Bhattarai²; ¹*Pacific Northwest National Laboratory*, ²*PNNL*

19RAM07: SERS II Sierra

Chairs: Colin Campbell, Roy Goodacre, Duncan Graham

- 9:15 AM (232) **Electrochemical SERS for Bacterial Detection;** Christa Brosseau¹, Taylor Lynk², Kaleigh McLeod³, Clarissa Sit³; ¹*Saint Mary's University*, ²*Organization ...*, ³*Saint Marys University*
- 9:35 AM (233) **Ultrasensitive and Reproducible Detection of int1 Enabled by Slippery Liquid-infused Porous Surface-enhanced Raman Scattering (SLIPSERS) and Hot-spot Normalization (HSN);** Peter Vikesland¹, Seju Kang¹; ¹*Virginia Tech*
- 9:55 AM (234) **SERS as an Analytical Tool for Synthetic Cannabinoid Screening in Oral Fluid;** Chiara Deriu¹, Chiara Deriu¹, Irene Conticello², Alexander M. Mebel¹, Bruce McCord¹; ¹*Florida International University, Miami, FL*, ²*University of Bologna, Bologna, Italy*
- 10:15 AM (235) **Rapid Identification and Quantification of Trace Fentanyl in Drugs of Abuse with Portable Raman;** Hao Wang¹, Zhaolin Xue¹, John Gilmore², Laura Fabris³; ¹*Rutgers, the State University of New Jersey*, ²*Hamamatsu Photonics*, ³*Rutgers University*
- 10:35 AM (236) **The Detection of Biomarkers Associated with Sepsis Using SERS;** Emma O'Connor¹, Karen Faulds¹, Duncan Graham¹; ¹*University of Strathclyde*

19SPSJ03: Near Infrared Spectroscopy I Smoketree B

Chair: Shigeaki Morita

- 9:15 AM (237) **Quantitative Analysis of Weakly and Strongly Interacting Three-component Solvent Systems: NIR versus Raman Spectroscopy;** Heinz Wilhelm Siesler¹, Hui Yan², Zhixin Xiong³; ¹*Department of Physical Chemistry, University of Duisburg-Essen*, ²*School of Biotechnology, Jiangsu University of Science and Technology, Zhenjiang, China*, ³*College of Light Industry Science and Engineering, Nanjing Forestry University, Longpan Road 159, 210037, Nanjing, China*
- 9:35 AM (238) **Anharmonic Quantum Mechanical Simulation of NIR Spectra. Applications in Physical and Analytical Chemistry;** Krzysztof B. Bec¹, Krzysztof Bec², Justyna Grabska², Yukihiko Ozaki³, Christian Huck²; ¹*Institute of Analytical Chemistry and Radiochemistry, University of Innsbruck*, ²*University of Innsbruck*, ³*Kwansei Gakuin University*
- 9:55 AM (239) **Spectral Analysis of Saccharides Focusing on the Anomer Structure;** Sae Tanaka¹, Dušan Kojić², Roumiana Tsenkova³, Masato Yasui²; ¹*Department of Pharmacology, School of Medicine, Keio University*, ²*Department of Pharmacology, Keio University School of Medicine, Tokyo, Japan*, ³*Biosystem Analysis, Graduate School of Agriculture, Kobe University, Kobe, Japan*
- 10:15 AM (240) **Gradient LC-NIR and Its Application;** Shigeaki Morita¹; ¹*Osaka Electro-Communication University*
- 10:35 AM (241) **ChemDetect Mid-IR Analyzer for Inline Chemical Identification of Liquid Chromatography Separations;** Craig Magee¹, John Craig¹, Jeremy Rowlette¹, Miles Weida¹; ¹*DRS Daylight Solutions*

TECHNICAL PROGRAM - TUESDAY
POSTER SESSION 11:00 AM – 12:00 PM
Exhibit Hall, Oasis

See page 85 for Tuesday posters by category. Posters will be displayed all day and attended again in the afternoon.

TECHNICAL PROGRAM – TUESDAY

WHAT'S HOT EXHIBITOR PRESENTATIONS 11:40 AM – 1:10 PM

Chair: Brian Dable

Exhibit Hall, Oasis

(Lunch is available from 12:00 – 12:30 pm; ticket required)

- 11:40 AM High-throughput polymorph screening with THz-Raman®
Ondax (Coherent): Anjan Roy
- 11:50 AM BLAZE: A New Dawn for NIR Spectroscopy
Teledyne Princeton Instruments: Alan Lichty
- 12:00 PM Advances in Wavelength Stabilized Lasers for Raman Spectroscopy
Innovative Photonic Solutions: Scott Rudder
- 12:10 PM Get the 'Spin' on AFM & Optics: From NanoRaman™ to Single Spin Magnetometry
HORIBA Scientific: Marc Chaigneau
- 12:20 PM Embedded technology for lab-to-process Raman spectroscopy
Kaiser: Igor Nazarov
- 12:30 PM Authentication of Ionic Salts in Seconds with XR
Thermo Fisher Scientific: Kyle Dumke
- 12:40 PM Latest Developments in Raman Spectroscopy
Renishaw: Tim Prusnick
- 12:50 PM Flexible Raman without Compromise
Wasatch Photonics: Paul Murphy
- 1:00 PM The New Era of Raman Spectroscopy
Timegate Instruments: Mari Tenhunen

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

19AES08: Biological and Pharmaceutical Applications

Mesquite D

Chairs: Wenwan Zhong, Mike Beauchamp

- 1:30 PM (242) **Isolation and concentration of proteins and small complex bioparticles with electric fields;** Mark Hayes¹, Yameng Liu¹; ¹*Arizona State University*
- 1:50 PM (243) **Capillary Electrophoresis-mass Spectrometry for Top-down Proteomics;** Liangliang Sun¹; ¹*Michigan State University*
- 2:10 PM (244) **Silica Fluorination - A Novel Electroosmotic Flow Control Approach;** Christopher R. Harrison¹, Sangho Yun¹, Jessica Torres¹, Kai Nguyen¹; ¹*San Diego State University*
- 2:30 PM (245) **Characterization of Molecular and Biomolecular Interactions with Lipid Bilayers Using Nanodisc Affinity Capillary Electrophoresis;** Christopher Palmer¹, Bethany Shetler¹; ¹*University of Montana*

- 2:50 PM (246) **Monitoring Phosphorylation and Methylation of Histone Peptides Using Host-assisted Capillary Electrophoresis;** Wenwan Zhong¹, Jiwon Lee¹; ¹*University of California, Riverside*

19ATOM03: Atomic Spectroscopy Techniques for Nuclear Applications *Pasadena*

Chair: Benjamin Manard

- 1:30 PM (247) **The Use of Automation to Improve Analytical Precision of Isotopic and Impurity Analysis;** Cole R. Hexel¹, Shalina Metzger², Brian Ticknor², Kayron Rogers², Ben Manard²; ¹*Oak Ridge National Laboratory*, ²*ORNL*
- 1:50 PM (248) **Balancing Actinide Measurement Quality with the Needs of the Data End-user: A Critical Evaluation of ICP-MS Instrumentation and Techniques in the Nuclear Sciences;** William S. Kinman¹; ¹*Nuclear and Radiochemistry Group, Los Alamos National Laboratory*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

- 2:10 PM (249) **Overview of Laser Ablation-based Optical Spectroscopy Techniques for Radiological Analysis;** Kyle C. Hartig¹; ¹*University of Florida*
- 2:30 PM (250) **Innovative Sample Preparation Methodologies for ICP-MS Analysis of Nuclear Materials;** John D. Brockman¹, Veronica Bradley², Taylor Weilert², Dana Wegge², Nicholas Hubley², John BROCKMAN²; ¹*University of Missouri*, ²*University of Missouri*

19AWD08: ANACHEM Award Symposium Honoring Robert Kennedy Mojave

Chair: Robert Kennedy

- 1:30 PM (251) **Microfluidic Design Advances Immunoblotting to the 21st Century;** Amy E. Herr¹; ¹*UC Berkeley*
- 1:50 PM (252) **Microfluidic Strategies for Measuring Adipocyte Signalling;** Michael T. Bowser¹, Rachel Harstad¹, Megan Weisenberger¹, Sarah Nelson¹, Sean Dembowski¹, Ryan Hunt¹, Michael Bowser¹; ¹*University of Minnesota*
- 2:10 PM (253) **Microfluidic Devices to Investigate Dynamic Signaling in Pancreatic and Liver Cells;** Michael Roper¹, Anna Adams¹, Basel Bandak¹, Joel Adablah¹, Weijia Leng¹, Wesley Eaton¹, Yao Wang¹, Michael Roper¹; ¹*Florida State University*
- 2:30 PM (254) **Microfluidic Tools for Epigenetic Profiling and Diagnostics;** Ryan Bailey¹, Steven Doonan¹, Yi Xu¹, Gloria Diaz¹, Jeong-Heon Lee², Tamas Ordog², Ryan Bailey¹; ¹*University of Michigan*, ²*Mayo Clinic*
- 2:50 PM (255) **Microfluidic Manipulation of Living Immune Tissue;** Megan Catterton¹, Megan Catterton¹, Rebecca Pompano¹; ¹*University of Virginia*

19BIM04: Spectroscopy and Precision Medicine Catalina

Chair: Michael Walsh

- 1:30 PM (256) **Investigating Scleroderma Skin Biopsies with Spectroscopy;** Hari Sreedhar¹, Shaiju Nazeer², David Martinez Marin³, John Varga⁴, Michael Walsh³; ¹*University of California San Diego*, ²*University of Alabama at Birmingham*, ³*University of Illinois at Chicago*, ⁴*Northwestern*
- 1:50 PM (257) **Biofluid Disease Diagnostics: A High-throughput Spectroscopic Method for the Detection of Brain Tumours;** James M. Cameron¹, Holly J. Butler², David S. Palmer^{1,2}, Matthew J. Baker^{1,2}; ¹*University of Strathclyde*, ²*ClinSpec Diagnostics*

- 2:10 PM (258) **Use of Raman Spectroscopy for the Study of Radiation Response in Brain Tumour Cells;** Iona E. Hill¹, Marie Boyd¹, Duncan Graham¹, Ted Hupp², Karen Faulds¹; ¹*University of Strathclyde*, ²*University of Edinburgh*
- 2:30 PM (259) **Fourier Transform Infrared Spectroscopy Reveals Mechanism of Bone Mineral Formation: From Amorphous Precursor to Mature Crystal;** William Querido¹, No'ad Shanas¹, Sakina Bookbinder¹, Maria Cecilia Oliveira-Nunes², Barbara Krynska¹, Nancy Pleshko¹; ¹*Temple University*, ²*Wistar Institute*
- 2:50 PM (260) **Multi-modal Imaging Analysis on Joint Capsule Tissue from Total Hip Replacement Patient;** Songyun Liu¹, Songyun Liu², Deborah Hall³, Stephanie McCarthy³, Si Chen⁴, Robert Urban³, Joshua Jacobs³, Robin Pourzal³; ¹*University of Illinois at Chicago*; ²*Rush University Medical Center*, ³*University of Illinois at Chicago, Rush University Medical Center*, ⁴*Argonne National Laboratory*

19IR10: Recent Advances in Using Molecular Spectroscopy for Pharmaceutical Research Smoketree E

Chair: Mike George

- 1:30 PM (261) **Introducing Selectivity and Improved Sensitivity for In-line Measurements of Stirred Suspensions with Ultrasound-enhanced Raman Spectroscopy;** Karin Wieland¹, Stefan Tauber², Christoph Gasser², Lukas Rettenbacher², Laurin Lux², Stefan Radel², Bernhard Lendl³; ¹*TU Munich*, ²*TU Wien*, ³*Technische Universität Wien*
- 1:50 PM (262) **Battling the Myths of Process FTIR Spectroscopy;** Dan Wood¹, Jonathon Speed¹; ¹*Keit Spectrometers*
- 2:10 PM (263) **Process Optimisation for Manufacturing with Light;** Mike George¹; ¹*University of Nottingham*
- 2:30 PM (264) **Speaker Roundtable;** Karin Wieland¹, Dan Wood², Mike George³; ¹*TU Munich*, ²*Keit Spectrometers*, ³*University of Nottingham*

19LIBS02: LIBS for Industry 4.0 Smoketree D

Chair: Francois Doucet

- 1:30 PM (265) **LIBS in the Aluminum Recycling Processes;** Amy J. Ray Bauer¹, Todd Hardwick¹, Christopher Stipe¹, Phil Bergman¹, Greg Petersen¹, Markus Gaelli¹; ¹*TSI, Incorporated*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

- 1:50 PM (266) **LIBS: The Ideal Tool for Industry 4.0;** Francois R. Doucet¹, Francois Doucet¹, Lutfu Ozcan¹, Kheireddine Rifai¹; ¹*ELEMISSION inc.*
- 2:10 PM (267) **Experimental Design: A Helpful Tool Before LIBS On-site Analyses of Agricultural Soils;** Bruno Bousquet¹, Julian Guezenoc¹, Anne Gallet-Budynek²; ¹*Université de Bordeaux*, ²*INRA*
- 2:30 PM (268) **LIBS for Quality Control in the Pharmaceutical Industry: Case of Asbestos in Cosmetic Powders;** Herve Sanghapi¹, Charles Ghany², krishna Ayyalasomayajula³, fang Yueh⁴, Jagdish Singh⁴; ¹*Alcorn State University*, ²*Mississippi College*, ³*Center for Informatics and Analytics, University of Mississippi Medical Center*, ⁴*JPS Advanced Technology LLC*
- 2:50 PM (269) **Temporal-spatial Resolved Laser-induced Breakdown Spectroscopy of T91 Steel of Different Aging Grades;** Meirong Dong¹; ¹*South China University of Technology*

19LIBS05: Archaeology and Anthropology *Smoketree C*

Chair: Matthieu Baudelet

- 1:30 PM (270) **pXRF and pLIBS for Archaeological Ceramics;** Mary Kate Donais¹, Brendan Connors², Peter Vandenabeele³, Mauro Martinez⁴, Matthieu Baudelet⁴; ¹*Saint Anselm College*, ²*SciAps Inc.*, ³*Univ Gent*, ⁴*Univ Central Florida*
- 1:50 PM (271) **Matrix-matched Standards for Anthropology Studies;** Matthieu Baudelet¹, Mauro Martinez¹, Courtney Bayne¹, Dylan Aiello¹, Matthew Julian¹, Romain Gaume¹; ¹*University of Central Florida*
- 2:10 PM (272) **Hot Tea Demineralizes Enamel While Cold Tea Protects: Spectroscopic and Microscopic Analysis;** Sinai H. C. Manno¹, Francis Manno¹, Condon Lau¹; ¹*City University of Hong Kong*
- 2:30 PM (273) **Speaker Roundtable;** Matthieu Baudelet¹, Mary Kate Donais², Sinai H. C. Manno³; ¹*University of Central Florida*, ²*Saint Anselm College*, ³*City University of Hong Kong*

19RAM08: SERS III *Sierra*

Chairs: Duncan Graham, Colin Campbell, Roy Goodacre

- 1:30 PM (274) **Charge transfer effects in the detection of proteins;** Zachary Schultz¹, Chelsea Zoltowski¹, Sian Sloan-Dennison¹, Carlos Lima de

Albuquerque¹, Brian Scarpitti¹, Lifu Xiao¹; ¹*The Ohio State University*

- 1:50 PM (275) **Chemically Imaging Cells with Super-resolution SERS;** Nathan C. Lindquist¹; ¹*Bethel University*
- 2:10 PM (276) **Gold Nanostars Enable Quantification of Cancer Biomarkers at the Single Cell Level;** Laura Fabris¹, Manjari Bhamidipati¹; ¹*Rutgers University*
- 2:30 PM (277) **Self-folding Hybrid Graphene Skin for 3D SERS Imaging of Single Live Cells;** Santosh K. Paidi¹, Weinan Xu¹, Qi Huang¹, Jayson Pagaduan¹, David Gracias¹, Ishan Barman¹; ¹*Johns Hopkins University*
- 2:50 PM (278) **3D Time-lapse SERS Imaging of Living Cells for Detection of Alkyne-tagged Drug Uptake;** Kazuki Bando¹, Kota Koike¹, Jun Ando², Naoki Terayama³, Kosuke Dodo³, Kimiko Sodeoka³, Satoshi Kawata¹, Katsumasa Fujita¹; ¹*Osaka University*, ²*Institute for Molecular Science*, ³*Riken*

19RAM17: Raman Spectroscopy for Security and Forensics Purposes *Ventura*

Chair: Igor Lednev

- 1:30 PM (279) **Point-of-use Raman Solutions for Security and Forensics Purposes: Opportunities and Challenges of Real-world Deployment;** Jürgen Popp¹; ¹*Leibniz Institute of Photonic Technology*
- 1:50 PM (280) **How Raman Spectroscopy Can Be Used to Assess Selective Drug Detection Using Molecular Imprinted Polymers;** Amanda J. Haes¹, Wenjing Xi¹; ¹*University of Iowa*
- 2:10 PM (281) **Development of Standoff Deep UV Resonance Raman Determination of Trace Explosives;** Sandy A. Asher¹, Sergei Bykov¹, Kyle Hufziger¹, Sandy Asher¹; ¹*University of Pittsburgh*
- 2:30 PM (282) **New Horizons in Organic Gunshot Residue Analysis;** Shelby R. Khandasammy¹, Lenka Halámková², Igor Lednev²; ¹*SUNY Albany*, ²*University at Albany, SUNY*
- 2:50 PM (283) **Standoff Detection of Threat Materials Using a FAST-SHS Raman Hyperspectral Imaging Sensor;** Nirmal Lamsal¹, Nathaniel Gomer², Haiyin Sun², Heather Gomer², Matthew P. Nelson³; ¹*ChemImge Corporation*, ²*ChemImage Corporation*, ³*ChemImage Corp*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

19SPECIAL02: SAS Session: Microplastics in the Environment I *Chino AB*

Chairs: Andrew Whitley, Shelly Moore

- 1:30 PM (284) **Microplastics Differ Between Indoor and Outdoor Air masses: Insights from Multiple Microscopy Methodologies;** Emily Welsh Gaston¹, Emily Gaston², Mary Woo², Clare Steele², Suja Sukumaran³, Sean Anderson²; ¹*CSU Channel Islands, ESRM*, ²*CSUCI*, ³*Thermo Fisher Scientific*
- 1:50 PM (285) **A Comparison Of multiple Techniques, FT-IR, Py-gcms, and Raman for Polymer Identification in Plastic Marine Debris;** Eunah Lee¹, Ashok Deshpande², Jennifer Lynch³, Kayla Brignac⁴, Melissa Jung⁵, Nigel Lascelles⁶, Dante Freeman⁷, Davielle Drayton⁷, Bridget O'Donnell⁸; ¹*HORIBA Scientific*, ²*National Oceanic and Atmospheric Administration*, ³*National Institutes of Standards and Technology, NOAA Affiliate*, ⁴*University of Hawaii, Global Environmental Sciences*, ⁵*Hawaii Pacific University*, ⁶*Florida A&M University*, ⁷*Savannah State University*, ⁸*HORIBA*
- 2:10 PM (286) **Detection and Analysis of Microplastics Using Raman Spectroscopy;** Sarah C. Shidler¹, Tim Prusnick¹, Richard Bormett¹; ¹*Renishaw Inc.*
- 2:30 PM (287) **Rapid, Automated Analysis of Microplastics Using Laser Direct Infrared Imaging and Spectroscopy;** Darren Robey¹, Dlpak Mainali², Christopher Moon²; ¹*Agilent Technologies Inc.*, ²*Agilent Technologies Inc*
- 2:50 PM (288) **Methods Workshop Held to Advance the Development of Standardized Methods to Measure Microplastics;** Shelly Moore¹, Steve Weisberg¹, Chelsea Rochman², Andrew Whitley³; ¹*Southern California Coastal Water Research Project*, ²*University of Toronto*, ³*HORIBA Scientific*

19SPR02: Sensing with Plasmonics *Smoketree A*

Chairs: Amanda Haes, Jean-Francois Masson

- 1:30 PM (289) **Pyrolyzed Photoresist Films: Utility of Carbon Substrates in Immunometric Assays Using Surface-enhanced Raman Scattering;** Marc D. Porter¹, Jason G.¹, Marc Porter¹; ¹*University of Utah*
- 1:50 PM (290) **3D Printing for Plasmonic Interfaces and Biosensing;** Quan Jason Cheng¹, Alexander Lambert², Kelvin Tran², Quan Cheng²; ¹*University of California*, ²*UC Riverside*

- 2:10 PM (291) **Going Green with Silver: Development of Sustainable Plasmonic Sensors;** Christa Brosseau¹, Taylor Lynk², Osai Clarke², Gaius St. Marie³; ¹*Saint Mary's University*, ²*Organization ...*, ³*Saint Marys University*
- 2:30 PM (292) **Sensitive, Selective, and Quantitative Copper Sensor Using Click-chemistry with Gold Nanoparticles;** ReJeana M. Cary¹, Ilaina Monroe¹, Joseph Holbrook², Olivia Hess¹, Sarah Unser³, Laura Sagle¹; ¹*University of Cincinnati*, ²*Eastern Kentucky University*, ³*Zoetis Inc*
- 2:50 PM (293) **The Plasmonic Stability of Gold Nanostars Synthesized Using Good's Buffers;** Amanda J. Haes¹, Wenjing Xi¹; ¹*University of Iowa*

19SPSJ04: Near Infrared Spectroscopy II *Smoketree B*

Chair: Shigeaki Morita

- 1:30 PM (294) **Novel Miniaturized Spectrometric Attempts to Monitor Quality of Food and Medicinal Plant Products;** Christian W. Huck¹; ¹*University of Innsbruck*
- 1:50 PM (295) **Improving Preprocessing of Spectral Data by the VSN (Variable Sorting for Normalization) Algorithm;** Federico Marini¹, Gilles Rabattel², Beata Walczak³, Jean-Michel Roger²; ¹*University of Rome La Sapienza*, ²*ITAP, Irstea, Montpellier SupAgro, University of Montpellier, Montpellier, France*, ³*University of Silesia, Katowice, Poland*
- 2:10 PM (296) **Relationship Between Bioactivity and Water Structure Analyzed by NIR Spectroscopy;** Mika Ishigaki¹, Yukihiro Ozaki²; ¹*Shimane University*, ²*Kwansei Gakuin University*
- 2:30 PM (297) **Optimization of Enhanced Near-infrared Spectroscopic Technique for Rapid Chemical Composition Analysis;** Kodai Murayama¹, Kodai Murayama¹, Risa Hara¹, Takuma Genkawa², Ichiro Tanabe³, Aiko Miyamoto², Fumie Watanabe¹, Nobuhiro Tomosada¹, Yukihiro Ozaki⁴; ¹*Yokogawa Electric Corporation*, ²*Food Research Institute, NARO*, ³*Osaka University*, ⁴*Kwansei Gakuin University*

TECHNICAL PROGRAM - TUESDAY
POSTER SESSION 3:10 PM – 3:50 PM
Exhibit Hall, Oasis

See page 85 for a listing of Tuesday posters by category. Student poster award winners will be announced the following morning during the plenary session.

TECHNICAL PROGRAM - TUESDAY
ORAL SYMPOSIA 3:50 PM – 5:30 PM

19AES06: AES: Leaders in the Field *Mesquite D*

Chairs: Sagnik Basuray, Adam Woolley

- 3:50 PM (298) **Precision Medicine Is Advanced by Profiling Cellular-to-molecular Diversity Using Electrophoretic Cytometry;** Amy E. Herr¹; ¹UC Berkeley
- 4:10 PM (299) **3D-printed Tools for Quantitative Bioanalysis;** Dana Spence¹, Cody Pinger¹, Andrew Heller¹, Dana Spence¹; ¹Michigan State University
- 4:50 PM (300) **Microfluidic Organic Chemical Analyzers for Detection of Solar System Biosignatures;** Richard A. Mathies¹, Anna Butterworth², Jeremy McCauley², Amanda Stockton³, Jungkyu Kim⁴, Matin Golozar⁵, James New⁶; ¹University of California, Berkeley, ²Berkeley Space Sciences Lab, ³Georgia Institute of Technology, ⁴Texas Tech University, ⁵UC Berkeley Space Sciences, ⁶UC Berkeley Space Sciences Lab

19ATOM09: High End ICP-MS Instrumentation *Pasadena*

Chair: Johanna Irrgeher

- 3:50 PM (301) **SAS Atomic Section Student Award Winner: A Comparative Analysis of Optical Spectrometric Methods and MC-ICP-MS for Stable Isotope Analysis of Magnesium in Geological Samples;** Carlos Abad¹, Stefan Florek², Helmut Becker-Ross², Stefan Muench³, Michael Okruss³, Jhanis Gonzalez⁴, Xianglei Mao⁴, Vassilia Zorba⁵, Norbert Jakubowski⁶, Michael Tatzel¹, Jochen Vogl¹, Sebastian Recknagel¹, Ulrich Panne¹; ¹Bundesanstalt für Materialforschung und –prüfung (BAM), ²Leibniz-Institut für Analytische Wissenschaften - ISAS - e. V., ³Analytik Jena AG, ⁴Lawrence Berkeley National Laboratory, ⁵Organization ..., ⁶Spetec GmbH
- 4:10 PM (302) **Application of Single Particle Inductively Coupled Plasma-mass Spectrometry (sp-ICP-MS/MS) in the Analysis of Nanoparticles in Hydrocarbons;** Jenny Nelson¹, Laura Poirier², Francisco Lopez-Linares²; ¹Agilent, ²Chevron

- 4:30 PM (303) **Optimizing ICP-MS/MS for Ultra Trace Analysis of Challenging Elements in Environmental Applications;** Daniel Proefrock¹, Anna Reese¹, Tobias Orth¹, Ole Klein¹, Nathalie Voigt¹, Tristan Zimmermann¹, Lars Hildebrandt¹, Fenna Nack¹; ¹Helmholtz-Zentrum Geesthacht
- 4:50 PM (304) **Sulfur Isotope Analysis at Ultra Trace Levels by EA-MC ICP-MS;** Michael Wieser¹, Aaron Wilkins², Thomas Prohaska³, Johanna Irrgeher³, Kerri Miller²; ¹Physics and Astronomy, University of Calgary, ²University of Calgary, ³Montanuniversität Leoben
- 5:10 PM (305) **Potential of MC-ICP-CC-MS in Cosmochemistry and Geochronology;** Justin Simon¹; ¹NASA Johnson Space Center

19CHEM03: Chemometrics at Work in Industry *Mesquite E*

Chair: Neal Gallagher

- 3:50 PM (306) **Application of NIR in the Oil/Gas Industry;** Randy T. Bishop¹, Randy Bishop², Paul Little²; ¹JP3 Measurement, ²JP3 Measurement
- 4:10 PM (307) **Autonomous Calibration;** Brian G. Rohrback¹, Randy Pell¹, Scott Ramos¹; ¹Infometrix, Inc.
- 4:30 PM (308) **Compression is Good for the Goal?;** Donal O'Sullivan¹, Manuel Palacios², Barry Wise²; ¹Eigenvector Research Inc., ²Eigenvector Research, Inc.
- 4:50 PM (309) **On-line, real-time monitoring for process control and optimization: processing nuclear materials;** Amanda Lines¹, Amanda Lines¹, Neal Gallagher², Heather Felmy¹, Shirmir Branch¹, Sergey Sinkov¹, Amanda Casella¹, Susan asmussen¹, Gregg Lumetta¹, Samuel Bryan¹; ¹Pacific Northwest National Laboratory, ²Eigenvector Research
- 5:10 PM (310) **Modern Tools for Model Development and Maintenance;** Paul Cammarata¹, Spencer Behling¹, Matt Chapman¹, J. D. Tate¹; ¹Dow Chemical

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19CTP03: Solving Developing World Chemistry Challenges: Where Are We Now? *Mojave*

Chair: Diane Parry

- 3:50 PM (311) **Spectroscopy and Alternative Plastics from Vegetable Oils**; Isao Noda¹; ¹*University of Delaware*
- 4:10 PM (312) **Hardware and Software Tools to Enable High-Quality Portable Mass Spectrometry Analyses**; Jacob Shelley¹, Garett MacLean¹, Courtney Walton¹, Jessica Hellinger¹, Yi You², George Chan³; ¹*Rensselaer Polytechnic Institute*, ²*Bundesanstalt für Materialforschung und -prüfung*, ³*Lawrence Berkeley National Laboratory*
- 4:30 PM (313) **Applying Chemistry to Confront International Humanitarian Problems**; Ronda L. Grosse¹, Bego Gerber¹, Bakarr Kanu², Ray Kronqist¹; ¹*Chemists Without Borders*, ²*Winston-Salem State University*
- 4:50 PM (314) **Strategies to Keep Research Moving Amidst Disaster Relief**; Ellen v. Misco¹; ¹*TeakOrigin*
- 5:10 PM (315) **High-speed Quantitation of More Than 30 Bioprocess Media Metabolites/nutrients with Miniature CE-MS**; Christopher D. Brown¹, Glenn A. Harris¹, Colin Gavin¹, Kenion Blakeman¹, Ji Young Anderson¹; ¹*908 Devices*

19IR06: Mid-IR Frequency Combs *Smoketree E*

Chair: Bernhard Lendl

- 3:50 PM (316) **Dual Comb Spectroscopy with Quantum Cascade Lasers: Development, Outlook, and New Possibilities**; Raphael Horvath¹, Raphael Horvath², Andreas Hugi², Markus Geiser², Markus Mangold², Pierre Jouy², Pitt Allmendinger², Jerome Faist³; ¹*IRsweep*, ²*IRsweep AG*, ³*ETH Zürich*
- 4:10 PM (317) **Molecular Spectroscopy with Frequency Combs**; Oliver Heckl¹, Jakob Feller², Aline S. Mayer², Georg Winkler², Lukas Perner², Bryce J. Bjork³, Thinh Q. Bui³, Jun Ye³; ¹*Faculty of Physics, University of Vienna*, ²*Christian Doppler Laboratory for Mid-IR Spectroscopy and Semiconductor Optics, Faculty Center for Nano Structure Research, Faculty of Physics, University of Vienna, Vienna, Austria*, ³*JILA, National Institute of Standards and Technology and University of Colorado, Department of Physics, University of Colorado*

- 4:30 PM (318) **Electro-optic Dual Optical Frequency Comb Generators: Evolution and Opportunities in Spectroscopy**; Pedro Martín Mateos¹, Pedro Martín Mateos¹; ¹*Universidad Carlos III de Madrid*
- 4:50 PM (319) **Semiconductor Laser Frequency Combs: From Fundamentals Towards Applications**; Johannes Hillbrand¹, Johannes Hillbrand¹, Hermann Detz¹, Aaron Maxwell Andrews¹, Harald Schneider², Robert Weih³, Federico Capasso⁴, Sven Höfling⁵, Gottfried Strasser¹, Benedikt Schwarz¹; ¹*TU Wien*, ²*Helmholtz-Zentrum Dresden Rossendorf*, ³*nanoplus*, ⁴*Harvard University*, ⁵*Universität Würzburg*
- 5:10 PM (320) **Multi-species Chemical Sensing Using QCL Based Dual Comb Spectroscopy**; Jonas Westberg¹, Chu C. Teng¹, Yifeng Chen¹, Charles L. Patrick¹, Gerard Wysocki¹; ¹*Princeton University*

19LIBS08: LIBS Elemental Imaging *Smoketree C*

Chair: Vincent Motto-Ros

- 3:50 PM (321) **Combining Spectroscopic and Tomographic Data**; Jozef Kaiser¹, David Prokop¹, Pavel Porizka¹, Tomas Zikmund¹; ¹*Central European Institute of Technology*
- 4:10 PM (322) **Multiscale Quantitative Mineral Analysis by Laser-induced Breakdown Spectroscopy**; Elton Soares de Lima Filho¹, Francis Vanier¹, Josette El-Haddad¹, Aïssa Harhira¹, Christian Padioleau¹, Mohamad Sabsabi¹, Alain Blouin¹; ¹*National Research Council Canada*
- 4:30 PM (323) **Multi-sensor Imaging by LIBS**; Jhanis J. Gonzalez¹, Charles Sisson², Juan Carlos Guerrero², Alan Koenig²; ¹*Applied Spectra, Inc. / Lawrence Berkeley National Laboratory*, ²*Applied Spectra*
- 4:50 PM (324) **Elemental Imaging by LIBS: Recent Advances and Remaining Challenges**; Vincent Motto-Ros¹, Vincent Motto-Ros²; ¹*Institut Lumiere Matiere*, ²*ILM*
- 5:10 PM (325) **Imaging Biochemical Signatures of Stress Events in Human Deciduous Teeth**; Bruno Bousquet¹, Eliza Orellana Gonzalez², Yannick Lefrais², Mona Le Luyer³, Priscilla Bayle², Vincent Motto-Ros⁴, Rémy Chapoulie²; ¹*Université de Bordeaux*, ²*IRAMAT-CRP2A, University Bordeaux Montaigne*, ³*PACEA, University of Bordeaux*, ⁴*PACEA, University of Bordeaux, France; Skeletal Biology Research Centre, School of Anthropology and Conservation, University of Kent, Canterbury, UK*, ⁴*ILM, University of Lyon, France*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19PAT06: PAT Enabled Flow Chemistry and Continuous Manufacturing *Smoketree D*

Chairs: Jim Rydzak, Savitha Panikar

- 3:50 PM (326) **Process Intensification Tactics in the Quest for Advancing Global Health Access;** Katherine Belecki¹; ¹*Department of Chemistry, Virginia Commonwealth University*
- 4:10 PM (327) **In-line FTIR Technology: Application to Continuous Flow Chemistry;** Norman A. Wright¹; ¹*Mettler Toledo Autochem*
- 4:30 PM (328) **Sampling Devices for In-line near Infrared Spectroscopy Monitoring of Powder Blend Homogeneity in Continuous Manufacturing;** Anders B. Sparen¹, Lisa Radovanovic Jansson², Marcus Josefsson², Heikki Savolainen², Solveig Wessberg², Håkan Wikström², Olof Svensson², Anders Sparen²; ¹*Pharmaceutical Technology & Development, AstraZeneca Gothenburg, Sweden*, ²*Pharmaceutical Technology and Development, AstraZeneca Gothenburg, Sweden*
- 4:50 PM (329) **The Tablet Press Feed-frame as a Optimum Point for Monitoring the Quality of a Tablet Product Made Using a Continuous Manufacturing Process;** Steve Hammond¹, Phil Doherty¹; ¹*Expo Pharma*
- 5:10 PM (330) **Development of Categorical Chemometric Models to Support Continuous Drug Product Manufacturing;** Caitlin Schram¹, Matt Kiesz, Sara Manteiga, Alex Clifford, Justin Pritchard, Kelly Swinney; ¹*Vertex Pharmaceuticals*

19PMA09: Pharmaceutical Forensics: Applying Analytical Science to Safe Manufacturing, Supply, and Screening *Madera*

Chairs: Ravi Kalyanaraman, Scott Huffman

- 3:50 PM (332) **USP Technology Review Program for Evaluating Screening Technologies for Medicine Quality Assurance;** Stephen Muendo Kimatu¹; ¹*United States Pharmacopeia (USP)*
- 4:10 PM (331) **Colombian Procedure for Handling of Falsified/Altered Products;** Miller Lysen¹; ¹*Bristol-Myers Squibb*
- 4:30 PM (333) **Combatting the Illegal Trade of Medicines: BMS Strategy Against Counterfeiting, Tampering, Diversion and Theft;** Ramon Armando Rivera¹, Joseph Connell¹, Simeon Wilson²; ¹*Bristol Myers Squibb*
- 4:50 PM (334) **SERS for the Detection and Analysis of Fentanyl;** Li-Lin Tay¹, John Hulse¹; ¹*National Research Council Canada*

- 5:10 PM (335) **Development of Pharmaceutical Tablet Authentication System using Spectroscopic Techniques in combination with Multivariate Method;** Md Naveem Hossain;

19RAM12: Emerging Raman *Ventura*

Chairs: Pavel Matousek, Duncan Graham, Ian Lewis

- 3:50 PM (336) **Interference-enhanced Raman Spectroscopy as a Tool for Developing Chip-based Sample Preparation Strategies;** Susanne Pahlow¹, Thomas Mayerhöfer¹, Uwe Hübner¹, Jürgen Popp¹, Karina Weber¹; ¹*Leibniz Institute of Photonic Technology*
- 4:10 PM (337) **Time-gated Raman Mapping Using Dmd-based Spectral Multiplexing;** Ioan Nottingher¹, Max Dooley¹, Felicity Rose¹, Jing Yang¹, Jane McLaren¹, Aruna Prasopthum¹; ¹*University of Nottingham*
- 4:30 PM (338) **Raman Fusion Spectroscopy: Multi-wavelength Excitation for Compact Devices;** Johannes Kiefer¹, Johannes Kiefer¹; ¹*University of Bremen*
- 4:50 PM (339) **Towards Raman-based cell sorting as a quality control step for highly efficient 3rd generation bio kerosene production;** Karin Wieland¹, David Bauer², Torben Schädler¹, Mahmoud Masri¹, Thomas Brück¹, Christoph Haisch¹; ¹*TU Munich*, ²*Technical University of Munich*

19RAM16: Stand-off Raman *Sierra*

Chair: Nathaniel Gomer

- 3:50 PM (340) **Standoff Chemical and Explosive Detection of Military Relevant Threats;** Jason Guicheteau¹, Jason Guicheteau², Phillip Wilcox², Ashish Tripathi², Erik Emmons²; ¹*U.S. Army Combat Capabilities Development Command, Chemical Biological Center*, ²*CCDC-CBC*
- 4:10 PM (341) **Standoff Raman and Raman Imaging Using a Monolithic Spatial Heterodyne Raman Spectrometer;** S. Michael Angel¹, J. Chance Carter², Joshua Ottaway², Abigail Waldron³, Ashley Allen³; ¹*University of South Carolina, Department of Chemistry and Biochemistry*, ²*Lawrence Livermore National Laboratory*, ³*Univ. of South Carolina*

TECHNICAL PROGRAM - TUESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

4:30 PM (342) **Underwater Time-gated Standoff Raman Spectroscopic Sensor for Detecting Hazardous Chemicals;** Shiv K. Sharma¹, Bruce Howe², Anupam Misra², Mark Rognstad², John Porter², Tayro Acosta-Maeda², Miles Egan²; ¹*Hawaii, University of Hawaii*

4:50 PM (343) **Advancements in Standoff Detection of Chemical, Explosive and Narcotic Threats Using Raman FAST Hyperspectral Imaging;** Matthew P. Nelson¹, Nathaniel Gomer¹, Chuck Gardner¹, Patrick Treado¹; ¹*ChemImage Corp*

5:10 PM (344) **Government Applications for Emerging Standoff Detection Equipment;** Michael Shepard¹, ¹*Naval Surface Warfare Center - IHEODTD*

19SPECIAL05: SAS Session: Microplastics in the Environment II *Chino AB*

Chair: Andrew Whitley

3:50 PM (345) **Increasing the Accessibility for Characterizing Microplastics: Introducing New Application-based and Spectral Libraries of Plastic Particles (SLOPP & Slopp-e);** Bridget O'Donnell¹, Keenan Munno², Hannah De Frond², Chelsea Rochman²; ¹*HORIBA Scientific, University of Toronto*

4:10 PM (346) **Open Specy: An Open Source, Online, Spectra Classification and Sharing Tool;** Win Cowger¹, Andrew Gray¹, Chelsea Rochman², Sebastian Primpke³, Jennifer Lynch⁴, Hannah Hapich⁵; ¹*University of California, Riverside, University of Toronto, Alfred Wagner Institute, University of Hawaii, UC Riverside*

4:30 PM (347) **Microplastic Identification Using Non-optimized Discriminant Fusion Classification Based on ATR-FTIR Spectroscopy;** John H. Kalivas¹; ¹*Idaho State University*

4:50 PM (348) **Development of Automatic Microplastic Measurement with Surface Z-axis Tracking Mode by μ -RAMAN Imaging Spectroscopy;** hyo jin kim¹, Soo Ah Cho², won bo cho³, yun cheol park⁴; ¹*Dongduk Womens University, Dongduk women's University, dongduk women's university, nanophoton korea*

5:10 PM (349) **Identification of Microplastic Particles Using Vibrational Spectroscopy Coupled to Multivariate Analysis;** Maria El Rakwe¹, Kada Boukerma¹, Florence Mazeas¹, Catherine Dreanno¹, Chantal Compère², Morgan Tardivel¹, Emmanuel Rinnert³; ¹*IFREMER, REM/RDT/LDCM, IFREMER, REM/RDT, IFREMER, REM/GM/LCG*

19SPR06: Rising Stars in Plasmonics *Smoketree A*

Chair: Jean-Francois Masson

3:50 PM (350) **Angstrom Scale Chemical Analysis of Metal-supported Regioisomeric Assemblies by Ultrahigh Vacuum, Tip-enhanced Raman Spectroscopy;** Nan Jiang¹; ¹*University of Illinois at Chicago*

4:10 PM (351) **Hot Electron Dynamics in Plasmonic Thermionic Emitters;** Matthew Sheldon¹, Nicki Hogan¹, Shengxiang Wu¹, Matthew Sheldon¹; ¹*Texas A&M University*

4:30 PM (352) **Point-of-Care Plasmonic Devices for Bacterial Pathogen Detection;** Laura Sagale¹, ReJeana Cary¹, Jie He¹, Ilaina Monroe¹, Laura Sagale¹; ¹*University of Cincinnati*

4:50 PM (353) **Digital Plasmonic Holography;** Ryan Spies¹, Alexandre Brolo², Nathan C. Lindquist¹; ¹*Bethel University, University of Victoria*

5:10 PM (354) **Surface Plasmon Resonance Biosensor Design for Domoic Acid Biomarker Detection and Evaluation of Chronic Exposure;** Betsy Jean Jean Yakes¹, Kathi A. Lefebvre²; ¹*U.S. Food and Drug Administration, National Oceanic and Atmospheric Admin.*

TECHNICAL PROGRAM - WEDNESDAY
AWARDS AND PLENARY LECTURES 7:45 AM – 9:00 AM
 Chair: Mary Kate Donais
Primrose A

7:45 AM Award Presentations

- 8:00 AM (355) **SAS Lester W. Strock Award; Remote LIBS, Raman and Hyperspectral Raman Imaging Using a Monolithic Spatial Heterodyne Spectrometer;** S. Michael Angel¹, Ashley Allen², Abigail Waldron³, Ivo Raimundo Jr.⁴, J. Chance Carter⁵; ¹*University of South Carolina, Department of Chemistry and Biochemistry*, ²*USC*, ³*Univ. of SC*, ⁴*Instituto de Química – Unicamp*, ⁵*Lawrence Livermore National Laboratory*
- 8:30 AM (356) **AES Electrophoresis Mid-Career Award; Digitizing Endocrine Tissue Secretions into Nanoliter Droplets for Analysis of Hormones and Metabolites at High Temporal Resolution;** Christopher J. Easley¹, Juan Hu¹, Xiangpeng Li¹, Nan Shi¹, Subramaniam Somasundaram¹, Jean Negou¹; ¹*Auburn University*

TECHNICAL PROGRAM - WEDNESDAY
ORAL SYMPOSIA 9:15 AM – 10:55 AM

19ATOM04: Atmospheric Pressure Glow Discharge Spectroscopies I (Instrumentation) Pasadena

Chair: R. Kenneth Marcus

- 9:15 AM (357) **A New Ionization Source for Environmental Mass Spectrometry;** Charles L. Wilkins¹, Michael Alves², Jon Sauer², Kimberly Prather³, Vicki Grassian⁴, Charles Wilkins¹; ¹*University of Arkansas*, ²*University of California, San Diego*, ³*University of California, San Diego*, ⁴*University of California, San Diego*
- 9:35 AM (358) **Factors Effecting Uranium Isotope Ratio Measurements in the Ls-apgd/orbitrap Coupling;** R. Kenneth Marcus¹, R. Kenneth Marcus¹, Edward Hoegg², David Koppenaal²; ¹*Clemson University*, ²*Pacific Northwest National Laboratory*
- 9:55 AM (359) **SAS Atomic Section Student Award Winner - Elemental Mass Spectrometry of Fluorine: Challenges and Innovations in Ionization and Detection;** Joseph E. Lesniewski¹, Kunyu Zheng¹, William McMahon¹, Samuel White¹, Kaveh Jorabchi¹; ¹*Georgetown University*
- 10:15 AM (360) **Investigations of Matrix Management Protocols for the Solution Cathode Glow Discharge (SCGD);** Stuart Schroeder¹; ¹*InnoTech Alberta*
- 10:35 AM (361) **New Approaches for a Combined Atomic and Molecular (CAM) Ionization Source;** David Koppenaal, Edward Hoegg¹, Ying Zhu¹, R. Kenneth Marcus², David Koppenaal¹; ¹*Pacific Northwest National Laboratory*, ²*Clemson University*

19AWD05: SAS Lester W. Strock Award Symposium Honoring S. Michael Angel Mojave

Chair: S. Michael Angel

- 9:15 AM (362) **Exploring the Planets with LIBS, Raman, and Luminescence Spectroscopies: Chemcam, Supercam and SHERLOC on Nasa's Mars 2020 Rover, and More to Come;** Roger Wiens¹, Roger Wiens², Sylvestre Maurice³, Luther Beegle⁴, Sam Clegg², Rohit Bhartia⁴, Shiv Sharma⁵, S. Michael Angel⁶; ¹*Los Alamos National Laboratory*, ²*LANL*, ³*IRAP*, ⁴*JPL/Caltech*, ⁵*U. Hawaii*, ⁶*U. South Carolina*
- 9:35 AM (363) **Advances in Combined Time-resolved Remote LIBS and Raman Spectroscopy;** Shiv K. Sharma¹, Anupam Misra², Tayro Acosta-Maeda², John Porter²; ¹*Hawaii*, ²*University of Hawaii-Manoa*.
- 9:55 AM (364) **Laser Ablation Spectrochemical Analysis;** Rick Russo¹; ¹*Lawrence Berkeley National Laboratory*
- 10:15 AM (365) **Characterizing Limiting Noises in Laser Induced Breakdown Spectroscopy: Still-challenging Issues;** Nicolò Omenetto¹; ¹*University of Florida*
- 10:35 AM (366) **Deployment of a LIBS System Using a Remotely Operated Vehicle at Seafloor Hydrothermal Vents;** Alan D. Chave¹, Susan Humphris¹, S. Michael Angel²; ¹*Woods Hole Oceanographic Institution*, ²*University of South Carolina*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

19AWD07: AES Mid-Career Award Symposium Honoring Chris Easley Mesquite D

Chairs: Jason Dwyer, Christopher Harrison

- 9:15 AM (367) **Microfluidic Systems for Studying the Gut Microbiome**; Charles Henry¹, Alec Richardson¹, Luke Schwerdtfeger¹, Stuart Tobet¹, Charles Henry¹; ¹Colorado State University
- 9:35 AM (368) **Electrophoretic Analysis of Small Molecules Released from Islets of Langerhans**; Michael Roper¹, Kimberly Evans¹, I-An Wei¹; ¹Florida State University
- 9:55 AM (369) **Integrating Microfluidic-based Cell Culture with Analysis**; R. Scott Martin¹; ¹Saint Louis University
- 10:15 AM (370) **Selective Assembly and Analysis of Melanoma Cells and Cell Clusters at an Array of Bipolar Electrodes**; Robbyn K. Anand¹, Darshna Pagariya¹, Joseph Banovetz¹, Min Li¹, Janis Borchers¹, Claire Campbell¹, Hannah Bishop¹, Sungu Kim¹, Baskar Ganapathysubramanian¹; ¹Iowa State University
- 10:35 AM (371) **3D Printed Integrated Microfluidic Devices for Extraction, Fluorescence Labeling, and Separation of Preterm Birth Biomarkers**; Anna V. Nielsen¹, Chao Pang¹, Mike J. Beauchamp¹, Greg P. Nordin¹, Adam T. Woolley¹; ¹Brigham Young University

19BIM05: Vibrational Spectroscopy: Toward Clinical Applications Catalina

Chairs: Karen Esmonde-White, Fay Nicolson

- 9:15 AM (372) **Investigating Term and Preterm Labor Using in Vivo Raman Spectroscopy**; Laura Masson¹, Christine O'Brien², Emad Elsamadicy³, Kelly Bennett³, J. Michael Newton³, Anita Mahadevan-Jansen⁴; ¹Vanderbilt University Department of Biomedical Engineering, ²Washington University in St. Louis, ³Vanderbilt University Medical Center, ⁴Vanderbilt University
- 9:35 AM (373) **Raman Imaging of Breast Microcalcifications from a Relevant Patient Cohort Reveals New Insights into the Vibrational Features of These Important Cancer Signs**; Renzo Vanna¹, Francesca Piccotti¹, Emanuele Torti², Beatrice Marcinnò², Carlo F. Morasso³, Manuela Agozzino¹, Luca Sorrentino⁴, Laura Villani¹, Francesco Leporati², Fabio Corsi¹; ¹Istituti Clinici Scientifici Maugeri IRCCS, ²Università degli studi di Pavia, ³ICS Maugeri, ⁴Università degli Studi di Milano

- 9:55 AM (374) **Red Blood Cell Degradation Evaluated by Raman Spectroscopy**; Richard A. Dluhy¹, Amareshwari Knoutham², Joo-Yuen Oh², Rakesh Patel²; ¹University of Alabama at Birmingham, ²University of Alabama at Birmingham
- 10:15 AM (375) **Study of Red Cell Concentrate (RCC) Supernatant for the Non-invasive Assessment of Storage-related Changes Using Deep Raman Spectroscopy**; Martha Vardaki¹, Dana Devine², Katherine Serrano³, Michael Blades⁴, Robin Turner⁵; ¹UBC, ²Department of Pathology and Laboratory Medicine/ Centre for Blood Research, UBC, ³Centre for Innovation, Canadian Blood Services, ⁴Department of Chemistry, UBC, ⁵Department of Electrical & Computer Engineering
- 10:35 AM (376) **A Tale of Diagnostic Imaging and Commercialization: Why Understanding Each Chapter Matters**; Katherine Cilwa¹; ¹Photocure Inc.

19CHEM04: Chemometric Opportunities in the Forensic Sciences Mesquite E

Chair: Rabi Musah

- 9:15 AM (377) **Food Authentication and Adulteration Detection with Data Fusion of Non-optimized Classifiers**; John H. Kalivas¹, Tony Lemos¹; ¹Idaho State University
- 9:35 AM (378) **Determining the Strength of Forensic Lubricant Evidence from DART-MS and GC-MS Data**; Candice Bridge¹, Mark Maric², Brooke Baumgarten³; ¹University of Central Florida & National Center for Forensic Science, ²UCF/NCFS, ³UCF
- 9:55 AM (379) **A Regression-based Algorithm to Maximize the Confidence in Mass Spectral Identifications**; Glen P. Jackson¹, Samantha Mehnert¹, Brandon Lowe¹, J. Tyler Davidson¹; ¹West Virginia University
- 10:15 AM (380) **Multi-label Classification Methods for the Forensic Identification of Fauna or Flora Within Mixtures**; Samira Beyramysoltan¹, Monica I. Ventura², Justine E. Giffen¹, Jennifer Rosati³, Rabi Musah¹; ¹University at Albany (SUNY), ²University at Albany (SUNY), ³John Jay College of Criminal Justice
- 10:35 AM (381) **Combining Advanced Statistical Methods and Laser-induced Fluorescence in Forensic Analysis**; George L. Donati¹, Jake A. Carter¹, Bradley T. Jones¹; ¹Wake Forest University

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

19FORENS05: Methods for Challenging Forensics Applications *Smoketree A*

Chair: Greg Klunder

- 9:15 AM (382) **Kinetic and Thermodynamic Models of Evaporation for Forensic Applications;** Victoria McGuffin¹, Ruth Smith¹; ¹*Michigan State University*
- 9:35 AM (383) **Evaluating the Impact of Preconcentration using Silicon Nanowire Arrays with Ion Mobility Spectrometry;** Matthew J. Mullen¹, Braden C. Giordano¹; ¹*US Naval Research Laboratory*
- 9:55 AM (384) **Predicting the lifetime of trace explosives materials on surfaces;** Michael Papantonakis¹, Robert Furstenberg², Viet Nguyen², Tyler Grissom³, Andrew Kusterbeck⁴, R. Andrew McGill¹; ¹*Naval Research Laboratory*, ²*US Naval Research Laboratory*, ³*NRC Postdoctoral Fellow / Naval Research Laboratory*, ⁴*Nova Research*
- 10:15 AM (385) **Adaptive Multivariate Chemical Imaging for High-throughput Detection of Illicit Substances in Mail;** Shawna K. Tazik¹, Matthew P. Nelson¹; ¹*ChemImage Corp*
- 10:35 AM (386) **Near-Infrared Spectroscopy of Gases from Heated Explosives;** Greg Klunder¹, Nick Muettterties¹, Taylor Miller¹, Evan Kahl¹, Peter Hsu¹; ¹*Lawrence Livermore National Laboratory*

19IR07: Time-resolved IR and 2D-IR Spectroscopy *Smoketree E*

Chair: Mike George

- 9:15 AM (387) **Pulse Radiolysis with Time-resolved Infrared Detection: A Powerful Method for Unraveling the Mechanisms of Redox Processes;** David C. Grills¹; ¹*Brookhaven National Laboratory*
- 9:35 AM (388) **Development and Applications of Quantum Cascade Laser Frequency Comb Spectroscopy for Fast Time-resolved IR Spectroscopy;** Raphael Horvath¹, Raphael Horvath², Urszula Szczepaniak², Markus Mangold², Pitt Allmendinger²; ¹*IRsweep*, ²*IRsweep AG*
- 9:55 AM (389) **Isolating Protein Amide I Signals in Water Using 2D-IR Spectroscopy;** Samantha M. Hume¹, Gregory Greetham², Paul Donaldson², Mike Towrie², Tony Parker², Matthew J. Baker³, Neil Hunt⁴; ¹*University of Strathclyde*, ²*STFC*

Central Laser Facility, ³*University of Strathclyde/ClinspecDx*, ⁴*University of York*

- 10:15 AM (390) **Time-resolved Resonance Raman Studies of Re(i) Complexes with Blended Intraligand and Metal-to-ligand Charge-transfer States;** Keith Gordon¹; ¹*University of Otago*
- 10:35 AM (391) **Filming Chemical Reactions at the Single-molecule Level Using Electron Beam;** Khlobystov N. Andrei¹, Stephen Skowron¹, Kecheng Cao², Kayleigh Fung¹, Craig Stoppiello¹, Johannes Biskupek², Ute Kaiser², Andrei Khlobystov¹; ¹*University of Nottingham*, ²*University of Ulm*

19LIBS04: Molecular Signal in LIBS *Smoketree C*

Chair: Michael Gaft

- 9:15 AM (392) **Progress in Laser Ablation Molecular Isotopic Spectrometry (LAMIS);** Alexander Bol'shakov¹, Xianglei Mao², Rick Russo²; ¹*Applied Spectra, Inc.*, ²*LBNL*
- 9:35 AM (393) **LIBS-MLIF method for halogens detection in air ambient conditions;** Lev Nagli¹; ¹*University Ariel, Israel*
- 9:55 AM (394) **Molecular Emissions in the Laser-induced Plasma in Simulated Martian Conditions: Calibration Models and New Insights from Plasma Imaging;** David S. Vogt¹, Kristin Rammelkamp², Peder B. Hansen², Simon Kubitzka², Sven Frohmann², Susanne Schröder², Heinz-Wilhelm Hübers²; ¹*German Aerospace Center*, ²*German Aerospace Center (DLR)*
- 10:15 AM (395) **Using Molecular Bands for Geological Purposes: An Exploratory Fluor Study;** Cécile Fabre¹, Cécile Fabre², Yann Foucaud²; ¹*Universite de Lorraine / GeoRessources*, ²*GeoRessources*
- 10:35 AM (396) **Molecule Formation in Calcium Carbonate and Calcium Hydroxide LIBS Plasmas: Model and Experiment;** Igor Gornushkin¹, Sergei Shabanov², Matthieu Baudalet³, Tobias Voelker⁴, Gerd Wilsch⁴; ¹*BAM Federal Institute for Materials Research and Testing*, ²*Department of Mathematics, University of Florida, Gainesville, FL 32611, USA*, ³*National Center for Forensic Science/Chemistry department, University of Central Florida, FL 12354, USA*, ⁴*BAM Federal Institute for Materials Research and Testing, 12489 Berlin, Germany*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

19PAT05: Advances in On-line Process Analysis

Smoketree D

Chair: Alison Nordon

- 9:15 AM (397) **Machine Learning and Online Analysis for Advanced Process Control and Optimisation;** Aparajith Bhaskar¹, Darren Whitaker¹, John Mack¹; ¹*Perceptive Engineering*
- 9:35 AM (398) **Rapid In-situ Measurement of Parahydrogen Fraction with Raman Spectroscopy and the Use of Parahydrogen for Enhanced Sensitivity Benchtop NMR Spectroscopy;** Andrew Parrott¹, Peter Richardson², Olga Semenova², Meghan Halse², Simon Duckett², Alison Nordon¹; ¹*University of Strathclyde*, ²*University of York*
- 9:55 AM (399) **Advantages of Measuring Moisture Content with Process Analytical Technology;** Adam J. Hopkins¹, Adam Hopkins¹, Kraig Kmietek¹; ¹*Metrohm USA*
- 10:15 AM (400) **A Digital Science Platform for Process Chemometric Model Maintenance;** David A. Joyce¹, Robert Carroll², Gary Walters³, Kathy Schulting⁴; ¹*Thermo Fisher Scientific - Digital Engineering*, ²*Shell*, ³*Thermo Fisher Scientific - Digital Science*, ⁴*Thermo Fisher Scientific*
- 10:35 AM (401) **Design and Development of a Samples and Variable Selection Method for a Robust Partial Least Squares (PLS) Regression;** Rajesh Morampudi¹, Joseph Medendorp¹; ¹*Vertex Pharmaceuticals*

19PMA08: Artificial Intelligence in Pharma *Madera*

Chairs: Steve Buckley, Peter Harrington

- 9:15 AM (402) **The Role of Ai-powered Computational Pathology to Advance Biomarker Discovery in Pharma;** Vipul Baxi¹; ¹*Bristol-Myers Squibb*
- 9:35 AM (403) **Machine Learning for Characterizing and Authenticating Natural Medicines;** Peter B. Harrington¹; ¹*Center for Intelligent Chemical Instrumentation*
- 10:15 AM (404) **Machine Learning Implementation in Practical Environments;** Steve Buckley¹, Teresa Nieten¹; ¹*Ocean Insight*
- 10:35 AM (405) **Limit of Detection Calculations in Multivariate Model Applications;** Doug Steinbach¹, Gary McGeorge¹, Dongsheng Bu¹, Lucy Hawarden¹, Patrick Wray¹; ¹*Bristol Myers Squibb*

19RAM01: Low Frequency Raman *Ventura*

Chair: Anjan Roy

- 9:15 AM (406) **Time-resolved (Ten Milli-second) Low Frequency Raman Spectroscopy: A Method of Evaluating Dynamic Behaviour in Drug Formulations;** Keith Gordon¹; ¹*University of Otago*
- 9:35 AM (407) **Low-frequency Raman Spectroscopy of Modern and Ancient Pigments;** Timothy M. Korter¹, Elyse Kleist¹; ¹*Syracuse University*
- 9:55 AM (408) **Quantification of Crystalline Active Pharmaceutical Ingredients by Transmission Low-frequency Raman Spectroscopy;** Motoki Inoue¹, Hiroshi Hisada², Takumi Osada², Tatsuo Koide³, Toshiro Fukami², Anjan Roy⁴, James Carriere⁴, Randy Heyler⁴; ¹*Meiji Pharmaceutical University*, ²*Meiji Pharmaceutical University*, ³*National Institute of Health Sciences*, ⁴*Coherent Incorporated*
- 10:15 AM (409) **Novel Method for Solubility Determination of Crystalline Drugs in Polymeric Matrices Using Hot Melt Extrusion and Terahertz-Raman Spectroscopy;** Ecaterina Bordon¹, Muhhamad T. Islam¹, Alastair Florence¹, Gavin Halbert¹, John Robertson¹; ¹*EPSRC Centre for Innovative Manufacturing in Continuous Manufacturing and Advanced Crystallisation, University of Strathclyde, Technology and Innovation Centre, 99 George Street, G1 1RD Glasgow, U.K*
- 10:35 AM (410) **THz-raman Measurements of Crystallinity and Form in Pharmaceuticals and Drug Development;** Anjan Roy¹, Lawrence Ho¹, Frank Havermeier¹, James Carriere¹, Tom Haw¹, Randy Heyler¹; ¹*Coherent Inc*

19RAM13: Biomedical Raman (CLIRSPEC) *Sierra*

Chair: Nick Stone

- 9:15 AM (411) **Multimodal, Label-free Detection of Ganglion Cells for Diagnosing Hirschsprung Disease;** James Chan¹, Che-Wei Chang¹, Marcos Oliveira¹, Payam Saadai¹, Laura Galganski¹, Christopher Pivetti¹, Karen Matsukuma¹; ¹*UC Davis*
- 9:35 AM (412) **Unique Nano-assemblies Built of "Off-the-shelf" Components for Raman Theranostics;** Priyanka Dey¹, Tanveer A. Tabish¹, Sara Mosca², Francesca Palombo¹, Pavel Matousek³, Nick Stone¹; ¹*University of Exeter*, ²*RAL, CLF, STFC*, ³*Science and Technology Facilities Council*

**TECHNICAL PROGRAM - WEDNESDAY
ORAL SYMPOSIA 9:15 AM – 10:55 AM**

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| <p>9:55 AM (413) Using Cholesterol Modified Nanoparticles as Agents for Cardiovascular Disease Systems; <u>Fatima Ali</u>¹, Karen Faulds¹, Duncan Graham¹; ¹University of Strathclyde</p> <p>10:15 AM (414) Breast Tumors Tissue Phantom: Mimicking and Modelling the Raman Spectra from Different Breast Cancers; <u>Rishikesh Pandey</u>¹, Machele Riccio Riccio², Gary Root², Michael sapack²; ¹CytoVeris Inc., ²CytoVeris Inc</p> | <p>10:35 AM (415) Assessing Liver Health for Transplant; <u>Colin Campbell</u>¹, Katie Ember¹, Stuart Forbes¹, Karen Faulds², Gabi Oniscu³; ¹University of Edinburgh, ²University of Strathclyde, ³Univeristy of Edinburgh</p> |
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**TECHNICAL PROGRAM - WEDNESDAY
POSTER SESSION 11:00 AM – 12:00 PM
*Exhibit Hall, Oasis***

See page 88 for Wednesday posters by category. Posters will be displayed all day and attended again in the afternoon.

**TECHNICAL PROGRAM – WEDNESDAY
WHAT’S HOT EXHIBITOR PRESENTATIONS 11:50 AM – 1:00 PM
Chair: Brian Dable
Exhibit Hall, Oasis
(Lunch is available from 12:00 – 12:30 pm; ticket required)**

- 11:50 AM Submicron Simultaneous IR and Raman Microscopy: A New Paradigm in Spectroscopy
Photothermal Spectroscopy Corp: Mustafa Kansiz
- 12:00 PM An Analyzer Framework for 21st Century Continuous Manufacturing
Tornado Spectral Systems: Scott Baker
- 12:10 PM New Advances (and New Products) for Laser Ablation Based Elemental Analysis
Applied Spectra: Alan Koenig
- 12:20 PM TBD
Barnett Technical Services
- 12:30 PM Identification of Microplastics Using the 8700 Laser Direct Infrared Imaging (LDIR) System
Agilent: Louis Tisinger
- 12:40 PM A-TEEM Fluorescence Spectroscopy: Molecular Fingerprinting with High Sensitivity for QC Applications in the Water and Pharma Industries
HORIBA Scientific: Adam Gilmore
- 12:50 PM New Nonlinear Methods in PLS Toolbox & Sol
Eigenvector: Neal Gallagher

**TECHNICAL PROGRAM - WEDNESDAY
ORAL SYMPOSIA 1:30 PM – 3:10 PM**

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| <p>19AES05: Biosensors Mesquite D
Chairs: Erin Henslee, Rucha Natu</p> <p>1:30 PM (416) High-throughput Deterministic Ratchet Devices for Organelle Separation; <u>Mukul Sonker</u>¹, Dai Hyun Kim¹, Alexandra Ros¹; ¹The Biodesign Institute, Arizona State University</p> | <p>1:50 PM (417) Detecting Single Nucleotide Polymorphism with Giant Magnetoresistive Biosensor; <u>Todd Klein</u>¹; ¹Zepto Life Technology</p> <p>2:10 PM (418) An Integrated Microfluidic Device with Nano-Magnetic Bead Capturing for Cancer-Derived Extracellular Vesicle Characterization; <u>Chenguang Zhang</u>¹, Ceming Wang¹, Satyajyoti Senapati², Hsueh-Chia Chang¹; ¹University of Notre Dame, ²University Of Notre Dame</p> |
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TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

2:30 PM (419) **A rapid and low cost peptide sensor for Pb²⁺ detection by direct interface capacitance measurement;** Jie J. Wu¹, Jian Zhang²; ¹*The University of Tennessee*, ²*Hefei University of Technology*

2:50 PM (420) **Borrowing from Packed Bed Reactors: A flow-through, nano-porous, shear-enhanced electrode for electrochemical spectroscopy - A sensitive and selective Biosensor;** Sagnik Basuray¹, Yu Hsuan Cheng¹, Zhenglong Li¹, Hansin Kim¹, Lixin Feng¹; ¹*New Jersey Institute of Technology*

19ATOM05: Atmospheric Pressure Glow Discharge Spectroscopies II (Applications) Pasadena

Chair: R. Kenneth Marcus

1:30 PM (421) **Analysis of Nanoparticles Using Novel Approaches to Solution-cathode Glow Discharge Atomic Emission Spectrometry;** Steven J. Ray¹, Jaime Orejas², Nicholas Hazel²; ¹*The State University of New York at Buffalo*, ²*SUNY-Buffalo*

1:50 PM (422) **Developments in Solution-cathode Glow Discharge for Elemental Analysis of Aqueous Samples;** Michael R. Webb¹, Wade Maresh¹, Joey Funderburg¹; ¹*University of North Carolina Wilmington*

2:10 PM (423) **Liquid-electrode Plasma Induced Vapor Generation Method;** Zhenli Zhu¹, Zhenli Zhu², Xing Liu², Hongtao Zheng², Chun Yang²; ¹*China University of Geosciences (Wuhan)*, ²*China University of Geosciences (Wuhan)*

2:30 PM (424) **Plasmas in Contact with Liquids: Physicochemical Processes at the Plasma-liquid Interface;** Selma Mededovic Thagard¹; ¹*Clarkson University*

2:50 PM (425) **Elemental Analysis in the Petroleum Industry Using Plasma Techniques;** Laura Poirier¹, Francisco Lopez-Linares²; ¹*Chevron/DTS*, ²*Chevron*

19CHEM05: Unraveling Sample Matrix Effects with Chemometrics Mesquite E

Chair: John Kalivas

1:30 PM (426) **The Development of Chemometric Functional Libraries;** Leonardo Ramirez-Lopez¹; ¹*BUCHI Labortechnik AG*

1:50 PM (427) **Local Calibration Using Multivariate Curve Resolution Methods;** Hamid Abdollahi¹, Ali Pahlavan², Somaiyeh Khodadadi², John Kalivas³; ¹*Department of Chemistry, Institute for Advanced studies in Basic Sciences, Zanjan, Iran*, ²*Institute for Advanced Studies in Basic Sciences*, ³*Idaho State University*

2:10 PM (428) **Quantification of Mixtures in Presence of Interferences and Matrix Effects by Multivariate Curve Resolution;** Roma Tauler¹; ¹*IDAEA CSIC*

2:30 PM (429) **Identifying Matrix Matched Samples by Leveraging Spectral Calibration Model Regression Vectors;** John H. Kalivas¹, Tony Lemos¹; ¹*Idaho State University*

2:50 PM (430) **Modeling and Performance Evaluation of a Real-time Molecular Chemical Imaging (MCI) Surgical Endoscope;** Arjun S. Bangalore¹, Marlina B. Darr¹, Alyssa B. Zrimsek¹, Shawna K. Tazik¹, Matthew P. Nelson¹, Patrick J. Treado¹; ¹*ChemImage Corp.*

19CTP04: Deviations from the Beer-Lambert Law: New Perspectives and Solutions Mojave

Chairs: Jürgen Popp, Thomas Mayerhöfer

1:30 PM (431) **The Bouguer-beer Lambert Law (re-)viewed from a Wave Optics Perspective;** Thomas G. Mayerhöfer¹, Susanne Pahlow¹, Sonja Höfer¹, Uwe Hübner¹, Jürgen Popp¹; ¹*Leibniz Institute of Photonic Technology*

2:10 PM (432) **Beyond the Beer-lambert Approximation, Considerations for Quantitative Chemical Analysis at the Nanoscale with the PTIR Technique;** Andrea Centrone¹; ¹*National Institute of Standard and Technology*

2:30 PM (433) **A Comparison of Computational Approaches to Remove "Artefacts" in IR Spectroscopy;** Shuxia Guo¹, Thomas Mayerhöfer², Jürgen Popp², Thomas Bocklitz²; ¹*Leibniz Institute of Photonic Technology Jena (IPHT Jena), Germany*, ²*Leibniz Institute of Photonic Technology Jena (IPHT Jena), Member of Leibniz Health Technologies; Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University of Jena*

2:50 PM (434) **Infrared Spectroscopic Imaging - From a Simple Combination of Spectroscopy and Microscopy to New Design Concepts;** Rohit Bhargava¹, Illia Rasskazov², Paul Carney², Rohit Bhargava³; ¹*University of Illinois Urbana-Champaign*, ²*University of Rochester*, ³*University of Illinois at Urbana-Champaign*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

19FORENS03: Forensic Analysis in the Lab and at the Crime Scene *Smoketree A*

Chair: Igor Lednev

- 1:30 PM (435) **Forensic Science R&D Funding at the National Institute of Justice: Opportunities for Novel Spectroscopic and Analytical Techniques Applied to Forensic Problems;** Gregory Dutton¹; ¹*National Institute of Justice*
- 1:50 PM (436) **Utilization of Portable Gas-chromatographic Systems Coupled with CMV for On-site Detection of Ignitable Liquid Residues;** Jose Almirall¹, Michelle Torres¹, Nicole Valdes¹; ¹*Florida International University*
- 2:10 PM (437) **On the Mass Spectral Interpretation of Cathinones and Fentanyl Analogs;** Glen P. Jackson¹, J. Tyler Davidson¹, Z. J. Sasiene¹, Younis Abiedalla², Jack DeRuiter², Randall Clark²; ¹*West Virginia University*, ²*Auburn University*
- 2:30 PM (438) **Nondestructive Analysis of a Bloodstain by ATR FT-IR Spectroscopy for Forensic Purposes;** Ewelina M. Mistek¹, Igor Lednev¹; ¹*University at Albany, SUNY*
- 2:50 PM (439) **On-scene Trace Identification of Materials of Grave Toxicity with Handheld Mass Spectrometry;** Christopher D. Brown¹; ¹*908 Devices*

19IR08: Recent Advances in Chemical and Material Detection Using Molecular Spectroscopy *Smoketree E*

Chair: Mike George

- 1:30 PM (440) **Standoff Detection of Threat Chemical Traces on Surfaces by active Long Wave Infrared Backscatter Imaging Spectroscopy;** Robert Furstenberg¹, Christopher Kendziora², Christopher Breshike², Yohan Yoon², Michael Papantonakis², R. Andrew McGill²; ¹*US Naval Research Laboratory*, ²*Naval Research Laboratory*
- 1:50 PM (441) **Detection and Identification of Deposited Biological Hazards Using Infrared Spectroscopy;** Kelly Curtis¹, Debbie Padgen¹, Camilla Robinson¹, Christopher Howle¹; ¹*Defense science and technology lab*
- 2:10 PM (442) **An Infrared Spectroscopic Study of Hazardous Chemicals Deposited Using a Piezoelectric Printer;** Linda Lee¹, Rhea Clewes¹, Siobhan Conner¹, Christopher Howle¹; ¹*Dstl*
- 2:30 PM (443) **Advances in Sorbent Materials for Detection and Protection Applications;** Tyler Grissom¹, Courtney A. Roberts², Michael Papantonakis², Andrew Kusterbeck³, R. Andrew McGill²; ¹*NRC Postdoctoral Fellow / Naval Research Laboratory*, ²*Naval Research Laboratory*, ³*Nova Research*

- 2:50 PM (444) **Frequency Comb Spectroscopy as a New Modality for Infrared Micro-spectroscopy;** Henry Timmers¹, Abijith Kowligy¹, Alex Lind¹, Nima Nader¹, Jonah Shaw¹, Dobryna Zalvidea², Jens Biegert³, Scott Diddams¹; ¹*NIST*, ²*IBEC*, ³*ICFO*

19LIBS11: 2019: International Year of the Periodic Table at the Speed of Light (New Methodology) *Smoketree C*

Chair: Sebastian Wachsmann-Hogiu

- 1:30 PM (445) **Elemental Concentrations Calibrations of Phosphate Slurries and Solid Pellets Using Laser Induced Breakdown Spectroscopy;** Driss Lahlou Kitane¹, Dimitris Bertsimas¹, Nawfel Azami², Francois R. Doucet³; ¹*Operations Research Center - Massachusetts Institute of Technology*, ²*INPT-UM6P*, ³*ELEMISSION inc.*
- 1:50 PM (446) **LIBS as a method to study and characterize biological materials;** Sebastian Wachsmann-Hogiu¹, Sebastian Wachsmann-Hogiu¹, Juanjuan Liu¹; ¹*McGill University*
- 2:10 PM (447) **2.5D LIBS Imaging Using Adaptive Optics;** Pablo Sobron¹, Christian Burlet², Yves Vanbrabant², Jose Antonio Manrique³; ¹*Impossible Sensing*, ²*Geological Survey of Belgium*, ³*Centro de Astrobiología | CAB · Unidad Asociada UVA-CSIC*
- 2:30 PM (448) **Fast Compositional Tomography of Ore Samples by Laser Induced Breakdown Spectroscopy;** Nicolas Montreuil, Kheireddine Rifai¹, Lütü Özcan², Francois Doucet³, François Vidal⁴; ¹*Dr.*, ²*Elemission.Inc.*, ³*Elemission.ca*, ⁴*INRS*
- 2:50 PM (449) **Molecules in Laser Induced Plasma: Plasma Characterization and Applications;** Timur A. Labutin¹, Andrey M. Popov², Sergey M. Zaytsev¹, Nikolay I. Sushkov¹; ¹*Lomonosov Moscow State University*, ²*Lomonosov Moscow State University*

19PAT03: Industrial Applications of Vibrational Spectroscopy *Smoketree D*

Chairs: Mark Rickard, Xiaoyun Chen

- 1:30 PM (450) **Advanced Fiber Spectroscopy in 0.3-16µm Range for Biomedical & Process Control Applications;** Viacheslav Artyushenko¹; ¹*art photonics GmbH*
- 1:50 PM (451) **Raman Spectroscopic Quantitative Analysis of a Water Soluble Polymer Synthesis: From the Lab to the Plant;** Peter J. Larkin¹, Boyu Li¹, Ian Anderson¹, Michael Lynch¹; ¹*Solvay*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

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| <p>2:10 PM (452) Detecting Organic Contaminants in Water via Mid-infrared Fiber-optic Evanescent Field Spectroscopy; <u>Carina Dettenrieder</u>¹, Yosef Raichlin², Abraham Katzir³, Boris Mizaikoff¹; ¹Ulm University / Institute of Analytical and Bioanalytical Chemistry, ²Ariel University / Department of Physics, ³Tel Aviv University / School of Physics and Astronomy</p> <p>2:30 PM (453) Novel Attenuated Total Reflection Sensor Concepts for Quantum Cascade Laser - Based Infrared Spectroscopy in Harsh Environments; <u>Andrea Teuber</u>¹, Robert Stach¹, Patrick Krebs¹, Boris Mizaikoff²; ¹Universität Ulm, ²Ulm University / Institute of Analytical and Bioanalytical Chemistry</p> <p>2:50 PM (454) Fabrication and Analysis Tools for Real-time Environmental Monitoring by Surface-enhanced Raman Spectroscopy (SERS); <u>Jason R. Dwyer</u>¹, Robert Chevalier¹; ¹University of Rhode Island</p> | <p>2:10 PM (460) Portable Raman Spectroscopy for Medical Applications; <u>Fay Nicolson</u>¹, Fay Nicolson¹, Neil Shand², Duncan Graham³, Karen Faulds³, Moritz Kircher¹; ¹Dana-Farber Cancer Institute, ²DSTL, ³University of Strathclyde</p> <p>2:30 PM (461) Raman-on-chip for High-throughput, High-resolution Handheld Spectroscopy; <u>Hilde Jans</u>¹, Frantz Agis¹, Victor Garcia Munoz¹, Hemant Kumar Tyagi¹, Harrie Tilmans¹, Xavier Rottenberg¹, Peter Peumans¹, Pol Van Dopre¹; ¹imec</p> <p>2:50 PM (462) Fiber-based Raman In-situ Chemical Sensing Using Modular and Monolithic Spatial Heterodyne Raman Spectrometers (SHRS); <u>J. Chance Carter</u>¹, S. Michael Angel², Joshua Ottaway¹, Ashley Allen², Abigail Waldron², William E. Hunt¹; ¹Lawrence Livermore National Laboratory, ²University of South Carolina, Department of Chemistry and Biochemistry</p> |
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19PMA11: Spectroscopy for Pharmaceutical Applications Madera

Chairs: Shengli Ma, Raphael Fish

- 1:30 PM (455) **Characterize Complex Drug Products Using Morphologically Directed Raman Spectroscopy (MDRS)**; Changning Guo¹, Changning Guo¹; ¹FDA
- 1:50 PM (456) **Characterization of linker Bond in Pharmaceutical Molecules by Vibrational Spectroscopy**; Shengli Ma¹; ¹Genentech
- 2:30 PM (457) **Raman spectroscopy with chemometrics enables a wide range of applications in supporting process development**; Michelle S. Raikes¹, Michelle Raikes¹; ¹Boehringer Ingelheim Pharmaceuticals
- 2:50 PM (473) **Speaker Roundtable**; Shengli Ma¹, Changning Guo², Michelle S. Raikes³; ¹Genentech, ²FDA, ³Boehringer Ingelheim Pharmaceuticals

19RAM05: Portable Raman Sierra

Chair: Neil Shand

- 1:30 PM (458) **Mobility Integration into Handheld Raman Devices**; Keith Carron¹, Keith Carron¹, Bryan Ray¹, Brett Miller¹; ¹Metrohm Raman
- 1:50 PM (459) **Sense and Sensitivity: Compact Raman Without Compromise**; David Creasey¹, Mark Zieg¹, Jonathan Faircloth², Robert Dickerson¹, Leigh Brady¹, Mike Sullivan¹, David Creasey¹; ¹Wasatch Photonics, ²Jonathan Faircloth

19SPECIAL01: SAS Session Commemorating John Jackovitz Chino AB

Chair: Robert Lascola

- 1:30 PM (463) **How a Spectroscopy Legend Helped a Pittsburgh Start Up**; Chuck W. Gardner¹, Patrick Treado¹, Matthew Nelson¹; ¹ChemImage Corporation
- 1:50 PM (464) **Deep Ultraviolet Standoff Photoacoustic Spectroscopy of Trace Explosives**; Sandy A. Asher¹, Alyssa Zrimsek¹, Sergei Bykov¹, Sandy Asher¹; ¹University of Pittsburgh
- 2:10 PM (465) **Biosensing with Raman Spectroscopy - A Career Influenced by John F. Jackovitz**; Bhavya Sharma¹; ¹University of Tennessee
- 2:30 PM (466) **Innovative Vibrational and Rotational Spectroscopy for Pharmaceutical Industry - From Small Molecules to Biologics**; Rina K. Dukor¹, Juanita Sanchez², Jordan Nafie², Justin Neill³, Laurence Nafie⁴; ¹BioTools, Inc, ²BioTools, ³Brightspec, ⁴Syracuse University
- 2:50 PM (467) **Hyperspectral Raman Imaging Using a Monolithic Spatial Heterodyne Raman Spectrometer**; S. Michael Angel¹, J. Chance Carter², Joshua Ottaway², Abigail Waldron³, Ashley Allen³; ¹University of South Carolina, Department of Chemistry and Biochemistry, ²Lawrence Livermore National Laboratory, ³Univ. of South Carolina

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

19SPR05: Multimodal and Multifunctional Plasmonics *Smoketree B*

Chair: Wei-Chuan Shih

1:30 PM (469) **Nanostructured Metasurfaces for Plasmon-enhanced Nonlinear Optical Spectroscopy**; Andrea R. Tao¹, Yuan Zeng²; ¹*Dept. of NanoEngineering, UC San Diego*, ²*Univ of California-San Diego*

1:50 PM (468) **Plasmonic Structures and Applications Fabricated Using Collapsible Nano-Fingers**; Boxiang Song¹, Yunxiang Wang², Zerui Liu², Pan Hu², Fanxin Liu, Steve Cronin², Adam Schwartzberg, Stefano Cabrini, Wei Wu²; ¹*University of Southern California*, ²*USC*

2:10 PM (470) **Plasmonic Bio-chip for RGB Cameras**; Wei-Chuan Shih¹, ¹*University of Houston*

2:30 PM (471) **Asymmetric Deposition of Platinum Atoms on Gold Nanorods Induced by a Substrate for Synthesis of Anisotropic Bimetallic Nanostructures**; Mahmoud Abdelwahed¹, Mahmoud Mahmoud¹; ¹*The University of Texas at San Antonio*

2:50 PM (472) **Utilization of Plasmonic Nanostructures for Highly Sensitive Vibrational Biospectroscopy**; Jürgen Popp¹; ¹*Leibniz Institute of Photonic Technology*

TECHNICAL PROGRAM - WEDNESDAY

POSTER SESSION 3:10 PM – 3:50 PM

Exhibit Hall, Oasis

See page 88 for a listing of Wednesday posters by category. Student poster award winners will be announced the following morning during the plenary session.

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

19ATOM06: Atmospheric Pressure Glow Discharge Spectroscopies III (Molecular) *Pasadena*

Chairs: Jacob Shelley, Steven Ray

3:50 PM (474) **Atmospheric Pressure Plasmas Coupled with Differential Mobility Spectrometry**; Theresa Evans-Nguyen¹, Ifeoluwa Ayodeji¹, Linxia Song¹, Nathan Grimes¹, Kenyon Evans-Nguyen², Theresa Evans-Nguyen¹; ¹*University of South Florida*, ²*University of Tampa*

4:10 PM (475) **Simple, Rapid Chemical Modification and Analysis of n-Alkanes with Flowing Atmospheric-pressure Afterglow (FAPA) Mass Spectrometry**; Brian Molnar¹, Sunil Badal², Garrett Maclean², Jacob Shelley²; ¹*Rensselaer Polytechnic Institute*, ²*Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute*

4:30 PM (476) **Molecular Analysis with High Repetition-rate Laser-induced Micro Plasma in Air**; Yi You¹, Andreas Bierstedt¹, Jens Riedel¹; ¹*Federal Institute for Materials Research and Testing (BAM)*

4:50 PM (477) **SAS Atomic Section Student Award Winner: An Exploratory Investigation of the Liquid Sampling – Atmospheric Pressure Glow Discharge for the Mapping of Molecular and Atomic Species of Biological Samples**; Htoo W. Paing¹, C Derrick Quarles², Terri Bruce¹, R. Kenneth Marcus¹; ¹*Clemson University*, ²*Elemental Scientific Inc*

5:10 PM (478) **Evaluating the Use of the LS-APGD Ionization Source for Protein Analysis**; Edward D. Hoegg¹, Edward Hoegg¹, David Koppelaar¹, R. Kenneth Marcus²; ¹*Pacific Northwest National Laboratory*, ²*Clemson University*

19AWD09: AES Lifetime Achievement Award Session Honoring Hsueh-Chia Chang *Mesquite D*

Chairs: Satyajyoti Senapati, Gongchen Sun

3:50 PM (479) **Isolation, Fractionation and Analysis of Exosomes**; Hsueh-Chia Chang¹; ¹*University of Notre Dame*

4:30 PM (480) **Acoustic-electric Interactions at Micron and Nanometre Scales**; Leslie Yeo¹, Heba Ahmed¹, Lillian Lee¹, Amgad Rezk¹, Kourosh Kalantar-zadeh¹, Connie Darmanin², Joseph Richardson³; ¹*Royal Melbourne Institute of Technology (RMIT)*, ²*LaTrobe University*, ³*University of Melbourne*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

5:10 PM (481) **Nanochannel Electroporated Cell Transfection and Vesicle Secretion for Nucleic Acid Delivery: Cancer Therapy, Immune Disease Treatment, and Regenerative Medicine;** James Lee¹; ¹*Ohio State University*

19CHEM06: Sample and Variable Selection: Memorial Session Honoring Frank Vogt *Mesquite E*

Chair: Barry Lavine

3:50 PM (482) **A Novel Multivariate Curve Resolution-alternating Least Squares (MCR-ALS) Methodology for Application in Hyperspectral Raman Imaging Analysis;** Joseph P. Smith¹, Erin C. Holahan², Frank C. Smith², Karl S. Booksh²; ¹*Merck & Co., Inc.*, ²*University of Delaware*

4:10 PM (483) **Variable Selection to Improve the Classification and Authentication of Edible Oils;** Barry Lavine¹, Isio Sota Uba¹, Matthew Bamidele¹; ¹*Oklahoma State University*,

4:30 PM (484) **Speciation of Dalbergia (Rosewood) via Hand-held Laser Induced Breakdown Spectroscopy (LIBS) and Chemometric Analysis;** James A. Jordan¹, Caelin Celani², Cady Lancaster³, Edgard Espinoza⁴, Karl Booksh²; ¹*National Geospatial-Intelligence Agency / US Geological Survey*, ²*Department of Chemistry and Biochemistry, University of Delaware*, ³*National Fish and Wildlife Forensics Lab, United States Forest Service*, ⁴*National Fish and Wildlife Forensics Lab, United States Fish and Wildlife Service*

4:50 PM (485) **Assessing Hand-Held LIBS for Speciation of Rosewood with PLS-DA and KNN;** Karl S. Booksh¹, Karl Booksh¹, Caelin Celani¹, James Jordan², Cady Lancaster³, Edgard Espinoza⁴; ¹*University of Delaware*, ²*USGS*, ³*US Fish and Wildlife Service*, ⁴*US*

5:10 PM (486) **Comparison of Spectroscopic Techniques Paired with Chemometrics for Determining the Peroxide Value of 19 Classes of Naturally Aged, Plant-based Edible Oils;** Joshua Ottaway¹, J. Chance Carter¹, Kristl Adams², Joseph Camancho³, Barry Lavine⁴, Karl S. Booksh³; ¹*Lawrence Livermore National Laboratory*, ²*Lawrence Livermore National Lab*, ³*University of Delaware*, ⁴*Oklahoma State University*

19CTP02: Women in Analytical Chemistry *Chino AB*

Chair: Rina Dukor

3:50 PM (487) **Women in Analytical Chemistry - Panel Discussion;** Bhavya Sharma¹, Amanda J. Haes², Diane Parry³, Anna Luczak⁴, Saumya Tiwari⁵; ¹*University of Tennessee*, ²*University of Iowa*, ³*Private Consulting*, ⁴*Bristol-Myers Squibb*, ⁵*University of Illinois*

Reception to follow

19LIBS07: Innovation in Instrumentation *Smoketree C*

Chair: Francois Doucet

3:50 PM (488) **Design and Development of Industrial Instrumentation;** Steve Buckley¹; ¹*Ocean Insight*

4:10 PM (489) **Evaluation of Portable LIBS and Portable XRF in the Frame of Multi-elemental Analysis of Agricultural Soils and Plants;** Bruno Bousquet¹, Julian Guezenoc¹, Anne Gallet-Budynek², Etonam Tete Kondo², Thomas Guzman², Alain Mollier², Pierre Masson³, Hugues Roussarie³, Martine Peypelut³, Thierry Dalix³, Guillaume Daugey³; ¹*Université de Bordeaux*, ²*INRA*, ³*INRA/USRAVE*

4:30 PM (490) **Application of Advanced Machine Learning Classification Techniques to Analyze Complex LIBS Spectra;** Prasoon K. Diwakar¹, Tejo Bheemasetti¹, Sofia Pozsonyiova², Melissa Fernandez³, Emily M. Orme⁴, Romila Pradhan⁵, Daniel Diaz⁶, David Hahn⁶, Shane C. Lee⁷; ¹*South Dakota School of Mines and Technology*, ²*Macalester College*, ³*Florida International University*, ⁴*Law Enforcement Officers Memorial High School*, ⁵*Purdue University*, ⁶*University of Florida*, ⁷*South Dakota School of Mines & Technology*

4:50 PM (491) **Plant Analysis by Laser-induced Breakdown Spectrometry (LIBS);** Aleksandr S. Zakuskin¹, Andrey M. Popov¹, Timur A. Labutin¹; ¹*Lomonosov Moscow State University*

19MASS01: MS Characterization of Proteins, Protein Complexes, and Therapeutic Proteins *Smoketree B*

Chair: Joseph Loo

3:50 PM (492) **The Role of Denaturing and Native-MS in Biopharma: From Target Validation to mAbs, ACDs and Beyond;** Iain D G Campuzano¹; ¹*Amgen Inc*

4:10 PM (493) **Measuring Membrane Interactions by Mass Spectrometry of Intact Lipoprotein Complexes;** Michael T. Marty¹, Michael Marty¹; ¹*University of Arizona*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

- 4:30 PM (494) **Native Mass Spectrometry and Surface Induced Dissociation for the Study of Membrane Proteins;** Sophie Harvey¹, Kevin Schey², Vicki Wysocki¹; ¹*The Ohio State University*, ²*Vanderbilt*
- 4:50 PM (495) **Probing Protein structure by Cyclic Ion mobility and IMSn: When Resolution Just isn't enough;** Roy Martin¹, Martin Palmer², Dale Cooper-Shepherd², James Langridge²; ¹*Waters Corp.*, ²*Waters*
- 5:10 PM (496) **Native Mass Spectrometry for a Top-down View of Protein Structures;** Joseph A. Loo¹; ¹*University of California, Los Angeles*

19PAT04: Online Analysis of Industrial Processes and Reactions *Smoketree D*

Chairs: Anna Sandlin, J.D. Tate

- 3:50 PM (497) **Shelterless Gas Chromatographs for On-line Analysis: Past, Present, and Future;** Eric Schmidt¹, J. D. Tate², Gerard Rogers², Eric Schmidt²; ¹*The Dow Chemical Company*, ²*Dow Chemical*
- 4:10 PM (498) **Implementing Process Optical Spectrometers;** Edward A. Orr¹, J. D. Tate², Allan Rilling³; ¹*ABB Inc.*, ²*Dow Chemical*, ³*ABB*
- 4:30 PM (499) **Microspectrometer Chips for Integrated Applications;** Nadia Pervez¹, Michael Gazes², Tanya Garza², Ioannis Kymissis²; ¹*Chromatation, Inc.*, ²*Chromatation*
- 4:50 PM (500) **Revolutionizing Process Monitoring in Mining Industry with Time-gated Raman Spectroscopy;** Mari Tenhunen¹, Bryan Heilala², Jyrki Savela³, Miia Mikkonen²; ¹*Timegate Instruments Ltd.*, ²*Timegate Instruments*, ³*Timegate Instruments Oy*
- 5:10 PM (501) **Deep UV Raman & Fluorescence Spectroscopy for in Situ Process Analysis;** William F. Hug¹, Quoc Nguyen¹, Michael Reid¹, Kripa Sijapati¹, Ray Reid¹; ¹*Photon Systems, Inc.*

19PMA04: Advanced Spectroscopic Techniques in Pharma *Madera*

Chair: Sergey Arzhantsev

- 3:50 PM (502) **Raman Optical Activity in Pharma: Studying Pharmaceutical Peptides in Solution;** Christian Johannessen¹; ¹*University of Antwerp*

- 4:10 PM (503) **Enabling Faster Route Discovery and Process Optimization with Molecular Rotational Resonance Spectroscopy;** Justin L. Neill¹; ¹*BrightSpec, Inc.*
- 4:30 PM (504) **Protein Solutions: Routine Higher Order Structure Analysis by Raman and Scattering Techniques;** Eunah Lee¹, Eunah Lee¹, Michelle Sestak¹, Jeff Bodycomb¹, Li Yan¹; ¹*HORIBA Scientific*
- 4:50 PM (505) **Analysis of Biomolecules by Raman Spectroscopy;** Shengli Ma¹; ¹*Genentech*
- 5:10 PM (506) **Real-time Monitoring of Polymorphic Transformations with Thz Spectroscopy;** Mark A. Arnold¹, Michaela Raglione¹, Tianyao Zhang¹; ¹*University of Iowa*

19PMA06: Counterfeits Food Products and Dietary Supplements *Catalina*

Chair: Sulaf Assi

- 3:50 PM (507) **At-Line Optical Porosity Measurements of Pharmaceutical Solids by GASMAS spectroscopy;** Jonas Johansson¹, Anders B. Sparen², Pirjo Tajarobi¹, Håkan Wikström², Patrik Lundin³, Anders Långberg³, Mikael Sebesta³, Märta Lewander Xu³; ¹*AstraZeneca*, ²*Pharmaceutical Technology & Development, AstraZeneca Gothenburg, Sweden*, ³*Gaspox AB*
- 4:10 PM (508) **Using Ion Chromatography to Judge Food Authenticity and Detect Adulteration;** Jeff Rohrer¹; ¹*Thermo Fisher Scientific*
- 4:30 PM (509) **Identification of Counterfeit Medicines Using Near-infrared Imaging;** Ian Robertson¹, Sulaf Assi²; ¹*Perkin Elmer Limited*, ²*Liverpool John Moores University*
- 4:50 PM (510) **PharmaChk: Testing the Quality of Medicines in the Field;** Darash Desai¹; ¹*Boston University*
- 5:10 PM (511) **Speaker Roundtable;** Jonas Johansson¹, Jeff Rohrer², Ian Robertson³, Darash Desai⁴, Muhammad Zaman⁴; ¹*AstraZeneca*, ²*Thermo Fisher Scientific*, ³*Perkin Elmer Limited*, ⁴*Boston University*

19RAM10: Raman Imaging/Microscopy *Sierra*

Chairs: Katsumasa Fujita, Duncan Graham

- 3:50 PM (512) **Raman Imaging of the Immune Cell Response to Local Environmental Changes;** Alison Hobro¹, Nicholas Smith¹; ¹*Osaka University*

TECHNICAL PROGRAM - WEDNESDAY

ORAL SYMPOSIA 3:50 PM – 5:30 PM

4:10 PM (513) **Saturated Stimulated Raman Scattering Microscopy for Super-resolution Vibrational Imaging;** Zhiwei Huang¹; ¹*National University of Singapore*

4:30 PM (514) **Novel Applications of SERS Labels in Molecular Sensing and Imaging;** Wei-Chuan Shih¹; ¹*University of Houston*

4:50 PM (515) **Imaging Intracellular Drug Distribution in Prostate Cancer Cells Using Ratiometric Raman and Stimulated Raman Scattering Microscopy;** William J. Tipping¹, Liam Wilson¹, Nicholas Tomkinson¹, Lauren Jamieson¹, Karen Faulds², Duncan Graham²; ¹*The University of Strathclyde*, ²*University of Strathclyde*

5:10 PM (516) **Evaluation of Single-cell Type, Function, and Heterogeneity Through Label-free Spectroscopic and Morphological Metrics;** Nicholas I. Smith¹, Nicolas Pavillon¹, Alison Hobro¹; ¹*Osaka University*

19RAM19: Raman with Spatial Light Modulators *Ventura*

Chair: Ioan Notingher

3:50 PM (517) **Integrated Holographic Optical Tweezers Raman (HOT-Raman) Imaging;** Wei-Chuan Shih¹; ¹*University of Houston*

4:10 PM (518) **Multi-beam Raman Microscopy Using Spatial Light Modulators;** Zhiyu Liao¹, Faris Sinjab², Ioan Notingher¹; ¹*University of Nottingham*, ²*University of Tokyo*

4:30 PM (519) **Compressive Raman Imaging via Digital Micromirror Devices;** Hilton B. de Aguiar¹, Hilton de Aguiar²; ¹*Physics Department, Ecole Normale Supérieure/Paris*, ²*Ecole Normale Supérieure/Paris*

4:50 PM (520) **Shaping Light Through a Single Multimode Fibre for Wide-field Raman Imaging;** Mingzhou Chen¹, Ivan Gusachenko¹, Kishan Dholakia¹; ¹*University of St Andrews*

5:10 PM (521) **Holographic Plasmonic Tweezing for Dynamic Trapping and Manipulation;** John McCauley¹, Joshua Kolbow¹, Nathan C. Lindquist¹; ¹*Bethel University*

19SPR04: Plasmon-enhanced Techniques *Smoketree A*

Chair: Gregory Wallace

3:50 PM (522) **Hybrid Gold-conductive Metal Oxide Films for Attenuated Total Reflectance Surface Enhanced Infrared Absorption Spectroscopy;** J. J. Burgess¹, Ian Andvaag¹, Tyler Morhart¹, Osai Clarke¹; ¹*University of Saskatchewan*

4:10 PM (523) **Single-molecule Spectrum and Polarization Reshaping by Plasmonic Nanoparticles;** Julie S. Biteen¹; ¹*University of Michigan*

4:30 PM (524) **Single Nanoparticle SPRI for Ultrasensitive Biosensing with Magnetic Hydrogel Nanoparticles;** Robert M. Corn¹, Esther Hussong¹; ¹*University of California Irvine*

4:50 PM (525) **Plasmonic Nanoparticles for Enhanced Nonlinear Photoabsorption Cross-Sections;** Andrea R. Tao¹, Yuan Zeng²; ¹*Dept. of NanoEngineering, UC San Diego*, ²*UC San Diego*

5:10 PM (526) **Rational Design and Synthesis of Tuneable Plasmonic Nanostructures for Sensitive and Direct DNA Mutation Detection by Surface Enhanced Raman Spectroscopy;** Yuan Liu¹, Alison Rodger¹, Yuling Wang¹; ¹*Macquarie University*

JOIN US WEDNESDAY NIGHT AT OUR SPECIAL EVENT FOR ALL SciX ATTENDEES

Name badge required; present your ticket at the door to exchange for two drink tickets.



TECHNICAL PROGRAM - THURSDAY
AWARDS AND PLENARY LECTURES 7:45 AM – 9:00 AM
 Chair: Mary Kate Donais
Primrose A

- 7:45 AM Award Presentations
- 8:00 AM (527) **SAS and Applied Spectroscopy William F. Meggers Award; Reflectance Spectra of Solids & Liquids - Easier to Obtain, Harder to Interpret: The Case for the Optical Constants;** Tim J. Johnson¹, Tanya Myers¹; ¹*Pacific Northwest National Laboratory*
- 8:30 AM (528) **Coblentz Society Clara Craver Award; Have Fun & Impact with in Situ Spectroscopy in the Chemical Industry;** Xiaoyun Chen¹, ¹*The Dow Chemical Company*

TECHNICAL PROGRAM - THURSDAY
ORAL SYMPOSIA 9:15 AM – 10:55 AM

19ATOM07: Atomic Spectroscopy Techniques for Nano & Bioanalysis *Pasadena*

Chairs: Martin Resano, Jose Manuel Costa-Fernandez

- 9:15 AM (529) **AF4 Coupled to ICP-MS/MS and Molecular Detectors for Quantitative Assessment of Nanoparticle Populations Present in Bioconjugate Mixtures;** Jose Manuel Costa-Fernandez¹, Diego Bouzas, Borja Moreira, Laura Cid, Mario Menendez Miranda, Jose Ignacio García Alonso, Jorge Ruiz Encinar; ¹*University of Oviedo / Spain*
- 9:35 AM (530) **SAS Atomic Section Student Award Winner: Single-particle ICP-MS for the Characterization of Nanoparticles: On Recent Improvements in Data Acquisition, Processing, Sensitivity and Dynamic Range;** Ingo Strenge¹, Bastian Franze², Darya Mozhayeva³, Antonio Montoro Bustos⁴, Karen Murphy⁴, Carsten Engelhard³; ¹*University of Siegen / NIST*, ²*TUV Rheinland*, ³*University of Siegen*, ⁴*National Institute of Standards and Technology*
- 9:55 AM (531) **New Developments in the Generic Quantification of Organic Compounds and Biomolecules Using Mass Spectrometry;** Jorge Ruiz Encinar¹, Francisco Calderón-Celiselis¹, Alicia Jiménez Nosti¹; ¹*University of Oviedo*
- 10:15 AM (532) **Copper and Iron Tissue Analysis: Clinical Significance and Analytic Challenges;** Sarah A. Erdahl¹, Jessica Fox¹, Elisabeth Steigerwald¹, Paul Jannetto¹, Joshua Bornhorst¹; ¹*Metals Laboratory / Mayo Clinic*
- 10:35 AM (533) **Dried Blood Spots for Elemental Analysis;** Martin Resano¹, Flavio Nakadi¹, Esperanza Garcia-Ruiz¹, Raul Garde¹, Maite Aramendia², Marcia A.M.S. da Veiga³, M^a Carmen Garcia-Poyo⁵, Christophe Pecheyran⁵, Julio Cruces⁶; ¹*University of Zaragoza*, ²*Centro Universitario de la Defensa, Carretera de Huesca s/n*, ³*Universidade de Sao Paulo*, ⁵*Centre National de la Recherche Scientifique (CNRS), University of Pau*, ⁶*Rafer S.L.*

19AWD04: SAS and Applied Spectroscopy William F. Meggers Award Symposium Honoring Tim Johnson *Mojave*

Chair: Tim Johnson

- 9:15 AM (534) **Accurate Methods to Determine the Optical Constants n/k for Liquids;** Tanya Myers¹, Tim Johnson¹, Russell Tonkyn², Oeck Ashley², John Loring², Catherine Banach², Bruce Bernacki², Steven Smith²; ¹*Pacific Northwest National Laboratory*, ²*PNNL*
- 9:35 AM (535) **Using Reference Spectra in the Form of n/k Values to Enable Improved Opticaltrace Surface Detection: Examples from IARPA'S SILMARILS Program;** Kristin M. Dewitt¹; ¹*Intelligence Advanced Research Projects Activity*
- 9:55 AM (536) **Applications of Optical Constants (n and k) to Standoff Detection of Threat Chemicals;** Robert Furstenberg¹, Christopher Kendziora², R. Andrew McGill²; ¹*US Naval Research Laboratory*, ²*Naval Research Laboratory*
- 10:15 AM (537) **First Principles Calculation of Reflectance Spectra of Solid Materials from N/k Values;** Bradley G. Henderson¹, Christopher Jeffery²; ¹*Los Alamos National Laboratory*, ²*Los Alamos National Lab*
- 10:35 AM (538) **Speaker Roundtable;** Tanya Myers¹, Kristin M. Dewitt², Robert Furstenberg³, Bradley G. Henderson⁴; ¹*Pacific Northwest National Laboratory*, ²*Intelligence Advanced Research Projects Activity*, ³*US Naval Research Laboratory*, ⁴*Los Alamos National Laboratory*

19BIM06: Machine and Deep Learning for Biomedical Diagnostics *Catalina*

Chairs: Thomas Bocklitz, Rohith Reddy

- 9:15 AM (539) **Toward a Thinking Microscope: Deep Learning-enabled Computational Microscopy and Sensing;** Aydogan Ozcan¹, Aydogan Ozcan¹; ¹*UCLA*

TECHNICAL PROGRAM - THURSDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

9:35 AM (540) **Classical Machine Learning and Deep Learning for Multimodal Imaging;** Thomas W. Bocklitz¹, Pranita Pradhan, Olga Chernavskaya, Shuxia Guo, Tobias Meyer, Michael Schmitt, Jürgen Popp¹; ¹*Leibniz-IPHT, Jena, Germany*

9:55 AM (541) **Your Deep Learning Toolbox: Selecting the Appropriate Architecture for Spectral Images;** David Mayerich¹, Sebastian Berisha², Saurabh Prasad², David Mayerich²; ¹*Department of Electrical and Computer Engineering, University of Houston*, ²*University of Houston*

10:15 AM (542) **Deep Representation and Transfer Learning for Infrared Spectral Imaging Data;** Arne Peter Raulf¹, Joshua Butke², Claus Kuepper², Fred Grosserueschkamp², Klaus Gerwert², Axel Mosig²; ¹*Ruhr-University Bochum, PRODI*, ²*Ruhr-University Bochum*

10:35 AM (543) **A Deep Learning Framework for Image Details Beyond the Infrared Spectroscopic Imaging Diffraction Limit;** Kianoush Falahkheirkhah¹, Kevin Yeh¹, Shachi Mittal¹, Rohit Bhargava²; ¹*UIUC*, ²*University of Illinois Urbana-Champaign*

19CHEM07: Chemotyping Complex Materials by Chemometrics *Mesquite E*

Chair: Mengliang Zhang

9:15 AM (544) **Classification of Cultivation Locations of Black Pepper (*Piper Nigrum* L.) Using DART-MS and Chemometrics;** Mengliang Zhang¹, Mengliang Zhang¹; ¹*Middle Tennessee State University*

9:35 AM (545) **Raman Mapping and Multivariate Image Analysis for Characterization of Transdermal Delivery Systems;** Daniel Willett¹, Huzeyfe Yilmaz¹, Anna Wokovich¹, Ahmed Zidan¹, Jason Rodriguez¹, David Keire¹; ¹*U.S. Food and Drug Administration*

9:55 AM (546) **Deconvolving Co-eluted Peaks in GC-MS Fuel Data via EWFA-MCR with Automated Library Matching;** Jeffrey Cramer¹, Mark Hammond¹, Thomas Loegel¹, Kevin Johnson¹, Robert Morris²; ¹*Naval Research Laboratory*, ²*Nova Research Inc.*

10:15 AM (547) **High-coverage and Quantitative Metabolome Analysis for Fingerprinting Complex Biological Samples;** Liang Li¹; ¹*University of Alberta*

19FORENS04: Environmental Forensics *Smoketree A*

Chair: Mark Cejas

9:15 AM (548) **Analysis of PCB and Dioxin/furan Data in Environmental Forensics: Experience and Application;** Glenn W. Johnson¹; ¹*University of Utah*

9:35 AM (549) **Forensic Problem-solving in the Subsurface with Multiple Lines of Evidence;** Mark J. Cejas¹, Ioana Petrisor²; ¹*Pace Analytical Energy Services*, ²*ToxStrategies*

9:55 AM (550) **The Application of Multi-proxy Statistical Techniques in Identifying the Sources, Fate and Transformation of Natural Organic Carbon in South Florida Wetlands;** Alice Chao Ya¹; ¹*KDC/ONE Thibiant international*

10:15 AM (551) **Development of an R-based Implementation of the Polytopic Vector Analysis Mixing Model;** Nicholas D. Rose¹, Timothy Negley¹, Glenn Johnson²; ¹*TIG Environmental*, ²*University of Utah*

10:35 AM (552) **Using Aqueous Geochemical Parameters and Isotopes to Investigate the Source of Surface Water Contamination;** Aaron D. Peacock¹, Aaron Peacock¹; ¹*Microbac Laboratories, Inc.*

19LIBS10: Environmental Monitoring *Smoketree C*

Chair: Cassiana Nomura

9:15 AM (553) **Laser-induced Breakdown Spectroscopy: An Interesting Tool for Monitoring Potentially Toxic Metal in Water;** Cassiana S. Nomura¹, Alexandrina Carvalho², Daniel Silvestre (in memoriam)², Flavio Leme³, Danielle Intima⁴, Juliana Naozuka⁵, Cassiana Nomura²; ¹*Institute of Chemistry - University of Sao Paulo*, ²*IQ-USP*, ³*UFABC*, ⁴*SABESP*, ⁵*UNIFESP*

9:35 AM (554) **Effect of Powder Compact Parameters on LIBS Quantitative Analysis;** Matthieu Baudelet¹, Sudeep Pandey¹, Richard Locke¹, Romain Gaume¹; ¹*University of Central Florida*

9:55 AM (555) **Solid Phase Extraction Combined with Laser-induced Breakdown Spectroscopy to Elemental Analysis;** Ivanise Gaubeur¹, Rodrigo Papai², João Manoel Lima Junior¹, Flavio Leme¹, Ivanise Gaubeur¹; ¹*Universidade Federal do ABC*, ²*Instituto de Pesquisas Tecnológicas (IPT)*

TECHNICAL PROGRAM - THURSDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

10:15 AM (556) **Monitoring the Uptake and Toxicity of Nanoparticles in Plants Using Laser-induced Breakdown Spectroscopy;** Pavel Porizka¹, Pavlina Modlitbova¹, Sara Stritezka¹, Karel Novotny², Jozef Kaiser¹; ¹Brno University of Technology, ²Masaryk University

10:35 AM (557) **Analysis of Plant Leaves Using Laser Ablation: Optical Emission Spectrometry;** Jhanis J. Gonzalez¹, Jose Chirinos², Dayana Oropeza², Vassilia Zorba², Rick Russo³; ¹Applied Spectra, Inc. / Lawrence Berkeley National Laboratory, ²LBNL, ³LBNL/Applied Spectra, Inc.

19PAT01: SAS PAT Technical section: PAT in the Pharmaceutical Industries Session I *Smoketree D*

Chair: Jim Rydzak

9:15 AM (558) **Interfacing PAT Sensors with Processing Equipment;** Steve Hammond¹, Phil Doherty¹; ¹Expo Pharma

9:35 AM (559) **Quantitative In-process Raman Measurements of Solids During Continuous or Batch Manufacturing Operations;** Karen A. Esmonde-White¹, Maryann Cuellar¹, Carsten Uerpmann², Sean J. Gilliam¹, Dave Strachan¹, Ian Lewis¹; ¹Kaiser Optical Systems, Inc., ²Kaiser Optical Systems SARL

9:55 AM (560) **In-Process Control Assessment of Final Blend Potency Using Loss-in-Weight Feeders and Near Infrared Analysis;** Caitlin Schram¹, Matt Kiesz, Sara Manteiga, Alex Clifford, Justin Pritchard, Kelly Swinney; ¹Vertex Pharmaceuticals

10:15 AM (561) **Distillation Process Understanding from In-situ Headspace Vapor Condensate Monitoring with Infrared Spectroscopy and Computational Modeling;** Charles Goss¹, Laura Wehmeyer¹, Rachel Janes²; ¹GlaxoSmithKline, ²Rowan University

10:35 AM (562) **Multi-spectroscopic Analysis of Crystallization Processes at Extreme Environmental Conditions;** Patrick Krebs¹, Robert Stach¹, Franca Jones², Boris Mizaikoff³; ¹Universität Ulm, ²Curtin University, ³Ulm University / Institute of Analytical and Bioanalytical Chemistry

19PMA05: Atomic Spectroscopy Applications in Pharmaceuticals *Madera*

Chair: Sharla Wood

9:15 AM (563) **Analysis of Common Counter-ions in Pharmaceuticals by XRF;** Sharla Wood¹, Keegan Hoose², Lydia Breckenridge¹; ¹Bristol-Myers Squibb, ²Lake Superior State University

9:35 AM (564) **Ion Chromatography for Determining Metals in Pharmaceuticals;** Jeff Rohrer¹, Jeff Rohrer¹; ¹Thermo Fisher Scientific

10:15 AM (565) **Determination of Total Vitamin B12 in Infant Formula by LC-ICP-MS;** Lee Yu¹, Laura Regalado Contreras¹; ¹National Institute of Standards and Technology

10:35 AM (566) **Speaker Roundtable;** Sharla Wood¹, Jeff Rohrer², Lee Yu³; ¹Bristol-Myers Squibb, ²Thermo Fisher Scientific, ³National Institute of Standards and Technology

19RAM02: Raman Spectroscopic Sensing *Ventura*

Chair: Torsten Frosch

9:15 AM (567) **Surface Enhanced Resonance Raman Spectro-electrochemistry for Target Specific Analysis;** Inez Weidinger¹, Ibrahim Halil Oener¹, Fabian Kruse¹, Huong Khoa Ly²; ¹Technische Universitaet Dresden, ²halil.oener@tu-dresden.de

9:35 AM (568) **New Developments in Raman Gas Sensing for Energy and Environmental Research;** Torsten Frosch¹, Anne Sieburg², Andreas Knebl², Timea Frosch², Juergen Popp², Torsten Frosch²; ¹Leibniz Institute of Photonic Technology, Jena; ²Institute of Physical Chemistry & Abbe Center of Photonics, Friedrich Schiller University, Jena, ³Leibniz Institute of Photonic Technology

9:55 AM (569) **Early Disease Detection by Raman Spectroscopy over Quantitative Polymerase Chain Reaction in Plant Disease Diagnostics;** Dmitry Kurouski¹, Dmitry Kurouski; ¹Texas A&M University

10:15 AM (570) **Enhancing DUV Raman Sensing and Imaging with Surface Plasmons;** Atsushi Taguchi¹; ¹Hokkaido University

10:35 AM (571) **Deuterium Uptake as Raman-based Antibiotic Susceptibility Test in a Clinical Scenario;** Christoph Haisch¹, David Bauer², Li Qui², Giuseppe Magistro³, Christian Stief³, Andreas Wieser³; ¹TU Munich, ²Technical University of Munich, ³Ludwig-Maximilians-University Munich

TECHNICAL PROGRAM - THURSDAY

ORAL SYMPOSIA 9:15 AM – 10:55 AM

19RAM15: Spatially Offset Raman Spectroscopy (SORS)

Sierra

Chair: Pavel Matousek

- 9:15 AM (572) **Surface-enhanced Spatially Offset Raman Spectroscopy for in Vivo Neurochemical Detection;** Bhavya Sharma¹; ¹*University of Tennessee*
- 9:35 AM (573) **In Vivo Imaging of Cancer Using Surface Enhanced Spatially Offset Raman Spectroscopy (SESORS);** Fay Nicolson¹, Fay Nicolson¹, Bohdan Andreiuk¹, Chrysafis Andreou², Hsiao-Ting Hsu³, Scott Rudder⁴, Moritz Kircher¹; ¹*Dana-Farber Cancer Institute*, ²*University of Cyprus*, ³*Memorial Sloan Kettering Cancer Center*, ⁴*Innovative Photonics Solutions*
- 9:55 AM (574) **Sensitivity of Transmission Raman Spectroscopy Signals to Temperature of Biological Tissue;** Adrian Ghita¹, Pavel Matousek², Nick Stone¹; ¹*University of Exeter*, ²*Science and Technology Facilities Council*
- 10:15 AM (575) **Spatially Offset and Transmission Raman Spectroscopy for Determination of Depth of Inclusion in Turbid Matrix;** Sara Mosca¹, Priyanka Dey², Tanveer A. Tabish², Francesca Palombo², Nick Stone², Pavel Matousek³; ¹*RAL, CLF, STFC*, ²*University of Exeter*, ³*Science and Technology Facilities Council*
- 10:35 AM (576) **Offset Geometry for Deep Tissue Raman Imaging with OCT;** Mingzhou Chen¹, Kishan Dholakia¹; ¹*University of St Andrews*

19SPECIAL06: SAB Special Session Chino AB

Chairs: Sara Tufi, Alessandro De Giacomo

- 9:15 AM (577) **Local Thermodynamic Equilibrium in a Laser-induced Plasma Evidenced by Blackbody Radiation;** Jörg Hermann¹, Jörg Hermann², David Grojo², Emanuel Axente³, Valentin Craciun³; ¹*French National Centre for Scientific Research (CNRS)*, ²*French National Center for Scientific Research (CNRS)*, ³*Romanian National Institute for Lasers, Plasma and Radiation Physics*
- 9:35 AM (578) **Investigation of the Atomization Mechanism of Gold Nanoparticles in Graphite Furnace Atomic Absorption Spectrometry;** Kerstin Leopold¹, Anja Brandt¹, Dominic Brucker¹; ¹*Ulm University*

- 9:55 AM (579) **Quantification of Water Content by Laser Induced Breakdown Spectroscopy on Mars;** William Rapin¹, Pierre-Yves Meslin, Sylvestre Maurice, Roger C Wiens, Didier Laporte, Boris Chauvire, Olivier Gasnault, Susanne Schroder, Pierre Beck, Steve Bender, Olivier Beyssac, Agnes Cousin, Erwin Dehouck, Christophe Drouet, Olivier Forni, Marion Nachon, Noureddine Melikechi, Benjamin Rondeau, Nicolas Mangold, Nancy H Thomas, Jeremie Lasue, Cécile Fabre, Jens Frydenvang, Jean-Luc Lacour; ¹*Caltech*
- 10:15 AM (580) **Depth Profile Analyses with Sub 100-nm Depth Resolution of a Metal Thin Film by Femtosecond - Laser Ablation - Inductively Coupled Plasma - Time-of-flight Mass Spectrometry;** Debora Käser¹, Lyndsey Hendriks², Joachim Koch¹, Detlef Günther¹; ¹*ETH Zurich*, ²*ETH Zurich / *currently TOFWERK, Thun, Switzerland*
- 10:35 AM (581) **Editing Spectrochimica Acta Part B: Personal Reflections and Considerations on the Development of Analytical Spectroscopy;** Nicolò Omenetto¹; ¹*University of Florida*

19SPECIAL07: New Developments in Measurement Science Smoketree B

Chair: Garth Simpson

- 9:15 AM (582) **Spectroscopy, whales, lifespan, phospholipids and the cause and cure for cataracts;** Douglas Borchman¹; ¹*University of Louisville*
- 9:35 AM (583) **The coffee ring effect for tap water fingerprinting;** Rebecca H. Lahr¹, Xiaoyan Li¹; ¹*Michigan State University*
- 9:55 AM (584) **An Electroanalytical Technique to Monitor Oxide Reduction Processes for Nuclear Safeguards;** Ammon Williams¹, Guoping Cao¹, Michael Shaltry¹, Jeff Sanders¹; ¹*Idaho National Laboratory*
- 10:15 AM (585) **Langmuir-Blodgett Films of Two-Dimensional Metal-Organic Frameworks;** Fangyuan Tian¹, Kristi Ishihara¹; ¹*California State University Long Beach*

TECHNICAL PROGRAM - THURSDAY
POSTER SESSION 11:00 AM – 12:00 PM
Primrose Foyer

See page 90 for Thursday posters by category. Posters will be displayed all day and attended again in the afternoon.

TECHNICAL PROGRAM - THURSDAY
ORAL SYMPOSIA 1:30 PM – 3:10 PM

19ATOM08: Atomic Spectroscopy Techniques for Clinical/Medical Pasadena

Chair: C Derrick Quarles

- 1:30 PM (586) **Accurate Quantification of Carboplatin Adducts with Serum Albumin by Monolithic Chromatography Coupled to ICP-MS with Isotope Dilution Analysis;** Christian L. Ward-Deitrich¹, Raquel Larios², M. Estela del Castillo Busto³, Daniel Garcia-Sar⁴, Heidi Goenaga-Infante³; ¹*UK National Measurement Laboratory (NML)*, ²*Agilent Technologies, Spain*, ³*LGC Ltd., UK*, ⁴*AGQ Labs, Spain*
- 1:50 PM (587) **Automated Sample Preparation Techniques for Clinical Analyses Using a Single Platform Sample Introduction System;** C Derrick Quarles¹; ¹*Elemental Scientific, Inc.*
- 2:10 PM (588) **Copper Isotopic Composition as an Indicator of Changes in Copper Processing in the Colon of Mice Due to Antibiotic Treatment;** Kerri A. Miller¹, Fernando A. Vicentini¹, Simon A. Hirota¹, Keith A. Sharkey¹, Michael Wieser¹; ¹*University of Calgary*
- 2:30 PM (589) **Gd-based Contrast Agents: A Clinically Significant Analytical Interference in ICP-MS Elemental Analysis;** Patrick Day¹, Sarah Erdahl¹, Steve Eckdahl¹, Joshua Bornhorst¹, Paul Jannetto¹; ¹*Mayo Clinic*
- 2:50 PM (590) **Enriched Stable Isotope Tracers in Medical Applications;** Johanna Irrgeher¹, Thomas Berger², Matthias Klose³, Christine Oppen¹, Thomas Prohaska¹; ¹*Montanuniversitaet Leoben*, ²*GLOCK Health, Science and Research G.m.b.H.*, ³*Glock*

19AWD11: Clara Craver Award Symposium Honoring Shawn Chen Mojave

Chair: Xiaoyun Chen

- 1:30 PM (591) **Molecular Structures of Buried Interfaces Involving Polymers;** Zhan Chen¹; ¹*University of Michigan*
- 1:50 PM (592) **Industrial Spectroscopist: The Joys and Challenges of Delivering Solutions;** Katherine A. Bakeev¹; ¹*B&W Tek LLC*
- 2:10 PM (593) **Theoretical Support to Industrial Spectroscopy Application;** William Wang¹; ¹*Lubrizol*
- 2:30 PM (594) **Agricultural Spray Droplet Characterization Using Raman Chemical Imaging;** Michael M. Bishop¹, Abrin Schmucker²; ¹*Corteva*, ²*Corteva Agriscience*
- 2:50 PM (595) **Measuring the Infrared Absorption and Scattering Coefficients of Polymeric Foams;** Mark Rickard¹, Anson Wong¹, Brian Meldrum¹; ¹*DuPont*

19BIM07: New Frontiers in Biomedical Analysis Catalina

Chair: David Mayerich

- 1:30 PM (596) **Dielectrophoretic Differentiation of Klebsiella pneumoniae Based on Antibiotic Resistance;** Shannon Huey Hilton¹, Mark Hayes¹; ¹*Arizona State University*
- 1:50 PM (597) **Isolation and Fractionation of Extracellular Vesicles by Size & Immuno-based Asymmetric Nanopore Membrane Filtration;** Ceming Wang¹, Chenguang Zhang¹, Satyajyoti Senapati², Hsueh-Chia Chang¹; ¹*University of Notre Dame*, ²*University Of Notre Dame*
- 2:10 PM (598) **Noninvasive Manipulation of Cells and Chemicals within Live Cultures via Addressable Microfluidics;** Anh Tong¹, Long Quang Pham¹, Vatsal Shah¹, Paul Abatemarco¹, Roman Voronov¹; ¹*New Jersey Institute of Technology*
- 2:30 PM (599) **Microfluidic Platform for Biomarker Detection; from Maternal Disease to Cancer;** Zeinab Ramshani¹, Chenguang Zhang¹, Satyajyoti Senapati¹, Hsueh-Chia Chang¹; ¹*University of Notre Dame*

TECHNICAL PROGRAM - THURSDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

19CHEM02: Exploiting Spatial and Spectral Information in Hyperspectral Images *Mesquite E*

Chair: Thomas Bocklitz

- 1:30 PM (600) **Very Important Pixels in MCR Analysis of Hyperspectral Images;** Cyril Ruckebusch¹, Cyril Ruckebusch², Mahdyieh Ghaffari², Nemat Omidikia³; ¹*LASIR CNRS UNIV LILLE*, ²*U LILLE LASIR CNRS*, ³*U. Systan and Baluchestan*
- 1:50 PM (601) **Can Deep Learning Beat Model-based Pre-processing of Infrared Spectral Data of Cells and Tissues?;** Uladzislau Blazhko¹, Johanne Solheim², Stanislaw Trukhan², Valeria Tafintseva², Volha Shapaval², Vassili Kovalev³, Achim Kohler²; ¹*NMBU*, ²*Norwegian University of Life Sciences*, ³*United Institute of Informatics Problems of the NAS of Belarus*
- 2:10 PM (602) **Chemical Imaging Modalities Combined with Chemometrics for Characterization of Interfacial Water: Potential and Current Challenges;** Junli Xu¹, Aoife Gowen¹; ¹*University College Dublin*
- 2:30 PM (603) **A Comparison of ANNS, SVMS, and XGBoost in Challenging Classification Problems;** Manuel A. Palacios¹, Donal O'Sullivan¹, Barry M. Wise¹; ¹*Eigenvector Research Inc.*
- 2:50 PM (604) **Investigations on the Data Analysis Pipeline Raman Spectroscopic Imaging;** Thomas W. Bocklitz¹, Nairveen Ali¹, Shuxia Guo, Mehul Chhallani, Jürgen Popp; ¹*Leibniz-IPHT, Jena, Germany*

19IR01: Optical Photothermal Infrared Spectroscopy I *Smoketree E*

Chairs: Curtis Marcott, Andrea Centrone

- 1:30 PM (605) **Bone and Ligament Structure and Failure as Studied by Photothermal Infrared Microscopy;** Mark Banaszak-Holl¹; ¹*Monash University*
- 1:50 PM (606) **Photothermal Infrared Spectroscopy: Growing Applications for Polymers and Materials Analysis;** Dennis J. Walls¹, Dennis Walls¹, Kathy Murschell¹; ¹*DuPont*
- 2:10 PM (607) **Biomedical Applications of Photothermal Spectroscopic Imaging;** Rohith Reddy¹, Chalapathi Gajjala¹, Licheng Zhang¹, David Mayerich¹, Rohith Reddy¹; ¹*University of Houston*

- 2:30 PM (608) **Investigation of Breast Calcification Microstructure in Ductal Carcinoma in Situ Using Multi-modal Spectroscopy;** Jayakrupakar Nallala¹, Doriana Calabrese¹, Sarah Gosling², Mustafa Kansiz³, Ferenc Borondics⁴, Jeffrey Marks⁵, Lorraine King⁵, Shelley Hwang⁵, Keith Rogers², Nick Stone¹; ¹*University of Exeter*, ²*Cranfield University*, ³*Photothermal Spectroscopy Corp.*, ⁴*Soleil Synchrotron*, ⁵*Duke University School of Medicine*
- 2:50 PM (609) **Recent Advances Is Submicron Photothermal Infrared Spectroscopy and Imaging;** Curtis Marcott¹; ¹*Light Light Solutions*

19LIBS06: Forensics and Security *Smoketree C*

Chair: Jose Almirall

- 1:30 PM (610) **Using LIBS for Elemental Signature Discovery in Forensic Applications;** Tatiana Trejos¹, Tatiana Trejos², Luis Arroyo², Emily Haase², Courtney Vander Pyl², Korina Menking-Hoggatt²; ¹*West Virginia University Department of Forensic and Investigative Science*, ²*WVU*
- 1:50 PM (611) **Improving the Forensic Relevance of LIBS by Quantifying Spectral Interferences;** Matthieu Baudelet¹, Jessica Chappell¹, Mauro Martinez¹; ¹*University of Central Florida*
- 2:10 PM (612) **Analysis of Nuclear Material with Heterogeneous Isotopic Composition by Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS) and Laser Induced Breakdown Spectroscopy (LIBS) Tandem System;** Jhanis J. Gonzalez¹, Andrew Duffin², Charles Sisson³, Juan Carlos Guerrero³, Alan Koenig³, Xianglei Mao⁴, Greg Eiden², Rick Russo³; ¹*Applied Spectra, Inc. / Lawrence Berkeley National Laboratory*, ²*PNNL*, ³*Applied Spectra, Inc.*, ⁴*LBNL*
- 2:30 PM (613) **Forensic Application of Micro-XRF: Glass Analysis;** Sergey Mamedov¹; ¹*HORIBA Instruments Incorporated*
- 2:50 PM (614) **Signal Processing of Handheld Libs-raman-xrf Multisensor Data for Soil Analysis;** Richard R. Hark¹, Chandra S. Throckmorton², Russell S. Harmon³, Karen A. Harmon³, John R. Plumer⁴, Jay L. Clausen⁵, Michael J. Morgan⁵, Jan M. H. Hendrickx⁶, James B. Harrison⁶; ¹*Institute for the Preservation of Cultural Heritage, Yale University*, ²*Signal Analysis Solutions*, ³*JRPlumer Associates*, ⁴*JRPumer Associates*, ⁵*USACE ERDC-CRREL*, ⁶*SoilHydrologyAssociates*

TECHNICAL PROGRAM - THURSDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

19MASS05: Mass Spectrometry of In-tact Proteins and Protein Complexes *Smoketree B*

Chair: Kermit Murray

- 1:30 PM (615) **Native ion-mobility mass spectrometry of *Staphylococcus aureus* α -hemolysin**; Jesse W. Wilson¹, Amber D. Rolland¹, Grant M. Klausen¹, James S. Prell¹; ¹*University of Oregon*
- 1:50 PM (616) **Direct Electrospray Photochemical Oxidation of Proteins**; Kermit K. Murray¹, Remilekun Lawal¹, Oluwatosin Ogundairo¹, Fabrizio Donnarumma¹; ¹*Louisiana State University*
- 2:10 PM (617) **Structural analysis of isolated heme protein based on gas-phase resonance Raman spectroscopy: Identification of the oxidation state, spin state, and coordination**; Hiroya Asami¹, Akihiro Kitazaki¹, Norishi Kawauchi¹, Jun-ya Kohno¹; ¹*Gakushuin University*
- 2:30 PM (618) **Determining what really counts: Modeling and measuring nanoparticle number concentrations**; Antonio R. Montoro Bustos¹, Elijah Petersen¹, Blaza Toman¹, Monique Johnson¹, Mark Ellefson², George Caceres¹, Anna Neuer³, Qilin Chan², Jonathan Kemling², Brian Mader², Karen Murphy¹, Matthias Roesslein³; ¹*NIST*, ²*3M*, ³*EMPA*

19PAT02: SAS PAT Technical section: PAT in the Biopharmaceutical Industries Session II *Smoketree D*

Chairs: Daniel Hill, Daniel Hill

- 1:30 PM (619) **Enabling Process Optimization, Scale-up and Technical Transfer Using Raman Spectroscopy in Production Bioreactors**; Karin M. Balss¹, Christopher Mahoney¹, Robert O'Brien¹, Wan Su¹, Nicholas Jacobyansky¹, David Latsahw¹, Emily Curtis¹, christopher Casey¹, felix Goldschmidt¹, simon Taennler¹, Olav Lyngberg¹, Olav Lyngberg¹; ¹*Janssen*
- 1:50 PM (620) **Streamlining CHO Cell Culture Process Development Using a Generic Model for Glucose Determination**; Kurtis Denny¹, Thomas Matthews¹, Chelsea Worley¹, Branigan Wheeler¹; ¹*Biogen*
- 2:10 PM (621) **Use of Integrated Process Models Towards Data Driven Risk Assessments and Optimized Characterization**; Christopher Mark Taylor¹, Christoph Herwig¹; ¹*Exputec GmbH*

- 2:30 PM (622) **A Hybrid Modeling Approach Using Monod Kinetics to Model Growth and Data Driven Methods for Modeling Protein Production and Product Quality Focusing on Analysis of Specific Consumption/secretion of Metabolites**; Chris McCready¹; ¹*Sartorius Corporate Research*
- 2:50 PM (623) **Fault Detection and Oligonucleotide Sequence Identification using an ATR-FTIR/Conductivity-based PAT Measurement System**; Daniel R. Hill¹; ¹*Biogen, Inc.*

19PMA10: Enable Intensified Downstream Manufacturing by Advanced Online Sensor Technologies *Madera*

Chair: Richard Wu

- 1:30 PM (624) **Raman as an Effective Tool in Downstream Measurements**; Sean J. Gilliam¹, Gregg Schorner², Tony Wang², Maryann Cuellar¹, David Strachan¹, Hervé Lucas³, Carsten Uerpman³; ¹*Kaiser*, ²*Amgen*, ³*Kaiser SARL*
- 1:50 PM (625) **Variable Pathlength Spectrophotometry as a PAT Tool for Downstream Processes**; Ramsey Shanbaky¹; ¹*C Technologies, inc.*
- 2:10 PM (626) **Raman Spectroscopy for Bioprocesses: How Hardware, Sampling and Data Analysis Decisions Drive Success**; Brian Marquardt¹, Sergey Mozharov¹; ¹*MarqMetrix Inc.*
- 2:30 PM (627) **Turning off "Autopilot" on an Adaptive, Handheld Raman Spectrometer**; Robert C. Brush¹, Lin Chen¹, Dean Stuart¹, Lin Zhang¹, Wayne Jalenak¹, Michael Hargreaves¹; ¹*Thermo Fisher Scientific*
- 2:50 PM (628) **Raman Spectroscopy in Biosensing**; Mehran Mojarad¹, Jim Loussaert¹, Robert Soto², David Semin¹, Heejin Lee¹; ¹*Amgen, Inc.*

19RAM04: Industrial Raman *Sierra*

Chair: Karen Esmonde-White

- 1:30 PM (629) **Real-time Monitoring of Amino Acid Consumption in CHO Fed-batch Production Media by Raman Spectroscopy and Regression Models**; Christopher Mahoney¹, Robert O'Brien¹, Nicholas Jacobyansky¹, Wan Su¹, Olav Lyngberg¹, Karin Balss¹; ¹*Janssen Pharmaceuticals*
- 1:50 PM (630) **Raman Spectroscopy: A Process Control Tool in Enzymatic Protein Hydrolysis**; Ulrike Böcker¹, Nils Kristian Afseth², Ingrid Måge², Jens Petter Wold², Sileshi Wubshet²; ¹*Nofima - Norwegian Institute of Food, Fisheries and Aquaculture Research*, ²*Nofima*

TECHNICAL PROGRAM - THURSDAY

ORAL SYMPOSIA 1:30 PM – 3:10 PM

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| <p>2:10 PM (631) Identification and Verification of Dietary Supplement Raw Materials and Finished Goods Using Handheld Raman Spectroscopy; <u>Mohamed Koroma</u>¹; ¹<i>Pharmavite LLC</i></p> <p>2:30 PM (632) Raman Concatenation for Enhanced Process Control in Biomedical, Pharmaceutical & Petrochemical Applications; <u>Scott Rudder</u>¹; ¹<i>Innovative Photonic Solutions</i></p> <p>2:50 PM (633) Industrial Applications of Raman Spectroscopy; <u>William Wang</u>¹; ¹<i>Lubrizol</i></p> | <p>2:30 PM (637) Drug Product Identification and Physical Stability Analysis by Transmission Raman Based Chemometrics; <u>Ashish Punia</u>¹, James Ormes¹, Michael McNevin¹, Matthew Lamm¹; ¹<i>Merck & Co., Inc.</i></p> <p>2:50 PM (638) Quantification and Control of Amorphous Contents by Raman. Applications and Case Studies in Pharmaceutical Processing; <u>Michelle S. Raikes</u>¹, Fredrik Nordstrom¹; ¹<i>Boehringer Ingelheim Pharmaceuticals</i></p> |
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19RAM14: Transmission Raman Spectroscopy *Ventura*

Chair: Mark Mabry

- 1:30 PM (634) **Evaluation of a Low Cost Portable Transmission Raman System for Content Uniformity Analysis of Solid Pharmaceutical Dosage Forms;** Jun Zhao¹, Katherine Bakeev¹, Kristen Frano¹, Pedro Martinez², Rodolfo Romanach², Maritza Reyna², Ana Moya², Adriluz Sanchez², Carlos Ortega², Faviola Villariny²; ¹*B&W Tek*, ²*University of Puerto Rico, Mayagüez Campus*
- 1:50 PM (635) **Comparison of Raman Imaging and Transmission Raman Spectroscopy Results on a Pharmaceutical Tablet;** Tim Prusnick¹; ¹*Renishaw Inc.*
- 2:10 PM (636) **Transmission Raman Spectroscopic Quantification of Active Pharmaceutical Ingredient in Coated Tablets of Hot-melt Extruded Amorphous Solid Dispersion;** Yemin Liu¹, Jayanth Doddi¹, Yanbing Zheng¹, Vivien Ho, Maurice Pheil¹, Yi Shi¹; ¹*AbbVie Inc*

19SPR03: Plasmon and Imaging: Catalysis *Smoketree A*

Chair: Zachary Schultz

- 1:30 PM (639) **Tailoring Plasmons and Interfaces Toward Optimized Hot Electron Generation and Injection;** Laura Fabris¹, Supriya Atta¹, Ashley Pennington², Fuat E. Celik¹; ¹*Rutgers University*, ²*Naval Research Laboratory*
- 1:50 PM (640) **Catalytic Nanoparticles as Labels for Biosensing;** Xiaohu Xia¹; ¹*University of Central Florida*
- 2:10 PM (641) **Quantifying Plasmon-generated Hot Carrier Energies;** Katherine Willets¹; ¹*Temple University*
- 2:30 PM (642) **Imaging Plasmons with Electrons: Coupling Molecular Vibrations and Infrared Plasmons;** Jon Camden¹, Jon Camden¹; ¹*University of Notre Dame*
- 2:50 PM (643) **Hybrid Plasmonic/semiconductor Materials for CO2 Reduction;** Zachary Schultz¹; ¹*The Ohio State University*

TECHNICAL PROGRAM - THURSDAY

POSTER SESSION 3:10 PM – 3:50 PM

Primrose Foyer

See page 90 for a listing of Thursday posters by category. Student poster award winners will be announced the following morning during the plenary session.

TECHNICAL PROGRAM - THURSDAY
19AWD10: FACSS INNOVATION AWARDS 3:50 PM – 5:30 PM
Chair: Mary Kate Donais
Primrose A

- 3:50 PM (644) **Accelerated Restricted Boltzmann Machines**; Peter B. Harrington¹; ¹*Center for Intelligent Chemical Instrumentation, OHIO University*
- 4:10 PM (645) **Molecular Basis for Chirality-regulated A β Self-assembly and Receptor Recognition Revealed by Ion Mobility-mass Spectrometry**; Gongyu Li¹, Lingjun Li²; ¹*University of Wisconsin-Madison*, ²*UW-Madison*
- 4:30 PM (646) **Chemical Approaches to Improve Nanopore Single-Molecule Sensing**; Jason R. Dwyer¹, James Hagan¹; ¹*University of Rhode Island*
- 4:50 PM (647) **Enhancing Enantioselective Absorption with Plasmonic and Dielectric Metasurfaces**; John M. Abendroth¹, Michelle Solomon¹, Jack Hu¹, Lisa Poulikakos¹, Amr Saleh¹, Yang Zhao², Jennifer Dionne¹; ¹*Stanford University*, ²*University of Illinois at Urbana-Champaign*

TECHNICAL PROGRAM - FRIDAY
FACSS INNOVATION AWARD PRESENTATION
AND CLOSING PLENARY 7:45 AM – 10:00 AM
Chair: Garth Simpson
Sierra-Ventura

- 7:45 AM 2019 FACSS Innovation Award Presentation
Closing Plenary: Data Science Meets Measurement Science
- 8:00 AM (648) **Phase Engineering for Targeted Super-Resolution Applications**; Christy Landes¹; ¹*Rice University*
- 8:30 AM (649) **Multiplexing spatial and hyperspectral imaging with dynamically structured illumination**; Randy Bartels¹; ¹*Colorado State University*
- 9:00 AM (650) **Spectral deep learning for prediction and prospective validation of functional groups for autonomous instrumentation**; Gaurav Chopra¹, Jonathan Fine¹, Armen Beck¹, Anand Rajasekar²; ¹*Purdue University*, ²*Indian Institute of Technology, Madras*
- 9:30 AM **Preview of 2020**
Linda Kidder-Yarlott, General Chair
Mary Kate Donais, Program Chair

TECHNICAL PROGRAM – MONDAY POSTERS
POSTERS SESSIONS 9:45 AM - 10:45 AM & 3:10 PM - 3:50 PM

Primrose Foyer; Hang posters 8:30-9:30 AM; Remove at 4:00 PM

19MP-AES: MONDAY POSTERS: AES

(M-P1) **Design of Custom Electrical Signals for fine-tuning dielectrophoretic particle separations;** Cody J. Lentz¹, Blanca H. Lapizco-Encinas¹, Samuel Hidalgo-Caballero²; ¹Rochester Institute of Technology, ²Benemérita Universidad Autónoma de Puebla, Mexico

(M-P2) **Quantifying miRNA Transience in On-Chip Myocardial Infarctions;** Stuart R. Blood¹, Hsueh-Chia Chang¹; ¹University of Notre Dame

(M-P3) **Microparticle Separations using Cascade Devices;** Nicole Hill¹, Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology

(M-P4) **Characterization of Exosomes and Nanoparticles Using Biphasic Nanopore Resistive Signals.;** Sebastian Sensale¹, Vivek Yadav¹, Hsueh-Chia Chang¹; ¹University of Notre Dame

(M-P5) **Insulator-based Dielectrophoresis to Characterize the Electrokinetic Behavior of Bacterial and Yeast Cells and Create a Library;** Adriana Coll De Peña¹, Anutthaman Parthasarathy¹, Abbi Miller¹, Andre O. Hudson¹, Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology

(M-P6) **Carbon-electrode Dielectrophoresis to Identify Candida Strains;** Emma A. Barnett¹, Max Vogel¹, Carly Hammond¹, Cora Bisbee¹, Devin Keck¹, Rodrigo Martinez-Duarte¹; ¹Clemson University

(M-P7) **3D Carbon-electrode Dielectrophoresis to Identify Candida Dubliensis;** Emma A. Barnett¹, Devin Keck¹, Rodrigo Martinez-Duarte¹; ¹Clemson University

(M-P8) **The Investigation of Phenolic Acids to Increase UV-detection of Titanium Dioxide Nanoparticles in Capillary Electrophoresis;** Madison R. Noroña¹, Ana Clara Fernandes², Dosil Pereira de Jesus², Carlos García³; ¹San Diego State University, ²Universidade Estadual de Campinas, ³Clemson University

(M-P9) **Using Capillary Isoelectric Focusing to Differentiate between Fresh and Stored Red Blood Cells to Aid in the Detection of Blood Doping;** Adrian Colazo¹, Madison R. Noroña¹, Christopher R. Harrison¹; ¹San Diego State University

(M-P10) **High-throughput Deterministic Ratchet Devices for Organelle Separation;** Mukul Sonker¹, Dai Hyun Kim², Alexandra Ros³; ¹The Biodesign Institute, Arizona State University, ²Arizona State University / Biodesign Institute, ³Arizona State University / The Biodesign Institute

(M-P11) **Impedance Spectroscopy Based Evaluation of Phytoplankton Health;** Margaret Jett¹, Karina Henson¹, Mohamed Rashed¹, Susan Hendricks², Stuart Williams¹; ¹University of Louisville, ²Murray State University

(M-P12) **Concentration and Characterization of Proteins by DC-iDEP;** Yameng Liu¹, Mark Hayes¹; ¹Arizona State University

(M-P13) **A Novel Method to Determine the Dielectric Properties of a Cell Population with Optoelectronic Tweezers;** Devin Keck¹, Rodrigo Martinez-Duarte¹; ¹Clemson University

(M-P15) **Electrokinetic characterization and sorting of protein nanoparticles;** Cody J. Lentz¹, Daniel Quevedo², Joerg Lahann², Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology, ²University of Michigan - Ann Arbor

(M-P16) **High-Resolution 3D-Printed Microfluidic Devices for Dielectrophoretic Applications;** Mohammad Towshif Rabbani¹, Mukul Sonker², Jorvani C. Villarreal³, Alexandra Ros³; ¹Arizona State University, ²The Biodesign Institute, Arizona State University, ³Arizona State University / The Biodesign Institute

(M-P17) **Characterization of PHMB as a dynamic capillary coating for fused silica capillaries;** Jessica Torres¹, Christopher R. Harrison¹; ¹San Diego State University

(M-P18) **Improving the Streaming Dielectrophoresis (DEP) Model Based on Various Geometric Electrode Arrays;** Sindora R. Baddam¹, Rodrigo Martinez-Duarte¹; ¹Clemson University

(M-P19) **Portable immersed AC Electrospray (iACE) using single and double barrel glass micropipettes for cell encapsulation and material synthesis;** Vivek Yadav¹, Zehao Pan², Satyajyoti Senapati², Hsueh Chia Chang¹; ¹University of Notre Dame, ²University Of Notre Dame

(M-P20) **High Resolution Separations of Neural Stem and Progenitor Cells;** Yameng Liu¹, Mark Hayes¹; ¹Arizona State University

(M-P21) **Electrically Triggered Water-in-Oil Droplets for Sample Reduction in Serial Femtosecond Crystallography;** Dai Hyun Kim¹, Austin Echelmeier², Jorvani C. Villarreal², Sahir Gandhi², Sebastian Quintana², Alexandra Ros²; ¹Arizona State University / Biodesign Institute, ²Arizona State University / The Biodesign Institute

(M-P22) **Microparticle Separations using Dielectrophoresis Chromatography;** Nicole Hill¹, Blanca H. Lapizco-Encinas¹; ¹Rochester Institute of Technology

(M-P23) **Multiplexed In-situ Profiling of Tissue-specific Gene Expression in Whole C. elegans by Ion Concentration Polarization Enhanced smFISH;** Gongchen Sun¹, Jason Wan¹, Hang Lu¹; ¹Georgia Institute of Technology

(M-P47) **Characterization and design guidance for chemical stripping of immobilized protein targets in microfluidic hydrogel scaffolds for multiplex target detection;** Anjali Gopal¹, Amy E. Herr¹; ¹UC Berkeley

19MP-IR: MONDAY POSTERS: MOLECULAR (IR)

(M-P24) **Optimization of Turn-Key Tools for Entry Level Users of Electrochemical ATR-SEIRAS;** J.J. Burgess¹, Jessica Sigrist², Erick S. Lins¹, Tyler Morhart², Jenni Briggs³; ¹University of Saskatchewan, ²Jackfish SEC, ³PIKE Technologies

(M-P25) **IR Spectroscopy combined with Porous SiO₂ and TiO₂: Trace Analysis, Adsorption Processes and Catalytic Reaction Monitoring;** Bernhard Lendl¹, Bettina Baumgartner², Jakob Hayden², Greta Haselmann³, Jérôme Loizillon⁴, David Grosso⁴, Dominik Eder²; ¹Technische Universität Wien, ²TU Wien, ³RWTH Aachen, ⁴Aix-Marseille Université

(M-P26) **Structural and Optical Characteristics of Aqueous Solutions of Ethanol, Dimethyl Formamide and Tetrahydrofuran;** Shukur Gofurov¹, Urol Makhmanov¹, Abdulmutallib Kokhkhharov², oksana B. Ismailova³; ¹Institute of Ion-Plasma and Laser Technologies, ²Tashkent, ³Uzbekistan-Japan Innovation centre of Youth

(M-P27) **Exploring the Performance and Utility of Low-Cost Silicon Attenuated Total Reflection Elements for Infrared Spectroscopy;** Barry Havens¹; ¹PPG Industries, Inc.

(M-P28) **Performance Comparison of Four Portable FTIR Instruments for Direct-on-Filter Measurement of Respirable Crystalline Silica;** Elizabeth L. Ashley¹, Lauren Chubb¹, Donald Tuchman¹, Elaine Rubinstein¹, Emanuele Cauda¹; ¹National Institute for Occupational Safety and Health/Pittsburgh Mining Research Division

(M-P29) **Predicting Progression of Interstitial Fibrosis in Kidney Transplants using FT-IR Imaging;** Siva Sreedhar¹, David Martinez Marin¹, Hari Sreedhar², Omar Shram³, Suha F. Mohiuddin¹, Suman Setty³, Michael Walsh¹; ¹University of Illinois College of Medicine Department of Pathology, ²University of California San Diego, ³Univ.of Illinois Chicago

(M-P30) **The Application of Online NIR in Flour Milling;** Nanning Cao¹; ¹Arden Mills

(M-P31) **Toward a handheld open source diffuse reflectance spectrometer for agriculture;** Francis Esmonde-White¹, Greg Austic²; ¹Esmonde-White Technologies, LLC, ²OurSci, LLC

(M-P32) **From a model to applications. Simulations of NIR spectra – melamine and thymol;** Justyna Grabska¹, Krzysztof B. Bec², Yukihiko Ozaki³, Christian W. Huck¹; ¹University of Innsbruck, ²Institute of Analytical Chemistry and Radiochemistry, University of Innsbruck, ³Kwansei Gakuin University

(M-P33) **Molecular spectroscopic study of anion doped lithium metal borates as cathode material for lithium-ion battery;** Youngil Lee¹, Chaewon Moon¹, Khoirul Umam¹; ¹University of Ulsan

(M-P34) **Modern Applications of Infrared Spectroscopy;** Jeff D'Agostino¹, Jeff D'Agostino¹, Todd Baker¹, Will Campbell¹; ¹Specac

(M-P35) **Microplastics Detection and Characterization using FTIR Microscopy;** Liang Zhao¹, Sudhir Dahal²; ¹Shimadzu Scientific Instruments Inc., ²Shimadzu Scientific Instruments

(M-P36) **Isotope analysis device with fine spatial resolution using UV laser ablation sampling coupled to hollow fiber based Mid-IR spectroscopy;** Jason M. Kriesel¹, Camille Makarem¹, James Moran², Timothy Linley², James Kelly¹; ¹Opto-Knowledge Systems, Inc. (OKSI), ²Pacific Northwest National Laboratory (PNNL)

19MP-NANO: MONDAY POSTERS: NANOTECHNOLOGY

(M-P37) **The Role of Gold Nanoparticle Size in the Quenching-to-Enhancement Transition of Plasmon Assisted Upconversion Luminescence;** Ana Egatz-Gomez¹, Diego Mendez-Gonzalez², Oscar Calderon³, Marco Laurenti², Eduardo Cabrera-Granado³, Enrique López-Cabarcos², Jorge Rubio-Retama², Elena Díaz⁴, Sonia Melle³; ¹Arizona State University, ²Department of Chemistry in Pharmaceutical Sciences, Complutense University of Madrid, ³Department of Optics, Complutense University of Madrid, ⁴GISC, Department of Materials Physics, Complutense University of Madrid

(M-P38) **Single Molecule Protein Patterning Using Hole Mask Colloidal Lithography;** William Lum¹, Dinesh Gautam², Jixin Chen², Laura Sagale¹; ¹University of Cincinnati, ²Ohio University

(M-P39) **Metrology of Sorted Single Walled Carbon Nanotubes by Raman Spectroscopy and Excitation Mapping;** Paul Finnie¹, Jianying Ouyang¹, Jianfu Ding¹, Jacques Lefebvre¹; ¹National Research Council Canada

(M-P40) **Selective Adsorption of DNA strands to Layered Double Hydroxide Nanomaterial;** Kyoung-Min Kim¹, Woo-Yong Park¹, Jinmi Jung¹, Ji Eun Jung¹, Hyun Kyoung Ju¹, Su Hyeon Lee¹, Ja Youl Yang¹, Nam Yee Kim¹, Yuna Kim², Ji-Sook Min², Jae-Min Oh³; ¹National Forensic Service / Seoul Institute, ²National Forensic Service, ³Department of Energy and Materials Engineering, Dongguk University

(M-P41) **DNA Adsorption Behaviour with Different Charged Layered Inorganic Nanomaterials;** Kyoung-Min Kim¹, Woo-Yong Park¹, Yuna Kim², Ji-Sook Min², Jae-Min Oh³; ¹National Forensic Service / Seoul Institute, ²National Forensic Service, ³Department of Energy and Materials Engineering, Dongguk University

(M-P42) **Time-dependent Study of Near-field Scanning Optical Microscopy Probes Forged Chemically and its Surface Functionalized for Sensing Applications;** Muhammad Nazmul Hussain¹, Xavier Udad¹, Eric Edwards¹, Jorg C. Woehl¹; ¹University of Wisconsin - Milwaukee

19MP-SPR: MONDAY POSTERS: SURFACE PLASMON RESONANCE

(M-P43) **Probing Quadrupole Modes in Gold Nano-rods Using Synchrotron Infrared Nano-spectroscopy;** Joseph J. Liberko¹, Jake Busche², Robyn Collette³, Philip Rack³, David Masiello², Hans Bechtel⁴, Jon Camden¹; ¹University of Notre Dame, ²University of Washington, ³University of Tennessee Knoxville, ⁴Advanced Light Source

(M-P44) **Influence of the Capping Material on Pyridine-induced Chemical Interface Damping in Single Gold Nanorods;** Ji Won Ha¹, Seong Woo Moon¹; ¹University of Ulsan

19MP-SPSJ: MONDAY POSTERS: SPSJ

(M-P45) **Understanding and Enhancing the Stability of a Well-Known Oxygen Sensitive Platinum Based Phosphorescent Molecular System;** Sindhu S. Konanur Shankar¹, Adil Basha¹, Mohammad Omary¹, Sreekar Marpu¹; ¹University of North Texas

(M-P46) **Surface plasmon resonance sensors utilizing far- and deep-ultraviolet lights;** Ichiro Tanabe¹; ¹Osaka University

TECHNICAL PROGRAM – TUESDAY POSTERS POSTERS SESSIONS 11:00 AM – 12:00 PM & 3:10 PM - 3:50 PM

Exhibit Hall, Oasisr; Hang posters 10-10:45 AM; Remove at 4:00 PM

19TP-IR TUESDAY POSTERS: MOLECULAR (IR)

(Tu-P1) **Optimising the Workflow for FTIR Microscopy Measurements of Microplastics;** Ian Robertson¹, Robert Packer²; ¹Perkin Elmer Limited, ²Perkin Elmer Corporation

(Tu-P2) **Plasmon-induced dissociation of acetic acid multimers detected by surface-enhanced near-infrared spectroscopy;** Ichiro Tanabe¹, Fumie Watanabe², Yuki Hanase³, Risa Hara², Nobuhiro Tomosada², Takuma Genkawa⁴, Kodai Murayama², Yukihiro Ozaki³; ¹Osaka University, ²Yokogawa Electric Corporation, ³Kwansei Gakuin University, ⁴The National Agriculture and Food Research Organization

(Tu-P3) **Evaluation of milk powder authenticity with a portable mid-infrared spectrometer and a non-targeted chemometric approach;** William Limm¹, Sanjeewa Karunathilaka¹, Betsy Jean Yakes², Magdi Mossoba¹; ¹FDA, ²U.S. Food and Drug Administration

(Tu-P4) **Characterization of the collagen structure in Normal, Wooden Breast and Spaghetti Meat chicken fillets by FTIR micro- and imaging spectroscopy and histology;** karen W. Sanden¹, Ulrike Bocker², Mona Pedersen¹, Nancy Pleshko³; ¹Nofima AS, ²Nofima, ³Temple University

(Tu-P5) **Brain Cell Phenotyping by Infrared Spectroscopy;** Lila Lovergne¹, Aris A. Polyzos¹, Edward S. Barnard¹, Michael C. Martin¹, Cynthia T. McMurray¹; ¹Lawrence Berkeley National Laboratory

(Tu-P6) **Study of Water Vapor as an Energy Relaxation Promoter for Methane Detection in Quartz-enhanced Photoacoustic Spectroscopy;** Pietro Patimisco¹, Angelo Sampaolo¹, Marilena Giglio¹, Arianna Elefante², Giansergio Menduni¹, Lei Dong³, Hongpeng Wu³, Vittorio Passaro¹, Frank K. Tittel⁴, Vincenzo Spagnolo¹; ¹Politecnico di Bari, ²University of Bari, ³Shanxi University, ⁴Rice University

(Tu-P7) **Broadband infrared dual comb spectroscopy with photonic chip-based frequency combs;** Nima Nader¹, Abijith Kowligy¹, Jeff Chiles¹, Eric J. Stanton¹, Henry Timmers¹,

Alexander J. Lind¹, Flavio Cruz¹, Daniel Lesko², Kimberly Briggman¹, Sae Woo Nam¹, Scott Diddams¹, Richard P. Mirin¹; ¹NIST, ²University of Colorado, Boulder

(Tu-P8) **Responsivity Corrected AFM-IR for Accurate, High-Sensitivity Nanoscale Chemical Imaging;** Seth M. Kenkel¹, Rohit Bhargava¹; ¹University of Illinois Urbana-Champaign

(Tu-P9) **Infrared Spectroscopy for Quantification of Diesel Particulate Mater;** David Parks¹, Andy Weakley², Peter Griffiths³, Arthur Miller¹; ¹NIOSH/SMRD, ²University of California Davis, ³Griffiths Consulting LLC

(Tu-P10) **Near infrared spectroscopy method for analysis of sorghum content in corn-sorghum flour bioethanol feedstock;** Kamaranga H. Peiris¹, Scott Bean², Michael Tilley²; ¹Kansas State University, ²USDA

(Tu-P11) **Dye sensitive corrosion detection with infrared attenuated total reflection spectroscopy on diamond like carbon coated waveguides;** Dervis Türkmen¹, Carina Dettenrieder¹, Mikael Karlsson², Lars Österlund², Fredrik Nikolajeff², Boris Mizaikoff¹; ¹Ulm University / Institute of Analytical and Bioanalytical Chemistry, ²Uppsala University / Department of Engineering Sciences

(Tu-P12) **Leveraging Mid-IR Spectroscopic Imaging to predict kidney transplant progression;** David Martinez Marin¹, Michael Walsh², Hari Sreedhar³; ¹University of Illinois College of Medicine Department of Pathology, ²University of Illinois at Chicago College of Medicine Department of Pathology, ³University of California San Diego

(Tu-P13) **Polymer Film Cross Section Studies using the AIM9000 FTIR Microscope;** Liang Zhao¹, Sudhir Dahal¹; ¹Shimadzu Scientific Instruments

19TP-LIBS: TUESDAY POSTERS: LASER-INDUCED BREAKDOWN SPECTROSCOPY

(Tu-P14) **How improve the direct quantification of lithium, using LIBS technique, for field applications;** Remi Schmitt¹, Nour Eddine Ourti¹, Jean Cauzid¹, Julien Mercadier¹, Vincent Motto-Ros², Cécile Fabre³; ¹GeoRessources, ²Institut Lumiere Matiere, ³Universite de Lorraine / GeoRessources

(Tu-P15) **Multiplexed detection of lanthanide-based labels by LIBS – the constraints and limits of spectral unmixing;** Bartek Rajwa¹, Carmen Gondhalekar¹, Euiwon Bae¹, Valery Patsekina¹, Jennifer Sturgis¹, Iyell-Joon Doh¹, Prasoon K. Diwakar², Xianglei Mao³, Vassilia Zorba³, Rick Russo³, J. Paul Robinson¹; ¹Purdue University, ²South Dakota School of Mines and Technology, ³Lawrence Berkeley National Laboratory

(Tu-P16) **The influence of plasma parameters and noise on partial least square regression of simulated laser-induced breakdown spectra of rocks;** Ebo Ewusi-Annan¹, Nouredine Melikechi¹; ¹University of Massachusetts Lowell

(Tu-P17) **Critical review on the use of normalization in LIBS;** Bruno Bousquet¹, Julian Guezennoc¹, Anne Gallet-Budynek²; ¹Université de Bordeaux, ²INRA

(Tu-P18) **Immobilization of Liquid and Oil Samples for Laser-Induced Breakdown Spectroscopy;** Max Vallone¹, Joshua Buttrick², Emily M. Orme³, Melissa Fernandez⁴, Prasoon K. Diwakar⁵, Claudia Ochatt⁶, Robert C. DuBard²; ¹Ransom Everglades, ²Ransom Everglades Upper School, ³Law Enforcement Officers Memorial High School, ⁴Florida International University, ⁵South Dakota School of Mines and Technology, ⁶Ransom Everglades High School

(Tu-P19) **Machine Learning for Metal Identification in Water Samples Using Laser-Induced Breakdown Spectroscopy;** Joseph Gross¹, Emily M. Orme², Melissa Fernandez³, Andrew Carter⁴, Rachel Silverstein⁴, Claudia Ochatt¹, Sofia Pozsonyiova⁵, Luis Felipe¹, Prasoon K. Diwakar⁶; ¹Ransom Everglades High School, ²Law

Enforcement Officers Memorial High School, ³Florida International University, ⁴Miami WaterKeeper, ⁵Macalester College, ⁶South Dakota School of Mines and Technology

(Tu-P20) **Measurement of Stark widths and shifts of O II and N II spectral lines in laser-induced plasma;** Aleksandr S. Zakuskin¹, Andrey M. Popov², Sergey M. Zaytsev¹, Timur A. Labutin¹; ¹Lomonosov Moscow State University, ²Lomonosov Moscow State University

(Tu-P21) **Quantitative Laser Induced Breakdown Spectroscopy (LIBS) for elemental analysis of doped battery electrode materials.;** Dibyendu Mukherjee¹, Ravi Pamu¹, Jagjit Nanda²; ¹University of Tennessee, ²Oak Ridge National Laboratory

(Tu-P22) **Study on variable selection methods for LIBS-based identification of geographical origins of sapphire samples;** Hoeil Chung¹, Chang Hwan Eum¹, Ji Hun Cho¹, Kyungjoon Cha¹; ¹Hanyang University

(Tu-P23) **Laser Ablation of a Eutectic BiSn Alloy: Incongruent Transfer and Hydrodynamic Effects in Crater Formation;** Tariq Alharby¹, Omar Musaev¹, Paul Rulis¹; ¹University of Missouri-Kansas City

(Tu-P24) **Bridging the Gap: Integrating Statistical Modeling and Machine Learning Methods to Better Classify and Visualize LIBS Data;** Sofia Pozsonyiova¹, Melissa Fernandez², Emily M. Orme³, Prasoon K. Diwakar⁴; ¹Macalester College, ²Florida International University, ³Law Enforcement Officers Memorial High School, ⁴South Dakota School of Mines and Technology

(Tu-P25) **Laser Induced Breakdown Spectroscopy of BaF2-Tm;** Michael Gaft¹, Lev Nagli², Yosef Raichlin³; ¹Ariel University, ²University Ariel, Israel, ³Ariel University / Department of Physics

19TP-OTHER TUESDAY POSTERS: OTHER

(Tu-P26) **A Painfully Detailed Look at Behavior of Stacked, Mutually-rotated Diffraction Gratings;** Alexander Scheeline¹, Jorge Guzman¹; ¹SpectroClick Inc.

(Tu-P27) **Inquiry-based Mini Learning Projects for Environmental Analysis Laboratory Course at Cal Poly Pomona;** Yan Liu¹; ¹California State Polytechnic University Pomona

(Tu-P28) **Bifunctional Cu2O-Ni electrocatalyst for oxygen evolution reaction and CO2 reduction;** Hanqing Pan¹, Christopher Barile¹; ¹University of Nevada, Reno

(Tu-P29) **Quantifying the Progression of Fibrosis in Nonalcoholic and Alcoholic Steatohepatitis Using FTIR Spectroscopy;** Suha F. Mohiuddin¹, Shaiju S. Nazeer², Siva Sreedhar¹, David Martinez Marin¹, Hari Sreedhar³, Ron Gaba⁴, Michael Walsh¹; ¹University of Illinois College of Medicine Department of Pathology, ²The University of Alabama at Birmingham, ³University of California San Diego, ⁴The University of Illinois at Chicago

(Tu-P30) **Quantitative determinations in thin-layer chromatography: development of a portable, low-cost system using digital image detection for direct analysis;** Taynara R. Machado¹, Alexandre Fonseca²; ¹University of Brasilia, ²Universidade de Brasilia

(Tu-P31) **Effect of the rate of silicic acid release from dissolving silica nanoparticles on the growth and fungal disease resistance ability of watermelon (Citrullus lanatus);** Hyunho Kang¹, Wade Elmer², Yu Shen², Jason White², Christy Haynes¹; ¹University of Minnesota, Twin-Cities, ²The Connecticut Agricultural Experiment Station

19TP-PAT TUESDAY POSTERS: PROCESS ANALYTICAL TECHNOLOGY

(Tu-P32) **HPLC and Visible Spectroscopic Analyses of Commercial Azo Dyes Relevant to the ASTM D6258 Method for Testing Dyed Fuels;** Kengkaj Sukcharoenphon¹, Thomas M. Rettberg¹, Jens Seltmann², Stephan Schöler², Katrin Fenzke²; ¹LGC Standards/VHG Labs, ²LGC Standards / LGC Labor GmbH

(Tu-P33) **Raman-Based Bioreactor Monitoring During Vaccine Manufacturing;** Brian C. Marks¹, John Higgins¹; ¹Merck & Co., Inc.

(Tu-P34) **Rapid Automated Tetrahydrocannabinol Extraction from Oral Fluid;** Marcus A. Tofanelli¹, Katrina M. Myers¹, Roxana F. Sandoval¹, George R. Farquar²; ¹BUZZKILL LABS INC, ²BuzzKill Labs

(Tu-P35) **In-line, label free, remote, non-contact optical detector for aqueous droplets in oil in fused silica capillaries;** Ana Egatz-Gomez¹, Jorvani C. Villarreal², Sahir Gandhi², Austin Echelmeier², Dai Hyun Kim³, Jose Manuel Lopez Alonso⁴, Oscar Calderon⁵, Sonia Melle⁵, Alexandra Ros²; ¹Arizona State University, ²Arizona State University / The Biodesign Institute, ³Arizona State University / Biodesign Institute, ⁴Optics Department, Universidad Complutense De Madrid, ⁵Department of Optics, Complutense University of Madrid

(Tu-P36) **A non-destructive monitoring method for the peptide chemosynthetic reaction by NIR spectroscopy;** Atsushi Itou¹, Kodai Murayama¹, Shun-Ichi Miyazaki¹, Mika Ishigaki², Keisuke Yoshikiyo², Tatsuyuki Yamamoto², Yukihiro Ozaki³; ¹Yokogawa Electric Corporation, ²Shimane University, ³Kwansei Gakuin University

(Tu-P37) **At-line NIR testing to replace HPLC API content measurement;** Anna Novikova¹; ¹Fette Compacting GmbH

(Tu-P38) **Development of HPLC - FLD Method for the Sensitive Analysis Of MSG in Food Samples;** Murat Soyseven¹, Goksel Arli¹; ¹Anadolu University

(Tu-P39) **Crystallization Monitoring of an Active Pharmaceutical Ingredient (API) by Raman Spectroscopy;** Lanfeng Zou¹, Daniel Patience¹, Vinny Couming¹, Chaomin Li¹, Tae Correia¹, Elliott Schmitt¹, John-David McElderry¹; ¹Biogen

(Tu-P40) **ChemCal, a tool used to generate uniform chemical(s)/biological(s) on surfaces for calibration/validation of surface contaminant measuring devices.;** Michael Reid¹, William F. Hug¹, Ken Nguyen², Ray Reid¹; ¹Photon Systems, Inc., ²Photon Systems Inc

19TP-RAM: TUESDAY POSTERS: RAMAN

(Tu-P41) **Rapid phenotypic approach for screening the major carotenoids of tomato in breeding selections;** Hacer Akpolat¹, David Francis¹, Luis Rodriguez-Saona¹; ¹Ohio State University

(Tu-P42) **Monitoring of gas compositions by use of enhanced Raman spectroscopy;** Timea Frosch¹, Anne Sieburg¹, Sebastian Schneider¹, Di Yan¹, Jürgen Popp², Torsten Frosch³; ¹Leibniz Institute of Photonic Technology, ²Leibniz Institute of Photonic Technology, ³Leibniz Institute of Photonic Technology, Jena; Institute of Physical Chemistry & Abbe Center of Photonics, Friedrich Schiller University, Jena

(Tu-P43) **Innovative Raman Techniques Using SORS and Transmission Raman for Analysis of Materials;** Dean H. Brown¹; ¹Agilent Technologies

(Tu-P44) **High-speed and High-density Multi-channel Raman Spectroscopy using a Back-illuminated sCMOS based Spectrometer;** Justin Cooper¹, Adam Wise¹; ¹Andor Technology

(Tu-P45) **Analysis of pharmaceutical tablets for labeled and unlabeled active ingredients using surface enhanced Raman scattering (SERS) with handheld devices;** Martin m. Kimani¹, Adam Lanzarotta¹, JaCinta Batson¹; ¹United States Food Drug Administration

(Tu-P46) **Detecting concentrations of Glucose, Sucrose and D-fructose in solutions by Means of Raman Spectroscopy, Support Vector Machine and Principal Component Analysis;** Jorge Castro-Ramos¹, Freddy Narea-Jimenez¹, Pilar Gomez-Gil¹; ¹National Institute of Astrophysics Optics and Electronics

(Tu-P47) **Highly sensitive detection of botulinum toxins A and B using SERS-based magnetic immunosensors;** Kihyun Kim¹, Namhyun Choi², Jaebum Choo¹; ¹Chung-Ang University, ²Hanyang University

(Tu-P48) **Fiber-Enhanced Raman Gas Spectroscopy for Isotopic Labeling Experiments with oxygen-18 and carbon-13;** Andreas Knebl¹, Robert Domes², Di Yan², Jürgen Popp², Susan Trumbore¹, Torsten Frosch³; ¹Leibniz Institute of Photonic Technology, Jena; Max-Planck-Institute for Biogeochemistry, Jena, ²Leibniz Institute of Photonic Technology, ³Leibniz Institute of Photonic Technology, Jena; Institute of Physical Chemistry & Abbe Center of Photonics, Friedrich Schiller University, Jena

(Tu-P49) **Application of SERS-based lateral flow biosensor for accurate diagnosis of dengue fever in tropical regions;** See Hi Lee¹, Jinhyeok Jeon², Jaebum Choo¹; ¹Chung-Ang University, ²Hanyang University

(Tu-P50) **Toward the application of Ball-lens hollow fiber Raman Probe for distinguishing lipid belong to the Farmed and Wild Tuna;** Bibin B. Andriana¹, Akinori Taketani¹, Riki Zakaria¹, Pradjna Paramitha¹, Yuya Kondo¹, Hidetoshi Sato¹; ¹School of Science and Technology, Kwansei Gakuin University

(Tu-P51) **Super-resolution imaging of SERS hotspots accessed with various polarization states;** Kallai Hokanson¹, Sarah Thorud¹, Alexandre Brolo², Nathan C. Lindquist¹; ¹Bethel University, ²University of Victoria

TECHNICAL PROGRAM – WEDNESDAY POSTERS
POSTERS SESSIONS 11:00 AM – 12:00 PM & 3:10 PM - 3:50 PM
Exhibit Hall, Oasisr; Hang posters 10-10:45 AM; Remove at 4:00 PM

19WP-BIM: WEDNESDAY POSTERS: BIOMEDICAL

(W-P1) **Multi-stage Electrokinetic Microsystem for the Purification and Assessment of Microbes;** Adriana Coll De Peña¹, Nicole Hill¹, Abbi Miller¹, Julie A. Thomas¹, Blanca H. Lapizco-Encinas¹; ¹*Rochester Institute of Technology*

(W-P2) **A Novel LC-MS/MS Method for Simultaneous Quantification of Amlodipine, Bisoprolol, Enalapril and its Metabolite Enalaprilat in Healthy Volunteers; Application to a Pharmacokinetic Study;** Ahmed M. Abdel-Megied¹, Samir Osman²; ¹*Kafrelsheikh University*, ²*October 6 University*

(W-P4) **Antimicrobial Cyclic Peptide Polymer Nanopores;** Kenan Fears¹, Luis Estrella¹; ¹*US Naval Research Laboratory*

(W-P5) **In situ Flow Measurements of Thermoresponsive Nanocarrier Delivery in Targeting-Free Cell Selection;** Darian J. Gamble¹, Marius Gollasch¹, Katarzyna Slowinska¹; ¹*California State University, Long Beach*

(W-P6) **Immunobinding-Induced Alteration in the Isotachophoretic Mobility of Proteins and Its Application in Multiplex Detection of Protein Markers on a Paper-Based Device;** Wen-Ji Dong¹, Shuang Guo¹, Cornelius Ivory¹; ¹*Washington State University*

(W-P7) **New two-step method of targeting GRP78 cancer receptor using collagen/cell penetrating hybrid peptide heterotrimers as carriers;** Phelicia Bell¹, Chelsea Del Rio¹, Katarzyna Slowinska¹; ¹*California State University, Long Beach*

(W-P8) **Diversity of Raman Spectra Obtained from the Employment of Ball-lens Hollow Fiber Optic Raman Probe (BHRP) to Immature mice's Esophagus Tissue;** Bibin B. Andriana¹, Riki Zakaria¹, Akinori Taketani², Anisa Maryani¹, Toshiya Ichiki², Yukako Kusaka¹, Hidetoshi Sato³; ¹*Kwansei Gakuin University*, ²*Sch. of Sci. Tech, Kwansei Gakuin University*, ³*School of Science and Technology, Kwansei Gakuin University*

(W-P9) **Effects of Electroporation and Cold Atmospheric Plasma on Human Lung Cancer Cells;** Kristen I. Haller¹, Nicole L. Miller¹, Jordan A. Hoops¹, Prasoon K. Diwakar¹, Timothy M. Brenza¹; ¹*South Dakota School of Mines and Technology*

(W-P10) **Development of immunoaffinity monolith extraction of preterm birth risk biomarkers in 3D printed microfluidic systems;** Taylor Fish¹, Haifa Almughamsi¹, Adam T. Woolley¹; ¹*Brigham Young University*

19WP- ENVIRON: WEDNESDAY POSTERS: ENVIRONMENT

(W-P11) **Comparative studies between bulk and suspension synthesis of a Hybrid Molecularly Imprinted Polymers (HMIPs) for extraction of saccharin from surface water;** Camila s. Dourado¹, Fabiana Casarin², Izabella Fernanda Domingues², Maria Vtória Villa Bande², Jez Willian Braga², Ana Cristi Dias²; ¹*University of Brasilia – UnB.*, ²*University of Brasilia – UnB*

(W-P12) **Colorimetric detection of nicotine – a marker for thirdhand smoke contamination;** Arrion A. Smith¹, Catrin A. Law¹, Christopher R. Harrison¹; ¹*San Diego State University*

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(W-P15) **Quantitative Determination of Coumarin in Cinnamon Barks and their Infusions;** GOKALP ISCAN¹, ESRA BEKTAS SARIALTIN¹, Murat Soyseven², Goksel Arli²; ¹*ANADOLU UNIVERSITY*, ²*Anadolu University*

(W-P16) **The Relationship Between Soil Properties and Essential Oil Components of Hypericum perforatum L.;** Yavuz B. Köse¹, Elif Dünder², Betül Demirci²; ¹*Anadolu University Faculty of Pharmacy*, ²*Anadolu University*

(W-P17) **Mycotoxin analysis of grounded and granulated coffees sold in local markets;** Bülent B. Ergun¹, Murat Soyseven², GOKALP ISCAN³, Goksel Arli²; ¹*Anadolu University Faculty of Pharmacy*, ²*Anadolu University*, ³*ANADOLU UNIVERSITY*

(W-P18) **Influence of stereochemistry on the partitioning of selected ortho and non-ortho polychlorinated biphenyls between aqueous solution and soil system.;** Gbadebo c. Adeyinka¹; ¹*University of KwaZulu-Natal, Durban, South Africa*

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(W-P21) **Non-targeted analysis and identification of counterfeit functional drinking water;** Yuna Kim¹, Min-Hui Son¹, Seok hoan Jeong¹, Ji-Sook Min¹; ¹National Forensic Service

(W-P22) **Characterizing Inorganic and Organic Gunshot Residue by Laser Induced Breakdown Spectroscopy and Electrochemistry;** Korina L. Menking-Hoggatt¹, Luis Arroyo², Colby Ott¹, Tatiana Trejos²; ¹West Virginia University, ²West Virginia University Department of Forensic and Investigative Science

(W-P23) **Development and Testing of a Real Time Man-in-Simulant-Test Sensor;** Jason M. Abbott¹, Keith Broekhuizen¹, Cyntia Jallad¹; ¹MRIGlobal

(W-P24) **Evaluation of Novel, Multifunctional Mesoporous Silica Sorbent Materials for Enhanced Sampling and Storage;** Colin Hessel¹, Dorin Preda², Min Song¹, John Lennhoff², Albert Wright², David Gamliel², Nicholas Craig², Kristina Bennett², Tyler Paul², Christopher Lang²; ¹Physical Sciences Inc., ²Physical Sciences Inc.,

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(W-P26) **Forensic Analysis of 3D Printed Polymers Pre- and Post-Manufacturing;** Brooke W. Kammrath¹, Ryan Zdenek¹, April Bowen¹, John Reffner², Maria-Isabel Carnasciali¹; ¹University of New Haven, ²John Jay College of Criminal Justice

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(W-P28) **Qualitative and Quantitative Fingerprinting of Petroleum Products in Drinking Water Sources using Simultaneous Absorbance-Transmittance Excitation-Emission Matrix Spectroscopy;** Adam M. Gilmore¹; ¹HORIBA

(W-P29) **The Potential for Forensic Organic Gunshot Residue Evidence Analysis Using Raman Spectroscopy;** Shelby R. Khandasammy¹, Lenka Halámková², Igor K. Lednev²; ¹SUNY Albany, ²University at Albany, SUNY

(W-P30) **Sex and Race Determination Based on Attenuated Total Reflection Fourier Transform-Infrared (ATR FT-IR) Spectroscopy of a Bloodstain;** Ewelina M. Mistek¹, Lenka Halámková¹, Igor K. Lednev¹; ¹University at Albany, SUNY

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(W-P32) **Feasibility of DDT degradation by bacteria isolated from pesticide-contaminated site in Salamanca city, Mexico: analytical study;** Bianey Garcia¹, Alma Rosa Corrales Escobosa², Katarzyna Wrobel², Francisco Javier Acevedo Aguilar², Kazimierz Wrobel²; ¹Universidad de Guanajuato, ²University of Guanajuato

(W-P33) **Simultaneous elemental and molecular analysis using solution cathode glow discharge mass spectrometry and optical emission spectroscopy;** Jessica Hellinger¹, Garrett M. MacLean¹, Malina Helling¹, Montwaun Young¹, Jacob Shelley¹; ¹Rensselaer Polytechnic Institute

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(W-P35) **Electrospray Ionization Zoom Time-of-Flight Mass Spectrometry;** Christopher J. Brais¹, Steven J. Ray¹; ¹The State University of New York at Buffalo

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(W-P39) **Evaluation of controlled release from piroxicam-loaded chitosan microspheres synthesized by different methods;** Sibel Büyüktiryaki¹, Rüstem Keçili¹, Murat Soyseven¹, Goksel Arli¹; ¹Anadolu University

(W-P40) **Development of a novel Reverse Phase HPLC method for the simultaneous analysis of metoprolol tartrate and phenol red in intestinal perfusion samples;** Mustafa Sinan Kaynak¹, Murat Soyseven¹, Goksel Arli¹; ¹Anadolu University

(W-P41) **Determination of Lactic Acid and Hydrogen Peroxide Quantities of Some Lactic Acid Bacteria;** sevda er¹, merih kıvanç²; ¹Department of Medical Services and Techniques, Yunus Emre Vocational School for Health Services, Anadolu University, Eskişehir, Turkey, ²Department of Biology, Faculty of Science, Eskişehir Technical University, 26555, Eskişehir, Turkey

(W-P42) **Simultaneous Analysis of 5-amino-2-chloropyridine and Tenoxicam using HPLC-DAD and HPLC-ELSD Systems;** Goksel Arli¹, Murat Soyseven¹, Rustem Kecili¹; ¹Anadolu University

(W-P43) **Assessing the Discrimination of Pharmaceutical Packaging Ink Through LIBS and ATR-FTIR;** Emily Haase¹, Mandy Ho², Tatiana Trejos¹, Luis Arroyo¹; ¹West Virginia University Department of Forensic and Investigative Science, ²West Virginia University

(W-P44) **Development of HPLC-DAD and HPLC-ELSD-based analytical methods for the analysis of potentially genotoxic impurity 2-aminopyridine in pharmaceutical compounds;** Rustem Kecili¹, Murat Soyseven¹, Goksel Arli¹; ¹Anadolu University

(W-P45) **Developing Mechanistic Understanding of Unconventional Growth in Pharmaceutical Crystals Using Scanning Electron Microscopy, Atomic Force Microscopy and Time-of-Flight Secondary Ion Mass Spectrometry;** Hector Polyzois¹, Monika Warzecha¹, Eleonora Paladino¹, Deborah L. Bowering¹, Rui Guo², Sarah L. Price², Gavin W. Halbert¹, Alastair J. Florence¹; ¹EPSRC CMAC Future Manufacturing Research Hub, University of Strathclyde, ²University College London (UCL)

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(W-P47) **Raman and SEM/EDX Characterization of Functionally Coated Pellets in Extended Release Capsules and Correlation of Dissolution Performance;** Wenjing Xi¹, Daniel Willett², Huzeyfe Yilmaz³, Zongming Gao⁴, Jason D. Rodriguez³; ¹FDA/CDER/DPA, ²U.S. Food and Drug Administration, ³US Food and Drug Administration, ⁴FDA

(W-P48) **Synthesis, Spectral Elucidation and Bioassays of 3-(Aminomethyl)-5-methylhexanoic acid Derivative and its Metal Complexes containing Imine moiety;** Khadija Shahid¹; ¹Riphah Institute of Pharmaceutical Sciences, Riphah International University, Islamabad, Pakistan

(W-P49) **Accelerated NMR techniques for Structure Elucidation of Pharmaceutical Candidates;** Kelsey L. Alexander¹, Brendan Duggan², William Gerwick³; ¹UCSD, ²Skaggs School of Pharmacy and Pharmaceutical Sciences, ³Scripps Institution of Oceanography

(W-P50) **Evaluating an Engineered Protein for Biocatalytic Production of a Chiral Pharmaceutical Intermediate;** Chanaka M. Amarasekara¹, Katherine Belecki¹; ¹Department of Chemistry, Virginia Commonwealth University

(W-P51) **Development of a Forced Degradation Platform for the Stability Indication of the Drug Substance Milbemycin oxime;** Mackenzie Lauro¹; ¹Merck & Co.

(W-P52) **Rapid Screening for Counterfeit Pharmaceutical Tablets by Near-Infrared Spectroscopy;** Ian Robertson¹, Robert Packer², Sulaf Assi³; ¹Perkin Elmer Limited, ²Perkin Elmer Corporation, ³Liverpool John Moores University

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(Th-P2) **Isotopic determination of LiOH-H₂O by Laser Induced Breakdown Spectroscopy;** Jason C. Wood¹, Michael B. Shattan¹; ¹Air Force Institute of Technology

(Th-P3) **Preparation and in housing characterisation of an americium working Standard solution for ICP AES measurements;** Didier Maloubier¹, Guillaume LEGAY¹; ¹CEA France

(Th-P4) **Determination of U, Pu, and Am in human keratinous samples using extraction chromatography and ICP-MS;** Dana Wegge¹, Sergei Y. Tolmachev², John D. Brockman³; ¹University of Missouri, ²United States Transuranium and Uranium Registries/ Washington State University, ³University of Missouri

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(Th-P6) **Total chloride analysis in petroleum feedstocks and products: some reflections;** Francisco A. Lopez-Linares¹; ¹*Chevron, Energy Technology Company*

(Th-P7) **Bioaccessibility of essential elements in açai (Euterpe oleracea M. and Euterpe spp.) pulps;** GISELAINA A. SANTOS¹, Aline P. Oliveira², Alexandrina A. C. Carvalho¹, Fernanda V. Matta³, Juliana Naozuka², Mônica Felipe-Sotelo³, Neil I. Ward³, Nádia C. F. Corrêa⁴, Cassiana S. Nomura¹; ¹*Universidade de São Paulo*, ²*Universidade Federal de São Paulo*, ³*University of Surrey*, ⁴*Universidade Federal do Pará*

(Th-P8) **Chemical analysis for adulteration identification in açai (Euterpe oleracea Martius) products;** GISELAINA A. SANTOS¹, Alexandrina A. C. Carvalho¹, Fernanda V. Matta², Juliana Naozuka³, Rômulo A. Ando¹, Mônica Felipe-Sotelo², Neil I. Ward², Nádia C. F. Corrêa⁴, Cassiana S. Nomura¹; ¹*Universidade de São Paulo*, ²*University of Surrey*, ³*Universidade Federal de São Paulo*, ⁴*Universidade Federal do Pará*

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(Th-P10) **Development of wearable device for a real-time monitoring of multiple in-vivo chemical information for self-health management;** hyo jin kim¹, Eun-jin park¹, won bo cho², Soo Ah Cho³, Sung chul Lee⁴, Chul Ku Hahn⁴, hyung hwan baik⁵, Ok kyun Kim⁶, Sung Ho Lee⁶; ¹*Dongduk Womens University*, ²*dongduk women's university*, ³*Dongduk women's University*, ⁴*Korea electronic technology institute*, ⁵*Kyung Hee University*, ⁶*kyung hee university*

(Th-P11) **Toward the Application of Ball-lens Hollow Fiber Optic Raman Probe (BHRP) For Studying the Biochemical Contents of Mice's Esophagus Tissue;** Riki Zakaria¹, Bibin B. Andriana¹, Akinori Taketani², Anisa Maryani¹, Toshiya Ichiki², Yukako Kusaka¹, Asri peni Wulandari³, Tatsuyuki Yamamoto⁴, Hidetoshi Sato⁵; ¹*Kwansei Gakuin University*, ²*Sch. of Sci. Tech, Kwansei Gakuin University*, ³*Departement of Biology, Faculty of Mathematic and Natural Science, University of Padjadjaran*, ⁴*Shimane University*, ⁵*School of Science and Technology, Kwansei Gakuin University*

(Th-P12) **Comparative study of the effects of cold atmospheric plasma and electroporation on bacterial cells to enhance the substrate utilization;** Payal Thakur¹, Tanvi Govil², Kristen I. Haller¹, Nicole L. Miller¹, Prasoon K. Diwakar¹, Sudhir Syal³, David Salem², Rajesh Sani²; ¹*South Dakota School of Mines and Technology*, ²*SDSMT*, ³*JUIT Biotechnology and bioinformatics*

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(Th-P14) **Coated Magnetic Iron Oxide Nanoparticles Conditioned with Phosphate as Curcumin Carriers Under Physiological Conditions;** Vladimir V. Zotov¹, Anselm Omoike¹; ¹*USC Upstate*

(Th-P15) **Phosphorescence-based Oxygen-Sensing Optrode for Improved Assessment of Compartment Syndrome;** Lilian Witthauer¹, Emmanuel Roussakis¹, Yenyu Chen¹, Juan Pedro Cascales¹, Conor Evans²; ¹*Wellman Center for Photomedicine / MGH / Harvard Medical School*, ²*Wellman Center for Photomedicine / Massachusetts General Hospital*

(Th-P16) **Hierarchical Detection and Assessment of Material Fatigue Damage of the Human Anterior Cruciate Ligament Caused by Repetitive Sub-maximal Mechanical Loading;** Jinhee Kim¹, Junjie Chen¹, Wenhao Shao¹, Stephen Schlecht¹, So Young Baek¹, Alexis Jones¹, Taeyong Ahn¹, James Ashton-Miller¹, Mark Banaszak-Holl², Edward Wojtys¹; ¹*University of Michigan*, ²*Monash University*

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(Th-P19) **Authentication of Omega 3 Fish Oil Dietary Supplements;** Debbie A. Peru¹, Gene S. Hall²; ¹*DP Spectroscopy & Training LLC*, ²*Rutgers, The State University of New Jersey*

(Th-P20) **Reduced Sensor Training Burden for a Short-Wave Infrared Conformal Filter Hyperspectral Imager via the Direct Calculation of Basis Vectors;** Robert Schweitzer¹, Shawna K. Tazik¹, Matthew P. Nelson¹; ¹*ChemImage Corp*

(Th-P21) **Fusion of similarity measures as an indicator of spectral uniqueness (ISU) to characterize differences in sample matrix effects;** Callan C. Norby¹, John H. Kalivas¹; ¹*Idaho State University*

(Th-P22) **Using Model Diversity and Prediction Similarity for Model Selection of Multivariate Calibration Updating Methods Based on Unlabeled Data;** Robert C. Spiers¹, John H. Kalivas¹; ¹*Idaho State University*

(Th-P23) **Dynamic Fluorescence Measurements of Rose Bengal Photosensitization in Octanol;** YINAN ZHANG¹, Sharon L. Neal²; ¹*UNIVERSITY OF DELAWARE*, ²*University of Delaware*

(Th-P24) **Development of Stable Spectral Processing Technique for Biomedical Raman Imaging Analysis;** Tsuyoshi Tanioka¹, Hiroko Matsuyoshi², Christian W. Huck³, Hidetoshi Sato¹; ¹*School of Science and Technology, Kwansei Gakuin University*, ²*School of Health Sciences, Gifu University of Medical Science*, ³*University of Innsbruck*

(Th-P25) **Novel Infrared and Raman spectroscopic Method for Saffron Authenticity;** Karla R. Borba¹, Luis Rodriguez-Saona², Didem P. Aykas², Maria Milani³, Greg Sigurdson², Monica Giusti²; ¹*School of Pharmaceutical Sciences, São Paulo State University-UNESP*, ²*The Ohio State University*, ³*Institute of Chemistry - São Paulo State University*

(Th-P26) **Determination of Caffeine in soft drinks by LCMSD Trap;** Zainab AlBallam¹; ¹*kuwait institute for scientific research*

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(Th-P29) **The Effect of Atmospheric Conditions on LIBS Precision;** Holly H. VerMeulen¹, Ashley M. Mossell¹, Michael J. Morgan¹, Komi S. Messan¹, Samuel A. Beal¹, Lizzie J. Corriveau¹, Jay L. Clausen¹; ¹*USACE ERDC-CRREL*

(Th-P30) **Optimized LIBS detection of lanthanide labels used to identify pathogens on paper immunoassay platforms;** Carmen Gondhalekar¹, Bartek Rajwa¹, Euiwon Bae¹, Valery Patsekin¹, Jennifer Sturgis¹, Iyul-Joon Doh¹, Prasoon K. Diwakar², Vassilia Zorba³, Richard Russo³, Xianglei Mao³, J. Paul Robinson¹; ¹*Purdue University*, ²*South Dakota School of Mines and Technology*, ³*Lawrence Berkeley National Laboratory*

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(Th-P32) **Gelation of Liquid Samples for Optimal Elemental Spectra Analysis Through Laser-Induced Breakdown Spectroscopy;** Emily M. Orme¹, Melissa Fernandez², Max Vallone³, Prasoon K. Diwakar⁴, Claudia Ochatt⁵; ¹*Law Enforcement Officers Memorial High School*, ²*Florida*

International University, ³*Ransom Everglades*, ⁴*South Dakota School of Mines and Technology*, ⁵*Ransom Everglades High School*

(Th-P33) **Submersible Laser Induced Breakdown Spectroscopy sensor for monitoring groundwater quality impacted by environmental and geologic carbon storage activities;** Daniel A. Hartzler¹, Chet R. Bhatt¹, Jinesh C. Jain¹, Dustin L. McIntyre²; ¹*LRST / National Energy Technology Laboratory*, ²*US National Energy Technology Laboratory*

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(Th-P35) **Rapid and direct trace element analysis of solids with laser ablation spectroscopy;** Yuanchao LIU¹, Condon Lau¹; ¹*City University of Hong Kong*

(Th-P36) **Application of Laser Induced Breakdown Spectroscopy in the Reconstruction of Firearm Related Incidents;** Courtney H. Vander Pyl¹, Oriana Ovide², Tatiana Trejos¹; ¹*West Virginia University Department of Forensic and Investigative Science*, ²*West Virginia University*

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(Th-P44) **Using Inkjet Dispense SERS (ID-SERS) to overcome the superhydrophobicity of optimally designed SERS substrates when using water-based analytes;** Milo Overbay¹, Christopher Young², Fausto D'Apuzzo¹, Raghuvir N. Sengupta¹, Jason Aronoff¹, Anita Rogacs², Ken Ward², Steven Barcelo¹; ¹*HP Inc / HP Labs*, ²*HP, Inc*

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