SOCIETY FOR APPLIED SPECTROSCOPY

DECEMBER 2024 NEWSLETTER

SciX Recap!
A huge thank you to the following session chairs and attendees that wrote blurbs about their experiences at SciX!

Overview (Abigail Bauer, Incoming Marketing Chair): SciX 2024—The Great Scientific Exchange—was held 20–25 October in Raleigh, NC. SciX is organized by the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). More than 1,000 attendees met at the Raleigh Convention Center to enjoy a week of intensive scientific sessions, short courses, career fair, and abundant networking opportunities. SciX 2024 in Raleigh boasted 580 oral presentations and 213 posters which covered a wide range of topics in analytical chemistry and its allied sciences. Topical presentations were organized around instrumental techniques and applications. Technical areas included molecular spectroscopy (Infrared and Raman), atomic spectroscopy (conventional and laser-induced breakdown (LIBS) methods), mass spectrometry, and chemometrics. Applications focus areas included plasmonics, forensics, biology/medicine, process analysis, and pharmaceutical analysis. SciX historically features substantial cross-programming between the sections, so that attendees can find talks of interest across the program.

Preparations for next year's SciX are already underway, and the program is sure to feature the same rich range of content related to pharmaceutical analysis. The conference will be held 5-10 October, in Covington, KY. Oral abstract submissions will be solicited starting in February, and sponsors and exhibitors are welcome to participate in SciX.
Visit www.scixconference.org for complete details.

Chemometrics (Caelin Celani): The chemometrics section at SciX 2024 had seven sessions covering a wide array of topics from fundamental advancements in the field to the application of multivariate methods in food/agriculture, forensics, materials science, and conservation science. All sessions were very well attended with roughly 50 or more attendees per session. The state of the field was addressed, with talks framing chemometrics within the new artificial intelligence (AI) revolution and establishing which problems we are uniquely suited to solve. CHEM03 was a session dedictated to highlighting key points from the National Science Foundation (NSF) workshop led by Drs. Karl Booksh, Sharon Neal, and Barry Lavine "Data-Driven Measurements and Instruments for Chemistry" and focused on the future of chemometrics in terms of current weak points like establishing best practices (including metadata, sharing vetted datasets,

etc.), educational needs for a diverse and data-oriented workforce, and integration of inductive multivariate modelling into deductive theoretical models. Application-focused sessions were also well received, with a diverse array of domestic and international speakers. These sessions led to numerous discussions in sessions and networking events about the application and implementation of chemical data science into the larger chemistry community as well as how we can best collaborate across academia, industry, and government in the future.

Early Career Interest Group (Anthony Stender): The Early Career Interest Group (ECIG) would like to take this opportunity to thank everyone who attended our activities at SciX 2024. We had a great turnout for the Monday night social event, and it proved to be a relaxing night to catch up with old friends and make new acquaintances. We also were pleased to once again hold a special session at SciX that focused on career paths in spectroscopy. We are already looking ahead to planning similar events for SciX 2025!

SciX gala in Raleigh, NC featured a local marching band. Photo Credit: Glen Jackson

Thursday poster session. Photo Credit: Glen Jackson

Attendees pose with Rameses, the University of North Carolina Chapel Hill mascot.

Join us in Covington, KY for the 2025 SciX Conference!

Photo from the ECIG special symposium “Showcasing Career Paths in the Spectroscopic Sciences” with (left-to-right) Fay Nicolson, Cyril Soliman, Chelsea Goetzman, Alexis Weber, Sara Mosca, Sam Mabbott. Fay and Sam were the organizers while the others in the photo were session speakers.

SAS 2024 Awards Handed Out During SciX2024:

William J. Poehlman Award – granted to the regional section of the Society which has contributed to the most towards accomplishing the goals and ideals of the Society during the preceding year: **University of Utah Student Chapter**, **Intermountain Section**

William F. Meggers Award – given to the authors of the outstanding paper appearing in *Applied Spectroscopy* during the previous calendar year: **Ioan Notingher, Nathan Woodhouse, Jan Majer, Peter Marshall, and Steve Hood** - "Quantification of Drugs in Brain and Liver Mimetic Tissue Models Using Raman Spectroscopy"

Lester W. Strock Award – established by the New England Section and is given annually to an author or authors of an outstanding paper or series of papers which are collectively outstanding: **Benjamin Manard, Oak Ridge National Labs**

Lippincott Award – given by Optica, the Coblentz Society, and SAS to honor the memory of Ellis R. Lippincott. The recipient of the award shall have made significant contributions to vibrational spectroscopy (this year, the award was given by Optica): **Steven Boxer, Stanford University**

Distinguished Service Award – established to recognize individual members for their long-time service to the Society: **Jay Kitt** – currently serving as Parliamentarian

Barbara Stull Graduate Student Award – given to graduate students in recognition of outstanding research in the area of spectroscopy: **Piyush Raj, Johns Hopkins University**

Undergraduate Award in Applied Spectroscopy – given to undergraduate students in recognition of outstanding research in the area of spectroscopy:

Kate Sherlock, The Ohio State University
Lillian Christensen, University at Albany
Alexander Cikanek, University of Rochester
Sofia Mehmood, Temple University

Emeritus Membership Award – recognizes members who have contributed to spectroscopy and have been members of the Society for 15 years and have retired from active scientific endeavor: **Gary M. Hieftje, Indiana University**

Fellows Award – established to recognize individual members for their outstanding achievements in and contributions to the science, the profession, and the Society: **Steven Ray, University of Buffalo**

SAS/NASLIBS Award – given to the authors of the outstanding LIBS paper appearing in the journal: **George C. Y. Chan, Richard E. Russo, and Leigh R. Martin** - “Characterization and Optimization of a Spectral Window for Direct Gaseous Uranium Hexafluoride Enrichment Assay Using Laser-Induced Breakdown Spectroscopy”

SAS Atomic Technical Section Student Award – given to students (undergraduate or graduate) who are Society members and who have excelled in the area of Atomic Spectroscopy:

Paula Menero-Valdés, University of Oviedo
Kyle Latty, University of Florida
Lhiam Paton, University of Graz
Maximilian Horstmann, University of Munster

Early Career Travel Grants - awarded to Early Career scientists who demonstrate merit in the field of spectroscopy and/or financial need: **Jay Kitt, Yeran Bai**

President’s Award – established to recognize individual members for extraordinary contributions in service within the preceding 24 months to the Society or for noteworthy achievement in the science of applied spectroscopy: **Brandye Smith-Goettler** - currently serving as Treasurer

SAS Poster Award Winners – established to recognize the top posters presented by students utilizing applied spectroscopy technologies and the allied sciences at the SAS national meeting, SciX:

- Design and Optimization of a new microwave microreactor for mass spectrometry. Presenting Author: **Buddhika T. Kumara, MSc (he/him/his) – The State University of New York at Buffalo**
- Machine Learning-Enhanced LIBS for Spectral Discrimination and Chemometric Analysis of Pu Oxalate Surrogates Presenting Author: Justin I. **Borrero Negrón, MS – University of Florida**
- Correction of Carbon-based Matrix Effects in MIP-OES Presenting Author: **Beatriz M. Fontoura, PhD – Wake Forest University**
- Zeta Potential as a Biosensor for Human Red Blood Cells in ECMO Bypass Circuits Presenting Author: **Brandon K. Eberl – Wake Forest University School of Medicine**
- Streaming Mode Dielectrophoresis to Characterize Micro and Nanoscale Particles Presenting Author: **A K M Fazlul Karim Rasel – Arizona State University**

SAS Service Awards - given to SAS members who have completed service positions within the Society:

Ed MacMillan – Ad Manager
Peter Larkin – Past President
Debbie Peru – Section Affairs
Dana Garcia – Section Affairs
John Wasylyk – Section Affairs

Topiaries in Raleigh, NC.

Attendees at the SciX Gala.

Attendees at the SAS student and early career event at Raleight Flying Saucer.

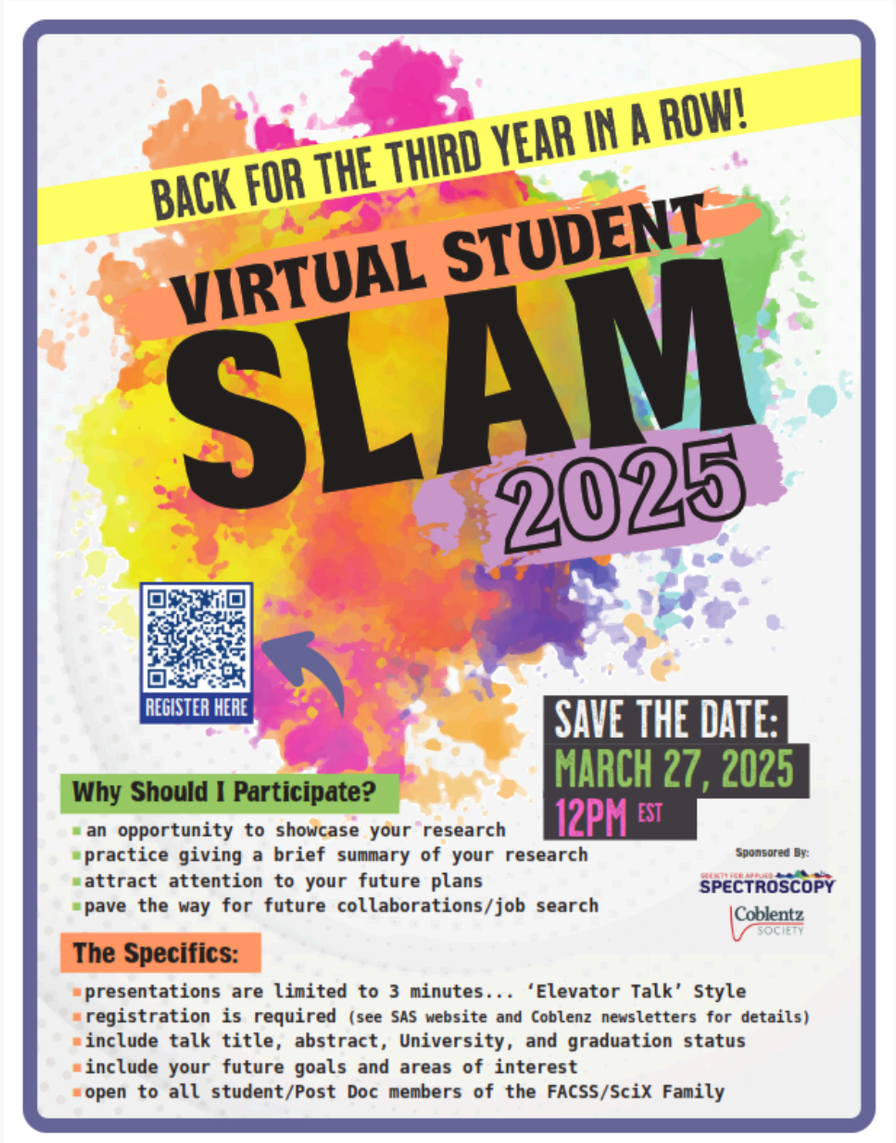
Virtual Student Slam 2025
Each Graduate Student will provide a three (3) minute synopsis of their research to be followed by a 30-minute Q&A session. Topics range from *Analysis of Automotive Paint Smears* to *Understanding Titan's Minerals to Single Molecule Detection*, all using various types of spectroscopies. Speakers are from graduate programs in both the United States and Europe. This event is held completely virtual.

Join us 27 March 2025 at 12:00 PM EST. The event is free to attend.

Register by 1 March 2025 here or use the QR code in the attached flyer.

Sponsored by the Coblentz Society, the New England Regional Section of the Society for Applied Spectroscopy, and the New York-New Jersey Regional Section of the Society for Applied Spectroscopy

John Wasylyk and Angela Gordon

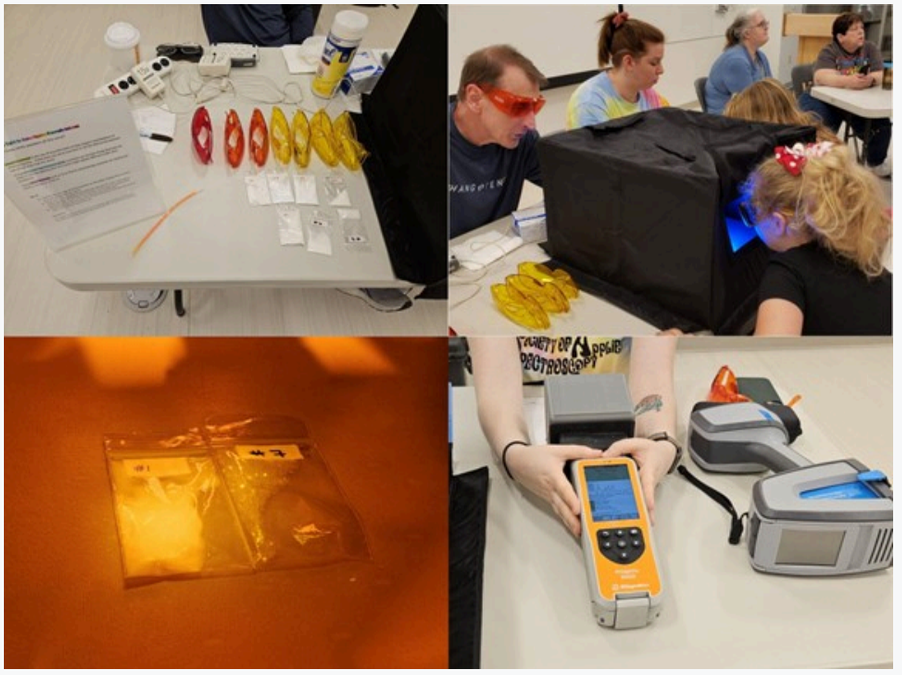


Illuminating Science: A Day of Light and Forensics

Back in May, the Cincinnati-Tristate section once again celebrated the International Day of Light by providing demos to local families at the Cincinnati Museum Center!

This year we added a demo showing how Forensic Scientists use light to analyze samples. The demo involved using Alternate Light Source (ALS) viewing paired with handheld Raman spectroscopy to identify components of similar looking samples. We provided the choice of six different white powders (e.g., talc, cellulose, commercial dishwashing formulations) and asked visitors to choose two to analyze. We then walked the visitor through viewing the samples with ALS while filtering the light using yellow or orange glasses. Next, we analyzed the two samples using a handheld Raman spectrometer (with a safety covering to protect the visitors from the laser source), and showed the viewers the output on the instrument, providing the identity of primary components of the powders. Throughout the process, the viewer filled out a slip of paper—their own “lab notebook” answering questions about their observations at each step. If you would like to receive the table signs sign and sample “lab notebook” sheet, contact gloria Story at ftirgirl@gmail.com.

View a short video clip from the event here.



Caption: (*top row left-to-right)* The “sample” options for visitors to select from and light-filtering glasses for ALS viewing; Demonstrators showing a visitor their samples under ALS and a second visitor looking at the Raman spectrum of their sample. (*bottom row*) Two samples under ALS with an orange filter for viewing; An example spectral output on the handheld Raman spectrometer.

Invitation to Participate in a Special Interlaboratory Study
Dear Colleagues:
We are in the early stages of planning a special, one-time interlaboratory study (i.e., a round robin) for Trace Elements in Caprine Liver. The principal goals of this study are to: 1) assess interlaboratory performance for trace element analysis of soft tissues; 2) assign robust values (± uncertainty) for several trace elements; and 3) produce a limited supply of caprine liver reference materials (RM) that may be useful to research laboratories in method development for trace element analysis of soft tissues. Participation will be entirely voluntary and there will be no charge for participation.

Over the last 38 years, the Wadsworth Center’s Trace Elements laboratory at the New York State Department of Health (NYSDOH) has collected whole liver post-mortem from goats. The animals were previously dosed with Pb during their adult life for the purpose of producing blood lead pools for the NYSDOH Proficiency Testing (PT) program. A few animals also received a one-time small dose of Pb, As, Hg, and Cd so that their major organs would be enriched with these elements as endogenous contaminants. Each caprine liver was frozen post-mortem, until being processed in the laboratory. Wet tissues were thawed and homogenized using a Stomacher™, then freeze dried. Dried tissues were homogenized via an ultra-centrifugal mill and sampled scooped into bottles. One “pool” of caprine liver was supplemented with trace elements (as an aqueous solution) including Rare Earth Elements before being homogenized.

We are inviting participation from laboratories with expertise in trace element analysis of soft tissues and an interest in this endeavor. We are interested in having participants conduct trace element analysis using their own validated method(s) for essential and non-essential elements. Study samples will be shipped in early 2025 with up to nine weeks allowed for analysis. Each participant will be assigned a confidential code number for use in this special event; this number will appear in all summary charts and tables. Each participant lab will receive a reporting spreadsheet containing the confidential code number and instructions for reporting results and methodological details. Participation in this interlaboratory study is intended for educational purposes only. No grading will be implied, nor will responses be deemed acceptable or unacceptable. Any remaining material can be kept and used at the participants' discretion.

If your laboratory is interested in participating, please provide a contact name, email, and address to dluneau@albany.edu by Monday, 16 December, 2024. Participants located outside of the United States should inform us of any restrictions they may have with respect to importing animal products of caprine origin into their country for research purposes. The caprine liver materials intended for this study are not of tissue culture origin and are not zoonotic. Please contact Deanna Luneau (dluneau@albany.edu) if you have any questions.

SAS Member News

CONGRATULATIONS to **Konnor Jones** (Newsletter Chair) on his recent successful dissertation defense, "Anionic: Cationic Surfactant Mixtures at the Oil-Water Interface" at the University of Oregon. Well done, Dr. Jones!

If you have news you want to share with SAS, email the Executive Director at exdir@s-a-s.org