New York/New Jersey SAS December 2021 Presentation

The NY/NJ SAS section cordially invites all interested Newsletter readers to join us for our December presentation by Woody Barton, of LLS Instruments, Inc., speaking on "NIR with Problem Data Sets". The presentation will be over Zoom, with details below.

The presentation will be at 12:00pm EST (9:00am PST) on 16 December 2021. For upcoming talks sponsored by the NY/NJ section of SAS, please see the schedule following December's information.

Join Zoom Meeting: https://us02web.zoom.us/j/2507362969?pwd=eGVsS2hYT0QzRnJyUzRoT1pJeXEzUT09

Meeting ID: 250 736 2969

Passcode: 1958

Find your local number: https://us02web.zoom.us/u/kbCHY7ZXuY

Abstract (Co-Author: J.A. de Haseth)

There are many approaches to developing a data set for near-infrared calibrations, some statistically valid, some not; but all with some interesting insights. There is the ideal situation with a large set of samples and ample laboratory resources for reference chemistry. Do you make a random selection or take every *n*th sample and scan and analyze? Do you start scanning and analyzing and build your calibration data set gradually as you go, with the big question? When do I stop? Yes, you can use the reference data to select a diverse range of samples ensuring that the ends as well as the range are adequately sampled. Some chemometric software packages will choose the most diverse set of samples based on the spectra. This provides a stopping point for initial calibrations and limits the amount of reference chemistry you may have to do. However, it is often not the situations that arise in the NIR lab that provide the most strenuous challenges. Usually, it is the real-world samples from commercial operations that have their limitations based on the process. The bottom line is you get to work with what you are handed.

Biography

Franklin E. (Woody) Barton, II received his B.S. in Chemistry from North Georgia College in 1964 and his Ph.D. in Chemistry from the University of Georgia in 1969. He entered active duty and served as a Field Artillery Battery Commander in Vietnam and returned to do post-doctoral research at the University of Georgia in 1970–1971. He accepted a position with the U.S. Department of Agriculture's Agricultural Research Service in Athens, Georgia, at the Russell Research Center from which he retired in 2008. During his 37 years there, he was the Research Leader of a multidisciplinary research group for over 25 years. He served as Location Coordinator/Center Director for his last four years, and earlier as an Acting Area Director for the South Atlantic Area (Virginia to Puerto Rico). He continued his military service in the U.S. Army reserves by teaching quantitative management course for the Command and General Staff College and retired from the YSAR in 1995. After retirement from the USDA in 2008, he became a partner in Light Light Solutions, LLC and as a senior officer in LLS Instruments, Inc. He is still active in solving analytical problems in the Agricultural and food industries.

Upcoming Presentations for NY/NJ SAS:

27 January 2022: The Power of Multivariate Analysis in Spectroscopy
Michael Roberto, Sartorius Stedim Biotech

27 February 2022: Research Scramble: Elevator Talks by 20 Graduate Students
Elevator Presentations by Selected Graduate Students

Call for Volunteers

The SAS Marketing Committee is looking for volunteers to help with the SAS Newsletter and other social media and journalism tasks starting in 2022. If you are interested please email marketing@s-a-s.org.

Technical SciX 2021 Overviews

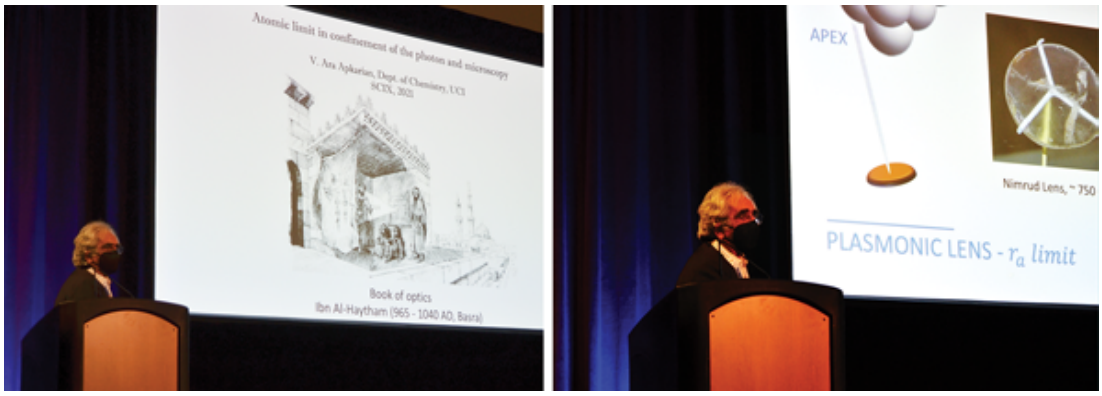
Chemometrics
The SciX 2021 Annual Meeting was exciting and informative for chemometricians. A distinguished chemometrician, Roy Goodacre, won the prestigious FACSS Charles Mann Award. Robert Spiers from John Kalivas' group won the SAS Undergraduate Student Award. Both awards were related to quantification by using multivariate chemometrics. There were five chemometric symposia. The first was, "Bringing it All Back Home: Data Integration Through Chemometrics", organized by Federico Marini of the University of Rome "La Sapienza". Pete Harrington presented the ISO Standard 11843-2 for the statistical determination of detection limits. The second symposium was Current Applications of Chemometrics organized by the Section Chair, Pete Harrington of Ohio University. "Chemometrics for Food and Drug Analysis" was organized by Mengliang Zhang of Middle Tennessee State University. "Chemometric Opportunities in the Forensic Sciences" was organized by Brooke Kammrath of University of New Haven. The final symposium was organized by SAS President Karl Booksh on "Chemometric Theory and Practice" that addressed the important topic of data discretization.

Contributed by Pete Harrington, Chemometrics Chair

SAS-Sponsored Award Sessions
Two SAS-affiliated awards were presented during SciX 2021 in Providence, Rhode Island.

The New England Section awarded the 2021 Lester W. Strock Award to Professor Uwe Karst of the University of Münster, recognizing his work in using mass spectrometry techniques to track the fate of metals in biological and environmental scenarios. His plenary presentation, delivered remotely due to the pandemic, described the tracking of gadolinium-based MRI contrast agents in the water systems of Germany. His award symposium, chaired by SAS Atomic Section co-chair Derrick Quarles, featured talks on the analysis and characterization of nanoparticles in various systems. Speakers included: Jacob Shelley (RPI), Jörg Bettmer (Oviedo), Derrick Quarles (Elemental Scientific), David Clases (University of Technology Sydney), and Ilona Norhorn (Münster).

SAS and *Applied Spectroscopy* presented the William F. Meggers Award for the outstanding paper in *Applied Spectroscopy* to Professor V. Ara Apkarian of the University of California, Irvine for the paper, "The Raman Spectrum of a Single Molecule on an Electrochemically Etched Silver Tip", which was published with co-authors Joonhee Lee, Nicholas Tallarida, and Laura Rios [Vol. 74, Issue 11, pages 1414–1420]. Professor Apkarian's plenary described the underlying physics of the interplay and eventual blurring of identities of the plasmonic electron and photon in the highly confined potential well of the metallic tip. The affiliated award symposium featured talks from Eric Potma (University of California-Irvine), Nan Jiang (University of Illinois-Chicago), Joonhee Lee (University of Nevada, Reno), Hrvoje Petek (University of Pittsburgh), and Bhavya Sharma (University of Tennessee).



Professor V. Ara Apkarian presents his work at the plenary session honoring him and his co-authors for their Applied Spectroscopy paper.

Readers are reminded that prerecorded versions of all talks at SciX 2021 will be available on the conference website, www.scixconference.org, until 31 December 31 2021. All attendees have access to the on-demand library. Persons who did not register for the conference may purchase access to the talks under the "Registration" section of the web site. This library is a great way to catch up on all the talks you might have missed during the conference!

Contributed by Rob Lascola, 2021 SciX Awards Chair

EAS 2021 Overview

Happy Diamond Jubilee (60th anniversary) to EAS!

EAS 2021 (15–17 November) was in-person at the Crowne Plaza Princeton convention center, after the COVID-19 hiatus of 2020. While not up to pre-COVID-19 attendance, there was a fair attendance compared to years past. The theme for this year was "Curiosity, Chemistry, and Perseverance", and there were a number of space related sessions.

Especially well attended was the keynote lecture given by Dr. Roger Wien, Los Alamos National Laboratory. Dr. Wiens gave a very interesting presentation on Mars Rover Perseverance and Curiosity Chemical Imaging with SuperCam Probe. Loads of really interesting pictures of the Mars surface and water-related features. He also described the instruments on the two Rovers and what kind of data they are collecting.

There was also a range of technical presentations covering a variety of interests. As COVID-19 restrictions continue to prevail, most sessions were a combination of in-person, pre-recorded or zoom presentations. The Zoom presentations were a bit of a challenge to connect, but fortunately speakers had also submitted recordings of their presentations. So, when Zoom failed—they could just turn on the recording. The recordings will also be made available to all attendees once the conference is over.

The in-person conference was also a good opportunity to meet up with fellow scientists and catch up. Despite there being less people present, it was still good to get together and talk science again. We hope to see everyone at next year's EAS where the theme is "Embracing Analytical Diversity".

Contributed by Suzanne Schreyer, Session Chair

Editor's Note: As 2021 Closes…

On behalf of the SAS Governing Board and the SAS Executive Committee, we hope that our readership has a pleasant holiday and New Year's season in the coming weeks. We appreciate the volunteers that help with SAS in various capacities, and our Newsletter readership who keeps providing valuable content and news for our spectroscopy community. We hope that 2022 brings back more in-person meetings and avenues for us all to connect and network further.

Luisa T.M. Profeta, SAS Newsletter Editor

Do you have something spectroscopy-related you want to discuss in the newsletter? Or something that will help our membership such as career tips or application tips? Please let us know by emailing luisaprofeta@gmail.com.

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