

SAS SPECTRUM eNEWS



HIGH SENSITIVITY SERS SUBSTRATES FOR TRACE LEVEL DETECTION

Newsletter Editor's Note

This issue and next issue will be mostly focused on SciX 2017, which just took place in Reno, Nevada, October 8–13. In this issue, we will highlight the various SAS sponsored technical sections including chemometrics, process analytical technology, and contemporary issues in analytical sciences. In the next issue, we will highlight the various awards, cool events, and the fun we had. I will also try to share some of my personal experience on chairing a session at SciX in the next issue.

It should be noted that many local SAS sessions continue to hold interesting and relevant events even though this newsletter does not have sufficient space to provide the details to do them justice. For example, the New York and New Jersey sections are organizing two very interesting seminars as noted below.

A picture of the venue (right). Photo courtesy of Luisa Profeta



New York/New Jersey SAS, November and December Meeting

Date: Thursday, November 9, 2017
Time: 5:30-8:30 PM. Dinner and networking 5:30-6:45, talk 6:45-7:45
Speaker: Dr. David W. Hopkins, "Using Derivatives Effectively — Norris Applications"
Location: Horiba, 3880 Park Ave, Edison, NJ 08820
Light Dinner: \$15 for adults, free for an SAS member who brings someone new, \$5 for students. You must email kathrynalee@hotmail.com for dinner reservation.

New York/New Jersey Society for Applied Spectroscopy Meeting at the Metropolitan Museum of Art, New York, New York

Date: Friday, December 1, 2017
Speaker: Dr. Eric Breitung, "Environmental Resting of Materials at The Met: Keeping the Art Safe During Display, Storage, and Shipping Using Advanced Materials Testing"

Contributed by Howard Mark
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SAS-Sponsored Chemometrics Section at SciX2017

Chemometrics symposia were strongly represented at SciX 2017. The leadoff symposium was New Frontiers in Chemometrics with Federico Marini from University of Rome, La Sapienza, in which methods that exploit experimental design were discussed. Neal Gallagher from Eigenvector Research discussed a method of finding anomalous spectra in hyperspectral images. Ludovic Duponchel from Lille University, France, presented his work on the topological analysis of multivariate data clusters. Xiang Zhang from the University of Louisville presented his work on chemometric pipelines for processing metabolomic data. The organizer of the session, Peter Harrington from Ohio University, demonstrated that the common approach of using a single set of validation data may result in misleading conclusions and a statistical approach of bootstrapped Latin partitions should be adopted.

The second symposium was on Spectral Fingerprinting for Characterization of Complex Materials and was organized by Mengliang Zhang of Middle Tennessee State University. This session focused primarily on food characterization with some talks on forensic applications. The third symposium organized by Steve Morgan of the University of South Carolina was Chemometric Opportunities in the Forensic Sciences. John Kalivas of Idaho State University gave an interesting case study of the use of chemometrics to recover removed VIN from a stolen motorcycle. Steve presented his work on the use of likelihood ratios in forensic chemistry. Michael Sigman from the University of Central Florida showed the value of receiver operating characteristic (ROC) curves for the interpretation of forensic evidence.

These three symposia all occurred on the first day of the conference. The Symposia resumed on Wednesday with the Bruce R. Kowalski Award in Chemometrics symposium honoring Joseph Smith that was organized by Barry Lavine, Oklahoma State University. Joseph Smith, University of Delaware, gave an interesting presentation on using chemometrics to find life on Mars using Raman spectroscopy. Renee JiJi from the University of Missouri discussed using deep UV resonance Raman to determine cholesterol in lipoproteins. Tim Corcoran from California State Polytechnic University Pomona showed the use of the Hadamard–Walsh transform for filtering Raman spectra. Frank Vogt from the University of Tennessee discussed hard modeling of micro-algal biosediment using attenuate total reflectance Fourier transform infrared (ATR FT-IR) spectroscopy.

The following day, the chemometric symposia resumed with Multiblock Methods: The Key to Measurement Fusion. We had some last-minute cancellations, but Pete Harrington took over the role of organizer and found some substitute speakers. Interestingly, this symposium turned out to be one of the best of the conference. Federico Marini started the session with an introduction to multiblock data using a favorite subject, beer, which was measured using a variety of spectroscopic methods. Benoit Jallais from AgroParis Tech, France, discussed the use of independent component analysis for modeling hyperspectral images. Pete talked about modifying restricted Boltzmann machines for multiblock modeling. Sergey Mamedov from Horiba gave a talk of multiblock analysis of forensic samples. In the afternoon, Dongsheng Bu of Bristol-Myers Squibb organized the last symposium, New Developments in Calibration Methods. A variety of new methods were presented. Chris Brown from 908 Devices discussed calibration free methods for quantification and Erik Andries from Central New Mexico Community College presented using augmented features and models to enhance calibration.

Contributed by Prof. Peter Harrington
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SAS-Sponsored Analytical Chemists Easing World Poverty at SciX2017

SciX 2017, marks the seventh year of the special symposium entitled Analytical Chemists Easing World Poverty. The session was founded in 2011 by SAS Past-President Diane Parry to highlight unmet measurement needs in developing nations. With the support of sponsors like SAS and Spectroscopy magazine, it has evolved into a popular session examining a variety of topics ranging from technical solutions to instrumentation problems to cultural challenges of Westerners working in developing nations. This year's symposium included five speakers from a wide array of backgrounds.

Laura Frame, a PhD student from the University Strathclyde lab of Duncan Graham and Karen Faulds, discussed her work on paper-based assays for malaria. This mosquito-borne parasitic disease is responsible for hundreds of thousands of deaths each year, primarily in sub-Saharan Africa. Stable, fast, simple, and cost-effective point-of-care detection is crucial in the fight against this disease. Using 3D paper diagnostic devices is a popular and growing area of research, and the subject received wide coverage at this year's SciX.

Dr. Peter Summers, University of Nottingham, Ningbo, China, highlighted the extensive problem of plastic waste recycling in China. Because these waste plastics are often contaminated, they are considered a low-value waste stream, which results in lack of incentive to invest. Instead, waste undergoes manual sorting, which exposes workers to toxic chemicals and other hazards. Dr. Summers' group is attempting to find better ways to sort and qualify waste plastics and add value for use in, i.e., plastic automobile parts. By adding such value, it becomes cost effective to mechanize the recovery process, leading to economic benefits and the reduction of hazards to human health.

Dr. Joaquin Rodriguez-Lopez, University of Illinois at Urbana-Champaign, discussed the myriad problems associated with sustainable energy efforts in developing nations. Among these, the problems of energy storage and smoothing variations in energy availability from, e.g., solar and wind energy loom large. Dr. Rodriguez-Lopez and his group are addressing this problem through development of large-scale, efficient, nonaqueous redox flow batteries based on a size-exclusion flow design that addresses many of these challenges.

Confronting the challenges faced by communities around the world must involve educating a new generation of science-literate citizens. Seth Thompson, from the University of Minnesota, in conjunction with the Mayo Clinic, introduced InSciEd Out (Integrated Science Education Outreach), a K-12 STEM education initiative that seeks to enhance the relevance of science in education and increase the sense of connectedness to nature among students and teachers. Increasing this sense of connectedness is both empowering and acts as a health intervention, as the connection between individual and societal behaviors, environmental health, and personal well being become clear. These initiatives are being carried out both at home and abroad, particularly with several partner schools in India.

Dr. Christopher Pierret, also with the Mayo Clinic in Rochester, Minnesota, expanded on Thompson's presentation by discussing the efforts of InSciEd Out using transgenic zebrafish as critical educational tools. These fish are also practical and useful diagnostic tools for the detection of water and watershed contamination and environmental toxicity, as well as tools for exploring heredity, genetics, and infectious disease. This work has blossomed into initiatives in higher education institutions in India that are providing new opportunities for scientific inquiry for both undergraduate and graduate students, creating a meaningful scaffold for cooperation between researchers and communities.

The Society for Applied Spectroscopy has been a strong supporter of this special session over the years. The symposium is a unique example of the cross-disciplinary nature of the SciX conference. It brings together practitioners from diverse communities, giving us the opportunity to use our expertise within our professions to make connections and find new ways to solve critical problems in under-served regions of the world. We look forward to seeing what next year's session brings.

Contributed by Rebecca Airmet
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SAS-Sponsored PAT Section at SciX2017

Seven PAT sessions were organized at SciX 2017. The first session on Monday, entitled "SAS PAT Technical Session: PAT in the Pharmaceutical Industry", was preceded by the SAS PAT technical section meeting. The meeting consisted of explaining that the section exists mainly to organize the PAT sessions at the SciX conference for the membership to attend. People were welcomed to attend this and the other six sessions. The sponsors were acknowledged and the group had no other business volunteered and was adjourned. The PAT sessions that were presented at SciX17 include:

1. SAS PAT Technical Session 1: PAT in the Pharmaceutical Industry organized by Brandye Smith-Goettler. This session is intended to show the new techniques being utilized for process monitoring in the pharmaceutical small molecule sector of the pharmaceutical industry.
2. SAS PAT Technical Session 2: PAT in the Biopharmaceutical Industry organized by Saly Romero. The intent of this session was to highlight the differences and technology used for process monitoring in the production of Biopharmaceutical and how spectroscopy is being used to enhance the bioprocessing.
3. Industrial Applications of Vibrational Spectroscopy organized by Mark Rickard and Shawn Chen. This session is intended to provide a forum to show how process monitoring and vibrational spectroscopy are being used in non-pharma industries, petrochemical, fine chemical, polymer, consumer, and other.

4. On-line Analysis of Industrial Processing and Reactions: Improvements and Best Practices organized by J.D. Tate and Anna Sandlin. The intent of this session is to show the use of all analytical techniques used in industrial processing and reaction monitoring such as gas chromatography, microwave, air monitoring and other techniques.
5. Advances in On-line Process Analysis organized by Allison Nordon from the University of Strathclyde in the UK. This session is intended to bring the academic perspective to the PAT field and perspectives from the UK and covers new technology such as ultrasonic imaging, NMR, terahertz and other technologies along with novel chemometric approaches for data analysis.
6. Process Monitoring Enhanced Flow API and Continuous Manufacturing organized by Jim Rydzak. This session is intended to bring the latest in monitoring techniques that are being applied to continuous flow chemistry synthesis of active pharmaceutical ingredients (API) and drug product manufacture.
7. Hand-Held and Portable Spectrometers: Applications and Instrumental Methods organized by David Schiering. This session's intent is to present the state of the art in hand held spectrometers that can be applied to various facets of analysis including field analysis, raw material, counterfeit identification and other industrial uses.

Process Monitoring Enhanced Flow API and Continuous Manufacturing organized by Jim Rydzak.

This session had a distinct flow designed into it. The first two speakers had academic and industrial perspectives on the development and use of flow chemistry to enhance, streamline and improve the economics of the synthesis of small molecule pharmaceuticals. Part of the discussion centered on improvements to pharmaceutical that could bring down the cost of drugs like antimalarial and other pharmaceutical desperately needed in the third world but beyond their reach because of cost. The third talk spoke of an industrial approach to developing continuous manufacturing that encompassed the entire production from flow chemistry API synthetic production to the finished continuous end product tablet production. The last two speakers concentrated on the continuous end product one from an academic-industrial collaboration and the other from the pharmaceutical industry.

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**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 xchen4@dow.com.**

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