

# 27th ASMS Sanibel Conference on Mass Spectrometry—Security and Forensic Applications

**José R. Almirall & Glen P. Jackson**

## Journal of The American Society for Mass Spectrometry

The official journal of The American Society for Mass Spectrometry

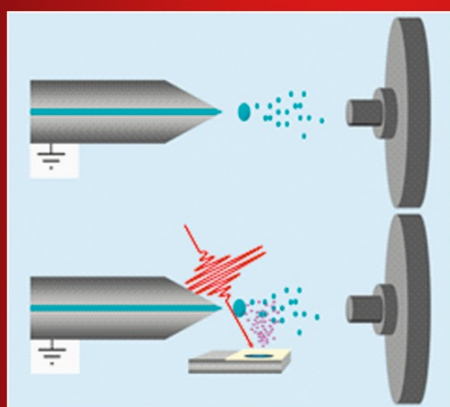
ISSN 1044-0305  
Volume 26  
Number 5

J. Am. Soc. Mass Spectrom. (2015)  
26:695-698  
DOI 10.1007/s13361-015-1107-0

Volume 26 Number 5

May 2015

## Journal of The American Society for **MASS SPECTROMETRY**



Protein charge states increase using supercharging additives in LEMS vs. ESI, see page 706.

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ISSN 1044-0305 • 26 (5) 695-846 (2015) • 13361



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## REVIEW

## 27th ASMS Sanibel Conference on Mass Spectrometry—Security and Forensic Applications

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The 27th Annual ASMS Sanibel Conference on Security and Forensic Applications of Mass Spectrometry was held from January 22 to 25, 2015 at the Hilton Clearwater Hotel in Clearwater Beach, FL. The co-organizers were José R. Almirall of Florida International University and Glen P. Jackson of West Virginia University. The conference brought together leading researchers and practitioners from universities, research institutions, and forensic laboratories to discuss the application of mass spectrometry to issues of national security and forensic science. Attendees represented many corners of the world, including Australia, Brazil, Canada, China, Czech Republic, Denmark, France, Germany, Sweden, United Kingdom, and the United States. Although the weather was very windy and cold by Florida standards, the enthusiastic spirit of the attendees was unaffected. Graham Cooks of Purdue University gave the conference a boost by providing NSF funds to support student travel. The grant (CHE-1262145) titled “Strengthening Forensic Science through Connections with the Analytical Sciences” provided 20 travel awards for students to attend the conference. ASMS provided an additional 20 awards, all of which were filled. The organizers and the students remain very grateful for the exposure to cutting-edge research and researchers in forensic mass spectrometry. The conference attracted a total of 150 registrants (Figure 1) and more than 56 poster presentations. In addition, five attendees signed up to receive two continuing education units (CEU) from West Virginia University.

The conference opened on Thursday evening with a fascinating keynote presentation by Sir Peter Fahy, Chief Constable of the Greater Manchester Police in the UK. Sir Peter Fahy, Knighted for his services to policing in 2012, provided fascinating insights into the history of policing and the continuously changing nature of crime. Many analogies exist between policing methods in the US and UK—like a civilian police force and funky hats—which is not true in most parts of the world. Sir Peter’s perspective on the implementation of science in law enforcement reminded the audience of the importance of buy-in from policy makers and the public. Most importantly, his

talk taught us about the importance of investigating criminals, not crime.

The plenary lecture on Friday morning was given by the charismatic Dr. Vahid Majidi, Deputy Assistant Secretary of Defense for Nuclear Matters. Vahid walked the audience through a ~15-year story of his personal perspective in national security positions, from Los Alamos National Lab, through the FBI, to his current position as Assistant Secretary at the Department of Defense. Vahid successfully educated and scared the audience about the realities and challenges of weapons-of-mass-destruction (WMD) scares, such as the famous Litvinenko polonium poisoning cases of 2006 and the Anthrax-letter cases of 2001. His talk injected a level of enthusiasm into the conference that reverberated throughout our time together. Doug Duckworth of PNNL talked about the application of ICP-MS to nuclear security issues. Doug’s group develops electrochemical methods to pre-concentrate attogram levels of uranium and plutonium for isotopic analysis using multicollector inductively coupled plasma mass spectrometry (ICP-MS). Impressive results included isotope-ratio measurements of plutonium from only a few tens of thousands of atoms in solution, and direct analysis of ultra-trace uranium and plutonium in glass using laser ablation ICP-MS.

Continuing the theme of isotopes and provenancing, Gabe Bowen from the University of Utah talked about the capabilities of geospatial forensics, a subject that seeks to predict the geographic origin of matter. Gabe presented the use of a Bayesian framework to help combine independent isotope measurements and other pieces of prior knowledge about a case to provide probabilities about the possible origin of forensic substrates. Gabe also taught us not to hunt deer illegally in California! Russell Frew of the International Atomic Energy Agency (IAEA) and the University of Otago, NZ, described the application of multi-isotope databases to support food authentication and biosecurity. His talk emphasized the importance of collaborating with stakeholders and the food industry to understand the factors that influence food distribution.

Glen Jackson described several forensic applications of isotope-ratio mass spectrometry (IRMS). He presented the capability of bulk and compound-specific isotope analysis to classify human hair to subject groups, including body mass index, age, and sex. The talk also described the use of isotope



Figure 1. Attendees getting blown away by the wind, and the quality of the presentations

ratios to link blowfly larvae, pupae, and adult flies to different food sources. Oliver Sutcliffe's group, at Manchester Metropolitan University, UK, uses a variety of analytical approaches, including mass spectrometry, to link precursor chemicals to new psychoactive substances (NPS). Oliver highlighted some of the major limitations to advancing knowledge in the area of NPS; these include the lack of chemical suppliers and lack of toxicological data. Whereas IRMS can link sources and products and discriminate products of different sources, IRMS cannot currently discriminate the products of different replicate syntheses.

From the nearby University of Tampa, Kenyon Evans-Nguyen talked about a variety of fieldable elemental and organic mass spectrometry approaches to help characterize street samples. Kenyon showed that on-site tandem mass spectrometry (MS/MS) of DART-generated drug ions enables better selectivity than full mass scanning. He discussed his group's recent progress towards a home-built plasma ion source at ambient pressure that can form both metal ions from refractory materials at high power and molecular ions of organic materials at low power. Facundo Fernandez of Georgia Institute of Technology talked about his well-known work using DART and MS/MS to help answer questions about counterfeit, substandard, and degraded medicines. Facundo also showed how a novel plasma ion source, in combination with portable ion mobility spectrometry, may provide an alternative and smaller instrument for field screening of drugs and medicines.

Guido Verbeck, from the University of North Texas, presented his work using nanomanipulation and nanoelectrospray mass spectrometry to screen forensic substrates for drugs, gunshot residue (GSR), and explosives. His group can detect attogram quantities of drugs on fibers and fingerprint residues, while preserving the integrity of the fingerprint ridges. They can also identify inorganic explosives in nano-manipulated samples by using sugar-adduct ions. Zheng Ouyang from Purdue University impressed the audience with his group's latest work in the area of fast, on-site detection of explosives and drugs using miniature ion-trap mass spectrometers. Using only 0.4  $\mu\text{L}$  of blood and 10  $\mu\text{L}$  of methanol in a paperspray

format, their portable MS system can detect a series of controlled substances below biologically relevant levels. Zheng described the clever yet simple slug flow microextraction spray of drugs in blood and urine, which enables liquid-liquid extraction in a capillary and produces more prolonged and stable ion signals relative to paperspray.

Arian van Asten, of the Netherlands Forensic Institute and the University of Amsterdam, continued the theme of paperspray MS from the perspective of an operational forensic laboratory. Arian courageously proposed the idea of integrating instrumental methods of analysis into the hands and workflow of regular police officers. The paradigm shift to move laboratory methods to non-chemists in the field poses many challenges, but the relevant government agencies are seriously considering his futuristic approach. His group is establishing an International Organization for Standardization (ISO) standard method for drugs in blood and urine using paperspray MS, and developing several other very interesting applications involving reactive paperspray. In another innovative vein, Arian also introduced the concept of estimation of error in chemical identifications, which is a vastly overlooked area of forensic science.

From the Forensic Science Program at Michigan State University, Ruth Smith presented her exciting preliminary work in the area of mass spectral filters to help keep up with the rapidly evolving designer drugs. Using accurate mass time of flight (TOF) data, Ruth demonstrated the potential and challenges of using mass defects and Kendrick mass defects of molecular ions and fragment ions to help identify and classify phenethylamines and cathinones. Bruce McCord from Florida International University introduced the audience to the complexities of post-blast detection of improvised explosive devices. In addition to presenting his work using crown ethers to help detect inorganic anions and cations in capillary electrophoresis, Bruce also presented interesting results on the transfer and persistence of inorganic explosives in fingerprints. He also presented some fascinating results of on-site measurements using paper microfluidics.

Libby Stern from the FBI Laboratory in Quantico, VA presented her work measuring the stable isotopes of explosives



and their precursors. Most manufacturers have enormous variability in the isotope ratios of their products, and this variability makes source identification a significant challenge. However, urea nitrate and TAT were amenable to classification/discrimination. In certain cases, carbon and nitrogen isotope ratios could be linked between precursors and products, but oxygen and hydrogen isotopes were not as reliable. John Goodpaster from IUPUI started his presentation with a bang, literally, by showing fascinating high-speed videos of pipe-bomb explosions. He presented a concept of total vaporization solid phase microextraction (TV-SPME) as a method of explosive preconcentration prior to fast GC-MS detection. He also showed how the mass of nitroglycerin was distributed among the various pipe bomb fragments. Mike Sigman of the University of Central Florida presented his group's recent work in applying chemometrics to fire-debris analysis. Mike guided the audience through chemometric schemes that have been used in the past to classify ignitable liquids. Initial testing using a variety of chemometric techniques has provided true positive classification rates on the order of 95% and false positive rates on the order of 13%. His results highlight the difficulty in classifying low levels of ignitable liquids in the presence of high matrix or background. He finished with a demonstration of how to employ an objective likelihood ratio approach to classify ILs.

José Almirall presented his group's research on the chemical characterization of printing inks using a variety of microscopic, spectroscopic, and instrumental methods of analysis to classify and discriminate a large number toners, offset inks, inkjets, and intaglio inks. His work compared scanning-electron-microscopy energy-dispersive X-ray spectroscopy (SEM-EDX) with laser-ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) for inorganic analysis of inks on substrates using a variety of chemometric approaches to show excellent association (~100%) of inks from the same source. Discriminating power is also quite good (>97%) for both SEM-EDX and LA-ICP-MS for toners, but only LA-ICP-MS performed well for the discrimination of all inks tested. A proprietary database search algorithm was demonstrated by searching several types of data including DART-MS data for more than 300 samples in the database. From the Brazilian Federal Police, Jorge Zacca presented cutting-edge applications of ambient ionization techniques to document analyses. Jorge's group has explored several ambient ion sources, including DESI and easy ambient sonic spray (EASI) coupled to a high resolution Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR-MS) or Orbitrap MS. He finished with the introduction of Venturi-assisted laser desorption ionization MS (VALDI-MS) as a way to decouple the desorption and ionization steps.

The Saturday evening session for promoted talks started with an impressive talk by Christian Reynolds of Wayne State University. He presented the use of laserless matrix-assisted ionization (MAI)-mass spectrometry as a novel method for use in airport security and field hospitals. Jenny Van from San Diego State University gave a clear account of her research in

the area of breath analysis. The last promoted talk was given by Stefanie Pleik of Justus Liebig University, who studies the composition and aging of fingerprint residues.

Sunday Morning opened with the presentation of certificates and checks to six poster award winners; three from each evening. The winners of the best student posters were Esme Candish, Brandon Stamper, Kristina Williams, William Hoffmann, Sarah Prebihalo, and Rhett Williamson.

The Sunday morning technical session began with Stephen Morgan of the University of South Carolina. His group uses LC-MS/MS to identify extracted dyes from individual fibers. The approach works well for most fibers with the exception of cotton fibers, which have different fundamental chemistry and high variability. Using a disposable tip device to extract and preconcentrate drugs, his group used LC-MS/MS to identify more than 40 drugs of abuse in blood and meconium in a fully automated manner. Karen Wahl from PNNL provided an enlightening summary of ricin production and toxicological effects. Karen described her group's work to link purified ricin preparations to castor bean sources. Acetone, carbohydrate, and oil content were also found to be significantly different for different preparations, and so can also be useful indicators of source and preparation route. She finished with a glimpse into a proteomic approach to identify ricin protein. Niels Morling from the University of Copenhagen, Denmark presented his unique work in the area of MALDI-TOF MS of DNA polymerase chain reaction (PCR) product analysis, such as single nucleotide polymorphisms (SNPs) and short tandem repeats (STRs). This approach has been used to identify individuals in mass disaster events and to identify ancestry and phenotypes such as eye color. On the theme of human profiles, Shari Forbes of the University of Technology, Sydney, Australia presented her group's work in the area of human decomposition odor analysis. Her group conducted a series of decomposition studies using pigs (as proxies for humans) under a variety of environmental factors. The number of identified volatile organic compounds (VOCs) was approximately twice as large for GCxGC-TOFMS compared with GC-MS, and several new ether and sulfur compounds were detected. The work is currently being used to help understand the training and tracking of cadaver-detecting canines.

Bryn Flinders from Maastricht University described his group's impressive efforts in mass spectrometry imaging of molecules in forensic applications in three important areas: distribution of drugs in hair, obliterated writing, and fine fingerprint structure. Finally, Adam Hall from the Barnett Institute at Northeastern University presented new approaches for fire-debris analysis using dynamic headspace concentration followed by DART-MS and chemometric analysis, including a nice comparison of GC-MS data with DART-MS data using American Society for Testing and Materials (ASTM) International Guidelines. DART-MS data provided some differences in MS profiles from different brands for the limited set of samples studied. Chemometric analysis of the information-rich spectra was applied and shows promise for interpretation and differentiation of gasoline samples from different brands.

On-line surveys conducted after the conference showed that most attendees liked the conference topic, the format, and the speakers. The attendees especially liked the number of young faculty in the program, the inclusion of promoted talks by students in the evenings, and the number of student posters. Regarding the breaks and 25-min cap on presentation times, one attendee reported, "It was good that presentations were kept short and punchy, and there were so many opportunities for discussion and networking." The most frequent critique in the surveys—which is not exactly a critique—was that forensic applications are not revisited often enough at Sanibel or Asilomar. This is the perfect time to remind readers that anyone can submit a topic suggestion to the Sanibel committee by using the on-line form (<http://www.asms.org/conferences/suggest-a-topic>).

Thanks again to ASMS for selecting, funding, and organizing the conference. We hope next year's meeting on Pharmaceutical Applications is as successful.

## Acknowledgments

The workshop was made possible with partial financial support by the National Science Foundation under grant CHE-1262145 to Purdue University. Any opinions, findings, and conclusions or recommendations expressed in this review are those of the participants and do not necessarily reflect the views of the National Science Foundation.