

ASMS 2018 Energy, Petroleum, and Biofuels Interest Group Workshop: “Expanding Compositional Space Coverage”

Marianny Y. Combariza and David D. Stranz presiding
Monday, June 4th, 2018 5:45 – 7:00 pm, Room 10

Format:

- Marianny Y. Combariza (University of Santander, Colombia) and David D. Stranz (Sierra Analytics, USA)
 - Welcome
 - Introduction and overview of workshop
 - ASMS oral and poster sessions on Energy, Petroleum & Biofuels
 - Rotation of interest group coordinators
- Four speakers (12 minutes each) on the topic of “Expanding Compositional Space Coverage”
 - Amy McKenna (NHMFL, FSU, USA): Segmented Data Acquisition and Spectral Stitching
 - Ryan P. Rodgers (NHMFL, FSU, USA): Online LC/MS on the 21T FT-ICR-MS
 - Carlos Afonso (University of Rouen, France): Ion Mobility / MS
 - Mark Barrow (University of Warwick, UK): Statistical Pretreatment of MS Data
- Question and answer session, with discussion

The ASMS Energy, Petroleum, and Biofuels Interest Group held its workshop on Monday evening (June 4th, 2018) as part of the 66th ASMS Conference on Mass Spectrometry and Allied Topics in San Diego, CA. Interest Group coordinators Marianny Y. Combariza (University of Santander) and David D. Stranz (Sierra Analytics) presided. Approximately 50 – 75 people were in attendance.

A brief business meeting started the workshop, with a call for greater submissions of oral and poster presentations for the 2019 conference and an emphasis of choosing appropriate categories when submitting. This year, there was only one oral session and a relatively small representation during the poster sessions. Choosing appropriate topic areas when submitting abstracts will help to increase the visibility and the representation of the interest group at future conferences.

A call was also made for a volunteer to replace outgoing interest group co-chair David Stranz for the 2019 – 2020 two-year cycle. Amy McKenna of NHMFL, Florida State University volunteered, and her name will be submitted to the ASMS Board for approval.

The workshop then proceeded to the main event, short presentations by the four speakers on “Expanding Compositional Space Coverage.” A number of techniques have been described in recent year which have greatly increased the number and reliability of chemical formula assignments to spectra of petroleum, biofuels, and related substances.

Direct complex sample analysis using FT-ICR-MS can be challenging due to analyzer overload or signal suppression for low-abundance analytes. Spectral stitching is an effective strategy to overcome these issues. Amy McKenna, from the NHMFL, described techniques for implementing segmented data acquisition and stitching on FT-ICR-MS instruments and how this has yielded orders of magnitude increases in the number of observed species, for the analysis of complex mixtures such as NOM and crude oil samples.

Ryan Rodgers presented recent results of online LC/MS data acquisition on the 21T FT-ICR-MS instrument at the NHMFL. As with segmented acquisition, lowering the density of species present in the FT-ICR cell coupled with higher field strength provides the ability to observe and assign a much

higher number of peaks even in broadband acquisition. An LC method that separates based on ring size was a key element in the experiment.

Ion mobility-mass spectrometry (IMMS) is becoming a powerful tool for analysis of highly complex mixtures. This method adds an additional postionization separation dimension to MS analysis. In an orthogonal approach, Carlos Afonso, from University of Rouen, described the use of IM coupled with high resolution TOF-MS to perform accurate mass measurements and size- and shape-dependent separation. This information, combined also with CID experiments, can be useful to determine structural features and to identify particular compound families within complex samples. The IM separation of ions occurs at time scales of milliseconds and is particularly useful when chromatographic separation is not possible.

FT-ICR-MS instruments, with high resolving power, can detect increasing numbers of components in complex mixtures such as NOM, biofuels and crude oil. Computer analysis of growing amounts of data requires versatile software tools and algorithms able to provide confidence in data handling. Mark Barrow, from University of Warwick, described work done in his laboratory on statistical evaluation of peak reproducibility in replicate analyses, the Themis algorithm, and how use of those results improves the reliability of composition assignments by eliminating spurious or noise peaks from assignment.

The workshop concluded with a brief question and answer session. The presenters were asked to provide a list of relevant references for their work. The coordinators plan to send these by e-mail to all members of the Interest Group.

Respectfully submitted,

Marianny Y. Combariza
David D. Stranz

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