

Report ASMS 2019 Energy, Petroleum, and Biofuels Interest Group Workshop: “Targeted Analysis, Fingerprinting, and Speciation in Complex Mixtures”

Presiding: Marianny Y. Combariza and Amy M. McKenna.

Date & Time: Monday, June 3, 2019. 5:45 to 7:00 p.m.

Place: Georgia World Congress Center, Building A, Level 3 Concourse, Meeting Room A304.

Workshop Outline

1. Marianny Y. Combariza (Universidad Industrial de Santander, Colombia) and Amy M. McKenna (National High Magnetic Field Laboratory, Florida State University, USA)
 - Welcome
 - Introduction and overview of the workshop
2. Four speakers (12 minutes each) on the topic of “Targeted Analysis, Fingerprinting, and Speciation in Complex Mixtures.”
 - Ralf Zimmermann. Full Professor, Analytical Chemistry Institute and Head of the Joint Mass Spectrometry Centre, University of Rostock, Germany.
Topic: Thermal Analysis MS for Complex Mixture Analysis.
 - Lieve Laurens. Senior Scientist in Biological Science, Bioenergy Center, National Renewable Energy Laboratory, USA.
Topic: Mapping the Algal Lipidome by FT-ICR MS to expand the Biofuel and Bioproduct Portfolio
 - Leonard Nyadong. Senior scientist, Phillips 66, USA.
Topic: Correlation of Asphaltene Structural Composition with Molecular Weight.
 - Remy Gavard. Ph.D. student in Mark Barrow's group, University of Warwick, UK.
Topic: Addressing the data Challenge of Complex Mixtures Analyzed by Hyphenated Ultra-High Resolution Mass Spectrometry.
3. Question and answer session, with discussion.

Workshop Summary

The ASMS Energy, Petroleum, and Biofuels Interest Group held its annual workshop on Monday evening (June 3, 2019) as part of the ASMS Conference on Mass Spectrometry and Allied Topics in Atlanta, GA.

Marianny Y. Combariza (Universidad Industrial de Santander) and Amy M. McKenna (NHMFL, Florida State University) organized the workshop. Approximately 45 – 55 people were in attendance.

A brief business meeting started the workshop, this year the ASMS was held at the Georgia World Congress Center, Building A, Level 3 Concourse, Meeting Room A304, on Monday, June 3, 2019, from 5:45 to 7:00 p.m.

The workshop then proceeded to the main event, short presentations by the four speakers on “Targeted Analysis, Fingerprinting, and Speciation in Complex Mixtures.” Correlating compositional data to macroscopic behavior is paramount to future energy research, with HRMS playing a vital role in providing molecular information. Complex organic mixture analysis by MS has prompted the development of new ionization sources and techniques, off- and on-line chromatographic methods, and data processing algorithms. Despite many efforts to overcome the limitation of ion suppression in these polydisperse systems, compound classes present in low concentration remain undetected. Often, these species are responsible for performance issues of final products derived from the raw feeds. Therefore, targeted analysis, fingerprinting and selective speciation of chemical functional groups are emerging as the next significant advancement in MS of complex mixtures.

Professor Ralf Zimmermann described the use of Thermal Analysis coupled with MS for Complex Mixtures Analysis. The technique allows observation of larger molecules behavior under increasing temperatures and also to study building blocks and to obtain diagnostic thermal fragments. The approach can be used for crude oil, asphaltenes, bitumen, deposits, polymers, and biofuels analysis.

Lieve Laurens explained how untargeted lipidomics could be helpful to create a compositional profile in biofuels; however, this approach does not allow unusual compounds (e.g., pigments) to be observed. Thus, separation/fractionation steps must be added to the workflow for lipidomics in novel biobased feedstocks analysis to increase formula assignment and compound identification.

Leonard Nyadong showed how selective fractionation strategies (based on polarity) coupled with high-energy collision-induced dissociation (HCD) can be used to observe differences in molecular structures (island vs. archipelago) for complex mixtures such as asphaltenes.

Finally, Remy Gavard described work done on a new workflow aimed to reduce HRMS data size (from GB to MB) without loss of information, and on shortening analysis time (from days to minutes) for large datasets like the ones obtained for chromatography - UHRMS coupling. The workflow involves use of the instrument's manufacturer software and the assignment software (e.g., Composer, PetroOrg) with a new algorithm (KairosMS) that allows fast data processing, integration, and interactive visualization of complex datasets.

The presentations concluded with a question and answer session.

Finally, a call was also made for a volunteer to replace outgoing interest group co-chair Amy M. McKenna for the 2020 – 2021 two-year cycle. Leonard Nyadong, Senior scientist, Phillips 66, was nominated and his name will be submitted to the ASMS Board for approval.

Respectfully submitted,

Marianny Y. Combariza and Amy M McKenna

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