

## Report on the 2015 ASMS Conference Workshop “Advanced MS and Separation Approaches for Biofuels and Petroleum”

Patrick G. Hatcher and Mark P. Barrow

The workshop was held on Monday, June 1 in Room 132 at 5:45 – 7:00 PM. Dr. Barrow moderated the workshop speakers and discussion after a short introduction by Dr. Hatcher. The following organization was prepared to spur discussion:

- Mark Barrow (University of Warwick, UK)
  - ❖ Introduction
- Florian Albrieux (IFPEN, France)
  - ❖ “Real world” areas of research
  - ❖ Experimental methods
  - ❖ Discussion
- Janne Jänis (University of Eastern Finland)
  - ❖ Data analysis and validation
  - ❖ Structure
  - ❖ Discussion

Slides for each of the speakers are included in this report and these served to stimulate abundant discussions in which a significant proportion of the 75-100 participants stepped up to make comments. Those attending represented a range of academic and commercial establishments, and the active discussion lasted the full duration of the available time.

It became quite clear in these discussions that we need better strategies to characterize both bio-oils and petroleum-derived oils. We also need to find ways to standardize the vast amounts of data being gathered for these materials. Along this line, we need to find approaches to better quantify products for which authentic standards are scarce or unavailable. In the case of biofuels, an important question is how do we utilize the MS approaches to predict pyrolysis product quality. In the areas of both petroleomics and biofuels, some important questions arose regarding:

- Chemical structure of molecules for which only elemental formulas are obtained
- The need to combine other characterizations methods (NMR, spectroscopy) with MS to obtain a more comprehensive view of sample composition
- Data analysis needs to be more automated and incorporate statistical treatment of large datasets
- Understanding of the chemistry will require the development of structural databases
- Can better progress be made by limiting the focus of examination to the 10 or 20 most abundant compounds or is it vital to include all of the minor components?

Overall, much discussion ensued on these topics with the hope that such discussion would promote added focus of research efforts and guide the work to be presented at future ASMS meetings.