

Report on Lipid Mass Spectrometry and Lipidomics workshop

61st ASMS 2013, Minneapolis

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The proposal for this inaugural workshop is stated below:

“The primary goal of the inaugural ASMS Lipids and Lipidomics workshop will be to bring together like-minded people in the field to gauge the potential interest in establishing an ASMS Interest Group in this area, as well as to discuss the current status and future needs of the various mass spectrometry technologies and data analysis strategies that are associated with worldwide lipidome analysis efforts. This discussion will be facilitated by several informal presentations, followed by an extensive discussion period, from several leading researchers in the field.”

The workshop was held on Wednesday June 12th (5:45-7:00 pm in convention centre 208A) and was attended by approximate 190 conference delegates (only a few seats were available in the room which had a capacity of 210). Discussions with attendees revealed that they included university- and industry-based researchers; representatives from instrument vendors (e.g., Waters, Thermo and AB Sciex representatives were all confirmed to be present - others may have also been in attendance); as well as representatives from lipid supply (e.g., Avanti Polar Lipids) and analysis companies (e.g., Zora Biosciences). The workshop attendees also covered the spectrum of expertise, with several participants being well-recognised experts in mass spectrometry while others had only recently been tasked with establishing lipidomics in their own laboratories.

Short presentations were made by three leading researchers in the field, namely, **Prof Robert Murphy** (University of Colorado Denver Health Sciences Centre); **Prof Xianlan Han** (Sanford Burnham Medical Research Institute); and **Dr Kim Ekroos** (Zora Biosciences, Finland). Presenters had been given only the following questions to guide their presentations:

“What do you think are the current challenges in lipid science and what opportunities are there for mass spectrometry to continue to expand its contributions to the field?”

Within this broad scope the speakers addressed several critical challenges in the application of mass spectrometry to lipid analysis in the context of their own recent work and there was wide-ranging discussion from the floor on several of these points. Three in particular were prominent, these were:

- (i) the need for strategies for identification of lipid structure, especially new structures encountered in discovery-type analysis. This also highlighted the need for clear lipid nomenclature that defines the level of knowledge and the implicit assumptions in the structural assignments. Recent contributions to classification and nomenclature for lipid mass spectrometry by Ekroos (“Lipidomics Perspective: From Molecular Lipidomics to Validated Clinical Diagnostics” in *Lipidomics*, Wiley 2012) and Liebisch *et al.* (“Shorthand Notation for Lipid Structures Derived from Mass Spectrometry” *Journal of Lipid Research* 2013, ASAP) were noted as important steps in this direction.
- (ii) the need for accurate and reproducible quantification of lipids in complex extracts. It was noted that vendors needed to be made aware of some of the specific requirements for lipidomics applications. The greater availability and cost-effectiveness of lipid standards was identified as an area for further development and the idea of a cross-laboratory validation study was also put forward.
- (iii) a large amount of research remains to make sure that methods for identification and quantification of lipids are robust, reproducible and validated, that could move the field beyond discovery to clinical applications.

A show of hands at the conclusion of the workshop indicated that the majority of those present found the discussion helpful and would be interested in further discussions on these topics to be facilitated by ASMS either through an ongoing conference workshop; the development of an interest group and/or specialist conferences on this topic (e.g., Fall workshop, Sanibel, Asilomar).