Report on workshop convened by Lipid Mass Spectrometry and Lipidomics Interest Group

62nd ASMS 2014, Baltimore

"Systems of annotation and reporting requirements for lipid mass spectrometry"

co-chairs:
Prof Stephen Blanksby (Queensland University of Technology)
A/Prof Christer Esjing (University of Southern Denmark)

The original proposal for this workshop is stated below:

"A recurring theme [from the inaugural workshop in 2013] was the importance of developing guidelines for the uniform reporting of mass spectrometry-based lipid and lipidome data, particularly in terms of an abbreviation code that encapsulates the exact level to which lipids can be structurally defined and/or quantified when using a particular MS or MS/MS approach. This workshop will invite opinion on systems of annotation and reporting requirements from leaders in the field that will then be opened for discussion and input from all workshop participants."

The workshop was held on Monday June 16th (5:45-7:00 pm in convention centre 343) and was attended by approximate 140 conference delegates (the room which had a capacity of 300).

Prof Stephen Blanksby facilitated the workshop that included 3 though provoking discussions led by three leading researchers in the field;

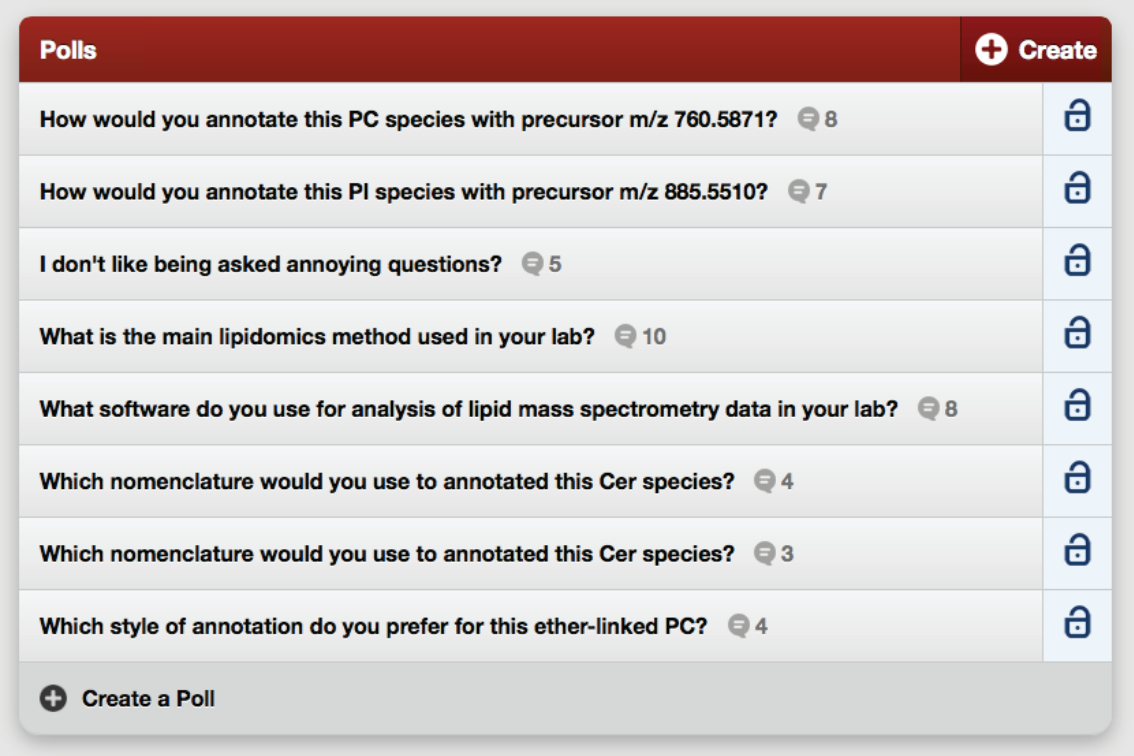
Prof Gavin Reid (Michigan State University and now University of Melbourne)
Emphasized the implications of increasing capabilities in high resolution and mass accuracy for lipidomics. Implications for lipid identification and also quantification were discussed. The ability (or inability) of contemporary data analysis tools to accommodate this additional information was mentioned and several delegates suggested that such findings might indicate a need to consider fractionation strategies (LC or ion-mobility) in combination with MS.

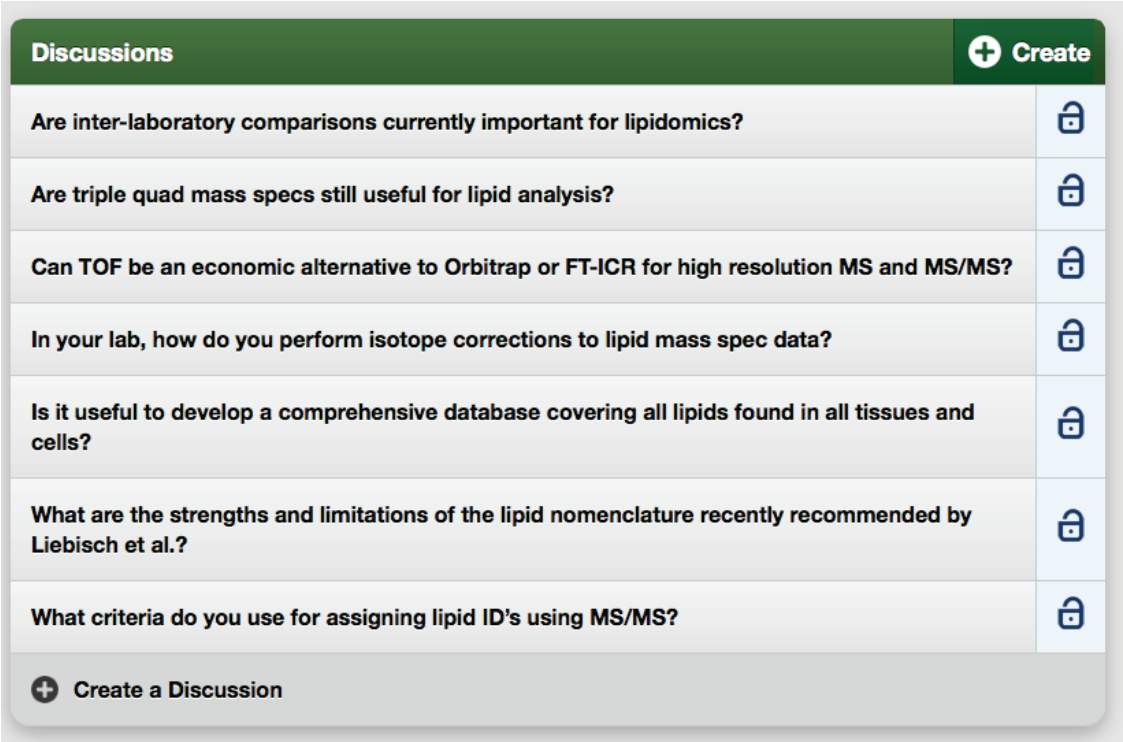
A/Prof Christer Esjing (University of Southern Denmark);
Led a discussion about the lipid structural assignments that could be made based on tandem mass spectra of common lipid classes and suggested several types of annotation that could be used that ensure that the hierarchy of assignment is consistent with the structural information available. A/Prof Esjing also proposed a structure for reporting the results of lipid identification and quantification (as outlined in his recent publication Husen P *et al. PLoS One* **2013** Nov 7;8(11):e79736). This prompted a discussion on what the minimum requirements for reporting lipid MS data should be. Views from the floor ranged from (i) no requirement - with some trust placed in the authors to provide data if required - through to (ii) full archiving of mass spectra used for lipid identification or quantification.

A/Prof Todd Mitchell (University of Wollongong).
Demonstrated how the same set of mass spectral data could be used to identify a wide range of lipid isobars and isomers. He showed that interrogation of widely used lipid databases (e.g., LipidMAPS) could yield large numbers of hits in each category and in general these hits were presented to the user in an unfiltered manner, *i.e.*, there is no ranking or scoring or identifications. This leads to the novice user often taking the top hit despite the fact that all other identifications may be equally likely based on the mass spectral information available and the known lipid biology of the system under examination. This prompted discussion as to how emerging commercial databases and software tools (e.g., LipidView from AB SCIEX and LipidSearch THERMO) could be improved to incorporate the ideas of hierarchical identification as proposed by Liebisch *et al.* (*Journal of Lipid Research* **2013**, 54, 1523) and extended by Esjing and co-workers (see above).

These presentations stimulated wide-ranging discussion that was further facilitated through an online forum (run as a gosoapbox event, https://app.gosoapbox.com/event/452985591/). Examples of the

types of questions used to stimulate this discussion are provided below. While these formed a useful basis for discussion, unfortunately the loss of WiFi during the session meant that very few online responses could be collected. We would ask that this failure (on the part of the Baltimore Convention Centre) is noted by ASMS and WiFi capacity is emphasized as critical criterion for.





Concluding remarks:
The discussion at this workshop will be extended by a working group; initially comprising the chairs and presenters (with others to be invited). The working group will look to bring together a summary of recommendations for ASMS 2015 and draft these for publication as a critical review in an appropriate journal (*e.g.*, *JASMS*).