ASMS Environmental Applications Working Group – Workshop Report 2017

This year's workshop was attended by about 120 scientists, and focused on data handling and processing, and ambient ionization applications. Andrew Ottens was announced as the incoming co-chair to replace Marc Engel starting June 30, 2017.

Each of our three invited discussion leaders gave a 5-10-minute informal synopsis, followed by lively questions and discussion. Their topics were; "Direct Analysis of Algal Biotoxins Using Ambient Ionization and High Resolution Mass Spectrometry" (Daniel Beach, National Research Council Canada, Halifax, Nova Scotia, Canada), "Themis: Pre-processing of complex mixture data" (Rémy Gavard, University of Warwick, UK), and "Analyzing, Searching, and Archiving Data Generated by Data Dependent Analyses" (Daniel Sweeney, MathSpec, Inc., Arlington Heights, IL). Daniel Beach examined the feasibility of direct analysis of various marine and cyanobacterial toxins with a focus on LAESI-HRMS and DART-HRMS. Rémy Gavard explained a new algorithm he's developing, Themis, a data analysis tool that processes replicate measurements, and detects aberrant data points (spectral noise), Themis improves differentiation of peaks from noise, and then produces an averaged spectrum. Daniel Sweeney showed modern strategies on how to handle modern high resolution LC-MS data that can produce thousands of MS/MS spectra per hour using data dependent analyses (DDA).

We did not use the Q&A mobile app because the audience preferred a more traditional approach to the discussion.

Following the workshop, approximately 30 attendees continued lively discussions at our annual working group dinner at a nearby restaurant.

In September we will survey the Environmental Applications interest group members for format and topic suggestions for next year. Two early suggestions are ion mobility in environmental analysis, and environmental contaminants and human health. If you have any suggestions for next years' workshop, either topics or speakers please send them to either Achille Cappiello (<u>achille.cappiello@uniurb.it</u>), Imma Ferrer (imma.ferrer@colorado.edu) Andrew Ottens (<u>andrew.ottens@vcuhealth.org</u>).

Sincerely,

Achille Cappiello, Marc Engel, and Imma Ferrer

Co Chairs, ASMS Environmental Applications Interest Group