

2020 ASMS Annual Conference Workshop Report

Getting Informatics Approaches to Work for You

(Virtual Workshop for the Flavor, Fragrance & Foodstuff Interest Group)

Organizers: James Redwine and Travis Falconer

Tuesday June 2, 2020

The 2020 workshop for the Flavor, Fragrance & Foodstuff Interest group consisted of four brief presentations delivered by invited panel members, followed by a question and answer session in which questions were submitted by attendees through the Zoom interface and the panel members spoke their responses; this Q&A session was moderated by the organizers. The four presenters were:

- Ann Knolhoff (U.S. Food and Drug Administration): “Considerations for Sample Preparation, Instrument Parameters, and Experimental Design for Non-Targeted Screening”
- Melanie Downs (University of Nebraska): “Non-Targeted Proteomics Data Analysis: Software and Practical Tips for Food Protein Analysis”
- Elisabeth Walker (ThermoFisher Scientific): “Uncovering Flavor Additives in Sake”
- Roy Martin (Waters): “Strategies for Targeted and Non-Targeted Screening and Differentiation of Cannabis Cultivars”

The participation peaked at 92 simultaneous attendees, including the speakers and organizers. Based on responses to a poll, there was approximately equal representation of the academic, student, industry, and government/regulatory sectors, as well as a few participants from non-government organizations. This distribution of participants is similar to that estimated for previous years.

The presentations were each approximately 10-15 minutes. The first two presentations covered practical topics related to non-targeted screening and the use of informatics, while the last two presentations described example applications of informatics/chemometrics related to flavors, fragrances, and foodstuffs. Of the participants who responded to the poll, ~70% indicated that they perform non-targeted, informatic/chemometric analyses using mass spectrometry. Interestingly, of those respondents, few are using the commercial off-the-shelf software provided by instrument vendors, instead opting for other custom solutions.

Ann Knolhoff discussed the effects that sample preparation and various experimental parameters have on the quality of the data processing results. Two interesting conclusions were that acquiring data in polarity switching mode yielded performance nearly comparable to separate positive and negative polarity injections, and that resolving power did not have a major impact on the number of features detected. Melanie Downs presented MS methods for non-targeted screening of food proteins and the large number of proteomics software packages and databases available. A significant challenge in this field is the limited sequence information available for many foods. Elisabeth Walker provided an example of the use of Thermo’s Compound Discoverer software to uncover flavor additives in sake, specifically,

how to look for a particular type of compound (i.e., how to search for compounds of a particular class). Finally, Roy Martin described the use of Waters' Progenesis Q1 software for the nontargeted data analysis of cannabis, including an application to distinguish cannabis cultivars from one another in which spectral libraries were used to identify the distinguishing compounds.

Unlike workshops of years past, the virtual format did not allow for real-time conversations between the audience and the panelists, so the level of engagement and exchange of information was reduced. However, the Q&A feature of the Zoom app allowed for participants to submit questions to the panelists, several which were submitted anonymously, perhaps an indication that some of the questions were asked by individuals that may not have felt comfortable asking a question in person. There were multiple questions for all of the panelists, with particular interest in the findings that Ann presented regarding experimental parameters and several specific questions for Elisabeth and Roy regarding their companies' respective software platforms.

The scheduling of the virtual workshops permitted attendance by individuals that may not have been able to attend in the traditional format; hopefully, the workshop content was relevant to the participants and maintains their interest for future workshops. The topic of nontargeted informatics/ chemometrics approaches was chosen with the intent of appealing to all members of the FFF interest group. The goal of the workshop was to make these approaches accessible to those who are unfamiliar with them or considering using them in the future. Based on the Q&A session, nontargeted screening plays a central role in the fields of flavors, fragrances, and foodstuffs, but that the use of informatics/ chemometrics for the analysis of nontargeted data has not yet been widely adopted. The FFF interest group workshop and forum may be useful platforms for interested users to share ideas and seek advice. Given the focus on food safety over the previous five years of the FFF workshop, next year we will again seek to explore a topic that includes the flavor and fragrance aspects of the interest group.

This year was James Redwine's second year of the two-year rotation. Joe Binkley (Leco Corporation) has volunteered to co-chair next year along with Travis Falconer. Marc Engel (Florida Department of Agriculture and Consumer Services) has offered to join as co-chair the following year.