2024 Flavor, Fragrance, and Foodstuff Interest Group Workshop:

"Flavor, Fragrance, and Foodstuff Discussion: Analyte Identifications and Sample Characterizations with GC, MS, and Software Tools"

Tuesday June 4, 2024, from 5:45 to 7:00 at ASMS in Anaheim, CA

Organizers: Liz Humston-Fulmer (LECO Corporation) and David Schroeder (Kraft Heinz)

Panelists: Jessica Prenni (Colorado State University), Sofia Nieto (Agilent), David Alonso (LECO Corporation), and Kurt Thaxton (Gerstel)

Attendees: There were approximately 75-90 people in attendance at the workshop. (An online polling app was used and there were 71 participants.) The workshop seemed to attract a broad audience, even beyond those working in the FFF market space.
Based on polling results,

- Approximately 40% of workshop attendees were new to ASMS
- Approximately 75% of workshop attendees were new to the FFF workshop
- The attendees had a variety of places of employment: 31% identified their place of employment as academia, 28% as industry, 24% as vendor, and 17% as government
- Nearly half (44%) of attendees do not currently work with food, flavor, or fragrance. Additional discussion on this polling question indicated that some attendees work in related fields and others work with the technologies (hardware and software) that were highlighted for the workshop, but on different sample types.

The workshop focused on two main discussion topics:

1. **Approaches to identification** - *using MS information with library databases, using chromatography to improve separation and spectral quality, connecting tentative identifications with sensorial descriptions, and using high-resolution MS data to support library matches and to help identify analytes without library matches.*
2. **Data analysis tools -** *comparing and characterizing data from sets of samples with clustering, machine learning, and various software and modeling tools*

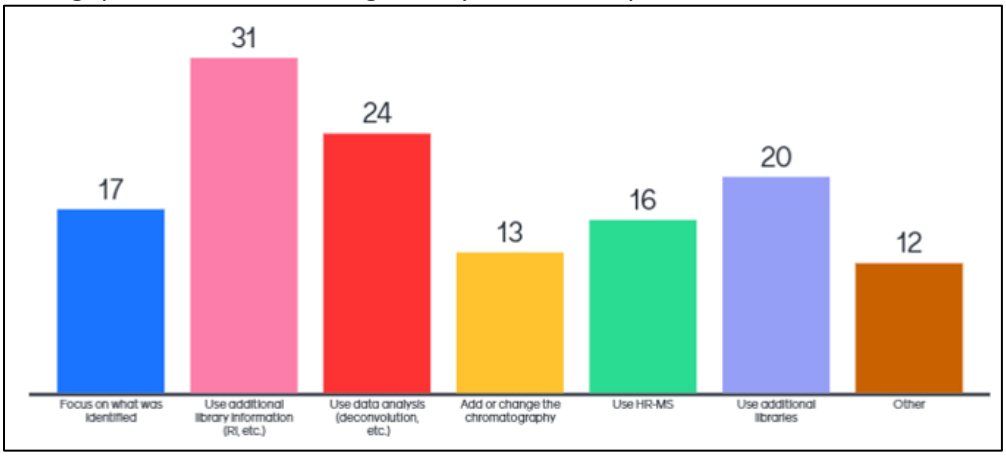
The discussion topics were covered with a mix of interactive polling, panelist presentations, application snapshots, and group discussion. Due to time limitations, the first discussion topic was explored in more detail than the second.

Outline of the workshop

1. The first topic was to try to get a sense of the typical work and interest of the attendees. This was explored through polling questions and discussion.
    a. Polling indicated that attendees do a fairly even mix of target and non-target work.
    b. Both LC and GC are commonly used by attendees, though GC was used more often: 63% use GC more and 37% use LC more.
    c. No matter the separation technique, analytes without reliable IDs are not uncommon and can be a challenge.

2. The second topic focused on non-target analyses with LC separations. This section included a panelist presentation and group discussion.
    a. Panelist presentation: Jessica Prenni (Colorado State University), "*Knowledge Gap in Food Composition*." This presentation provided an overview of the Periodic Table of Food Initiative and discussed standardization and how compiling this information in the database can allow for exploring interesting questions about food samples.

3. The next area of focus related to addressing analytes without reliable identifications in GC work. This section included polling questions, application snapshots, and two panelist presentations.
    a. Polling question: What strategies do you use to improve identifications?



    b. Each polling option was then discussed with group input and application snapshots.
        i. Focus on analytes that were identified: group discussion indicated that sometimes what was identified with library matching was enough to address the question of interest
        ii. Use additional library information: discussion covered using retention index to support analyte identifications or reject those that do not make sense based on chromatographic elution position. This is a common practice amongst the group
        iii. Use additional data analysis: sometimes the challenge with identification is related to coelutions that interfere with the spectra and getting cleaner spectral data to match to libraries can help. An application snapshot was shown to demonstrate benefits of deconvolution for providing cleaner spectra in instances of coelution. This can sometimes lead to improved identifications

iv. Add or change chromatography: An application snapshot was shown to highlight the benefits of GCxGC for instances where first dimension coelutions exceed deconvolution. When interferences are the cause for being unable to identify a feature, adding another dimension of separation is another way to get cleaner spectral information that can sometimes lead to improved identifications

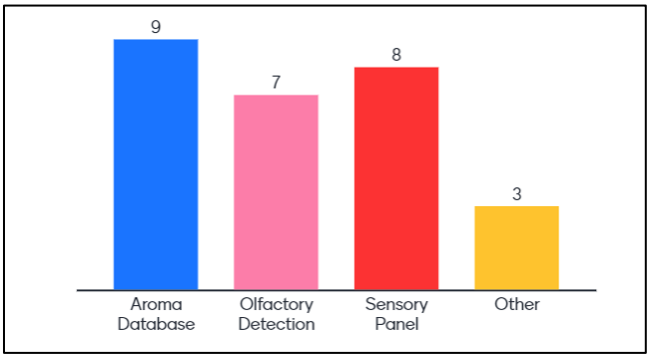
v. Add high resolution MS: Discussion about the benefit of accurate mass to support or reject library matches and to help propose identifications when analytes are not present in libraries

c. Panelist presentation: Sofia Nieto (Agilent), "*Accurate Mass GC/MS Benefits for Flavor and Fragrance Applications.*" This presentation discussed high-resolution MS and how it can be used to support or reject library hits. There was also discussion on using the spectrum to propose structures for unknowns that were not in the library.

d. Panelist presentation: David Alonso (LECO), "*Nepeta cataria Project.*" This presentation also discussed high-resolution MS with EI and CI and how it can be used to support or reject library hits. There was also discussion on using the spectrum to propose structures for unknowns that were not in the library

4. The final topic was about connecting analytes that have been tentatively identified to aroma or sensory characteristics. This section included polling questions and a panelist presentation

a. Polling question: How do you connect sensory details to data?



b. Panelist presentation: Kurt Thaxton (Gerstel), "*Connecting Mass Spectrometry to the Human Experience.*" This presentation focused on the use of olfactory detection with GC- MS and provided tips and suggestions.

c. Polling question: "What aroma databases do you use?"