2023 Flavor, Fragrance, and Foodstuff Interest Group Workshop

"Utilizing GC/MS Technologies and Associated Software Tools to Address Challenging Applications in the Flavor, Fragrance and Foodstuffs Laboratory"

Wednesday June 7, 2023, from 5:45 to 7:00 at ASMS in Houston, TX
Organizers: Joe Binkley (LECO Corporation) and Liz Humston-Fulmer (LECO Corporation)

The 2023 workshop for the Flavor, Fragrance & Foodstuff Interest group focused on using software tools with GC/MS (and/or GCxGC/MS) to address common tasks in Food/Flavor/Foodstuff work. The workshop was divided into three parts:

1. On-line polling for audience introductions and an opportunity to share initial questions
2. Three brief presentations from invited panel members on relevant topics
3. Q&A and open discussion with panel and audience

Attendees: There were approximately 45-50 people in attendance at the workshop. Thirty-five people participated in the online polling, but not all attendees did the polling. Based on polling results, there was an even mix of people from academia and industry and slightly fewer from government or other agencies. About 1/3 of attendees indicated that they do not do application work related to flavor/fragrance/food. Nearly everyone, however, does work with GC (or GCxGC). In addition to people doing flavor/fragrance/foodstuff work, it appears that the workshop attracted general GC users and those interested in the associated software tools.

Detailed descriptions of each section are listed below,

1. **On-line polling**

The polling section of the workshop provided an opportunity to understand the audience participants, and to gauge what types of questions people had at the beginning of the workshop. Many of the questions that came up during the polling section were addressed during the presentations and/or discussion sections.

- The audience participants were an even mix of industry and academia with a slightly smaller group of people from government and other agencies. There was also a much smaller group of instrument or software developers.
- Most people work directly on food/flavor/fragrance applications, but approximately 1/3 of the attendees indicated that they do not do this type of work. (Some indicated that they do GC-related work and/or were interested in software.)
- Those participating in the polling, indicated that their main application objective was sample characterization, followed by sample comparisons, R&D development tasks, and off-odor analysis. QA/QC and deformulation tasks were also listed, but were a smaller subset of application goals.
- A range of analytical methods are commonly used amongst the group. For separation techniques, nearly all of the attendees use GC or GCxGC and about half of the attendees use LC. Nearly all of the attendees use MS and about half use FID. A variety of software tools were mentioned.

- Desired software features to simplify work were ranked as: Analyte IDs (for features that are in libraries), Analyte IDs (for features not in libraries), sample alignment, and linking analytes to aroma characteristics. A few other various tasks were also mentioned. These were things like using retention index and determining compound class of analytes in a mixture.

2. Panel presentations

Three panelists shared snapshot presentations (approximately 10 minutes each) of relevant application work – these covered a range of sample types and highlighted various tasks, including off-odor analysis, sample characterizations, and comparisons of different samples. Each presentation included discussion of software tools and features that facilitated the work.

- Professor Albert Lebedev (Lomonosov Moscow State University): "Solving the mystery of the Chukotka stinky Gray whales" – This was an application project that used GC-MS to determine the chemical related to an off-odor in whale tissue. Once the chemical was identified, biological sources of the off-odor could be proposed.
- Liz Humston-Fulmer (LECO Corporation): "Buttery and Traditional Chardonnay Wines: Sample Characterization and Comparison" – This was an application project that used GC-MS to compare two types of wine with different processing (a traditional chardonnay and a buttery chardonnay). Chemical differences and similarities that connected to the sensory descriptions of each wine were determined and described.
- Caitlin Cain (University of Washington): "Uncovering the Volatile Profile of Potato Taste Defect in Roasted Arabica Coffee using GCxGC-MS and Chemometrics" – This was an application that used GCxGC-MS to investigate off-odors by comparing coffee samples with known potato taste defect and those without. Specific chemical differences were determined and described.

3. Q&A and Open Discussion

There was a good discussion during this portion of the workshop, and many topics and questions were covered. The discussion continued past the scheduled time, and likely could have continued a while longer. Some topics of note were:

- Use of Retention Index (RI) with GC analyses. How to calculate RI in samples and how to reference RI information from standard libraries. It was noted that NIST23 will have expanded coverage of RI information.
- There was discussion about spectral libraries that are used for searching. Which are most common and how many features remain unknown after library searching. What to do with unknowns without a library match is an ongoing question.
- There was discussion about determining how important the chemicals that are detected are to the aroma profile. There was discussion about using database information with aroma characteristics to connect aroma notes to the observed chemicals in the samples. (For example, the Good Scents Company.) There was also discussion about using olfactory detection with GC.
- There was discussion about the benefits and considerations with GCxGC – how is deconvolution done, sampling of first dimension separation, the increase in peak capacity, and how structured nature of chromatograms can give functional group information.