

Food Safety & Authenticity: HRMS Applications (Flavor, Fragrance & Foodstuff Interest Group)  
Organizers: David Schroeder and Sara Kern

This year we started off the meeting to discuss high resolution mass spectrometry for food and ingredients. David Schroeder (Kraft Heinz Company) presented a short discussion starter about some recent consumer complaints where High Resolution Mass Spectrometry was used to determine the identity of a contaminant that had been introduced post-packaging. Next, Brian Mussleman (IonSense) gave a long presentation regarding the use of DART-HRMS to quickly identify active pharmaceutical ingredients in dietary supplements. After this introduction we fielded discussion from the attendees.

We had approximately 130 attendees this year. The discussion was vigorous and interesting and lasted the allotted time. It was reported that there is a database called Cramer Toxtree that will assign hazards to compounds based on the structure that is entered, which is useful when encountering contaminants in complex food matrices.

A user cautioned the group to refrain from using background subtraction from their high resolution data, as it can create artifacts that can hinder correct identification. They also mentioned that complex matrices can result in many adducts being formed (well beyond  $[M+H]^+$ , ammonium, sodium, and acetate) that can make the chromatograms and mass spectra tremendously complicated, even though it is really the same analyte forming many different adducts. Another user mentioned that a searchable database similar to what is available for GC-MS data will be released shortly. It was generally agreed that the data analysis software is beginning to catch up to the sophisticated hardware, although there was some discussion that false positives can occur when the spectrum is noisy and/or complex and the software uses isotope patterns to definitively identify compounds, as many ions may be overlapping.

We briefly discussed resolution and asked the question "how much resolution is truly required"? No one seemed to have (or be willing to share) experience with the new 1,000,000 resolution instrument, but it seemed to be the consensus of the group that the required resolution depends on the application. The sensitivity and resolution of many commercially available systems meet current needs.

The role of HRMS in detecting allergens in foods was brought forth as an emerging topic and will be further explored next year. Additionally, using HRMS to look at leachables and extractables in food packaging was suggested as another new topic for next year.

It was suggested that in 2018 we continue discussing non-targeted food safety analysis and screening methodology. Sara Kern (U.S. Food and Drug Administration, Forensic Chemistry Center) will lead the discussion and Melanie Downs (Assistant Professor at University of Nebraska Lincoln) volunteered to serve as co-chair.