

Flavor, Fragrance and Foodstuff Interest Group

Organizers: Walter Hammack and Tim Croley

The Role of High Resolution Mass Spectrometry in the Regulatory Environment

June 3, 2015

This year we started off the meeting to discuss the increase in use of high resolution mass spectrometry for food and related commodities. I discussed the FDA's recent guidelines for the use of high resolution mass spectrometry (HRMS) in the regulatory environment. After this introduction we had Jonathan Litzau from FDA's Forensic Chemistry Center and Michel Nielen from RIKILT present examples of how they've incorporated HRMS in their work.

We had approximately 100 attendees this year. The discussion was lively and engaging and went beyond the allotted time. A lot of people were interested in the "magic" number of how much resolution is required and others were interested in the criteria that others were using. I think that it was unanimous that one would need at least two ions and some sort of retention time or standard confirmation before they would make a claim to identity. Both the US and EU are requiring (or going to require) 5 ppm mass accuracy on the precursor ion.

Other Issues that were raised:

1. Preference of Orbitrap vs. QTOF or TOF? No preference
2. The European point system. Why aren't we using it in the US? Too many moving parts and not enough uniformity.
3. How many data points beyond the decimal is realistic? Four. This was also part of a discussion of mass precision and how it's somewhat overstated.
4. How many scans across the peak are needed for confident capture? Depends on the application and the confidence of the technique.

Toward the end, the discussion shifted towards screening methods and what was being done in this area. It was suggested for next year that the focus be on non-targeted analysis and screening methodology. Walter Hammack will lead the discussion. David Schroeder from Kraft has volunteered to be the co-chair for next year.