

November 7, 2024 (13:30-14:15)

Waters™

VENDOR SEMINAR:

Tackling separation challenges: Strategies for identifying plant toxin isomers and analyzing Glyphosate & Co. in complex matrices

During our lunch seminar, we will explore various technologies that aid in resolving separation issues. You will discover how ion mobility introduces a highly resolved third dimension to your analysis, revealing the composition of plant toxins. Additionally, you will learn how combining modern mixed-mode column chemistries with a traditional 2D-LC approach offers new opportunities for routine food testing labs analyzing Glyphosate & Co. in complex matrices.

Ion mobility mass spectrometry to enhance the determination of natural toxins in food samples

Dr. Laura Carbonell-Rozas, University of Almeria, Spain

The main challenge related to the determination of some natural toxins such as pyrrolizidine alkaloids and ergot alkaloids (EAs) using LC-MS, is the existence of numerous co-eluting isomers that lead to identical product ions. In this context, ion mobility mass spectrometry (IMS) introduces a third dimension of separation to LC-MS workflows, allowing compounds to be differentiated based on their collision cross section (CCS). This seminar will present several IMS-based strategies aimed at enhancing analytical performance in the determination of EAs and PAs across a variety of food samples, including cereals, spices, herbs, and their derivatives. We evaluated different IMS technologies, such as travelling wave-IM (TWIMS) and cyclic-IMS, in conjunction with LC and high-resolution MS (LC-IM-HRMS), to address the current challenges associated with EAs and PAs determination. We constructed and cross-validated CCS libraries for EAs and PAs across multiple laboratories and additionally, utilized machine learning to support the experimental findings. The incorporation of IMS into LC-MS methodologies helped reduce background noise, enhance the signal-to-noise ratio, and consequently, improve signal sensitivity, yielding higher quality mass spectra for compound identification. This is particularly beneficial in non-targeted analysis and suspect screening. Moreover, cyclic IMS proved to be an effective alternative when a higher resolving power was required, as was the case for some PA epimers that could not be separated by TWIMS.

IMS has proven to be a powerful technique for enhancing the performance characteristics of LC-MS methods in the analysis of natural toxins within complex matrices, such as food samples and food-related products.

Bringing the direct analysis of Glyphosate & Co. in complex matrices into routine food testing labs

Dr. Claudia Rathmann, Waters GmbH

The task of analyzing Glyphosate & Co. in food without the necessity for sample derivatization appeared to be resolved with the numerous methods outlined in the QuPPE document. However, matrices such as dried lentils, lemon concentrate, or black tea challenge this assumption in routine environments. We will present a combined strategy, backed by data from renowned food testing laboratories, that leverages the unique retention capabilities of modern mixed-mode column chemistries and traditional 2D-LC chromatography. This approach effectively separates matrix interferences that suppress highly polar analytes like AMPA, MPPA, glufosinate, and glyphosate.