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VENDOR SEMINAR:

NEW LEVELS OF CONFIDENCE AND PRODUCTIVITY IN THE SCREENING AND QUANTITATION OF RESIDUES AND CONTAMINANTS BY UHPLC/Q-TOF/ MS

New levels of confidence and productivity in the screening and quantitation of residues and contaminants by UHPLC/Q-TOF/MS

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There is an ever increasing number of residues and contaminants which need to be tested in our daily food. The range of compounds includes pesticides, mycotoxins, packaging contaminants, and many others. For many control laboratories it would be extremely interesting to expand their scope of analysis to potentially include all these compound classes in one screening method. With modern Q-TOF LC/MS instruments, allowing the analysis of most pesticides and mycotoxins much below the regulatory limits, this is within the realms of possibility, not least since QuEChERS has proven its potential as generic sample preparation technique. Qualitative screening with Q-TOF analyzers in combination with comprehensive databases and libraries does not always require having expensive standards for each contaminant on hand. However, in complex matrices such as QuEChERS extracts of food, the challenge remains not only to find the targeted contaminants, but to successfully rule out potential false positives, and at the same time to be as productive as with LC triple quadrupole instruments.

In this presentation we show how this can be achieved when screening for pesticides and mycotoxins in various food matrices by applying Agilent's 1290 UHPLC system coupled to a Q-TOF LC/MS system operated in the All Ions MS/MS acquisition mode. The All Ions MS/MS allows for the CID fragmentation of compounds without precursor selection, enabling the accurate mass acquisition of molecular ions and fragments from the same compound. In combination with Agilent's unique offering of comprehensive databases and libraries and together with the industry leading MassHunter software, the All Ions MS/MS aids in the successful elimination of potential false positives. The workflow was successfully validated for the screening of pesticides in fruit and vegetables with a screening detection limit (SDL) below 5 µg/kg for most pesticides in all tested matrices. Further examples from the qualitative screening of mycotoxins in nuts and cereals will be shown, applying a new accurate mass database and library for mycotoxins and fungal metabolites.

The All Ions MS/MS workflow is perfectly integrated in the MassHunter software. Identification of contaminants is done on multiple levels using a unique co-elution score for the molecular ions and fragments, the comparison of area ratios, the accurate mass and isotope pattern matching of the molecular ions and the accurate masses of the fragments. Fast data review is aided by powerful graphical features of Batch- and Compounds-at-a-glance in combination of using all these ID criteria with MassHunter Quant outlier flagging.