November 7, 2013 (14:30-15:30)

Waters

THE SCIENCE OF WHAT'S POSSIBLE.™

VENDOR SEMINAR:

INNOVATIVE ANALYTICAL TOOLS FOR MULTI-RESIDUE ANALYSIS: FROM ULTIMATE SENSITIVITY TO EFFICIENT DATA HANDLING AND INTERPRETATION

Residue Analysis on the Crossroad: the Need of Non-Target Screening in Food and Animal Feed by UHPLC-HR-Q-TOF MS as Alternative for the Conventional Target Screening Approach

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Presently the prevailing method for determining pesticides, Vet drugs and other legislative relevant contaminants in food and animal feedstock is a targeted approach using LC/MS/MS or GC/MS/MS. The definitions of methodologies and its target compounds are mainly based on the juridical requirements as well as customer requests on known residuals of which relevance is mostly based on historical experiences.

New active substances, contaminants and substances, not in the mainstream of public awareness, are often overlooked hitherto the inherent methodology of targeted analytical technologies. In an increasingly globalised World with foodstuff and packaging materials from a multitude of suppliers and origins, a targeted screening will inherently risk of omitting potential unwanted and toxic contaminants.

The goal of our development project was to develop a sensitive non-targeted screening methodology for determination of pesticides, Vet Drugs and other contaminants in Food and Animal feedstock using high resolution UHPLC and QToF MS technology. The Screening Detection Limits (SDL) for these substances should be below the MRL and/or no more than 5 % false negatives should be accepted.

After intensive investigations on routine screening equipment in the high resolution mass spectrometry range, the selection was made on a UHPLC QToF (Acquity UPLC and Xevo G2-S QToF, Waters Corporation). This UPLC-MS system uses the so-called MS^E technology with a large library which can rapidly identify and quantify targeted compounds using a sophisticated software approach. Furthermore and in the same sample run, unknowns can also be isolated and possibly identified using compound-specific characteristics, such as accurate mass, the identification of adducts, fragmentation patterns, retention time and isotope ratios.

The validation of this non-targeted screening method was carried out using the current SANCO document 12495/2011 and also the Guidelines for the Validation of Screening Methods for Residues of Veterinary Medicines (Community References Laboratories Residues) and was successful for more than 600 selected pesticides, 200 Vet Drugs and 250 other contaminants of relevance. The SDLs were in the range from 1 to 10 µg/kg. This novel approach in analytical work will in the near future replace the tandem MS systems, which will be continued in the usage for confirmatory analytical work.

New technology solutions to increase the scope of food analysis capabilities

Sara Stead

Waters Corporation

Ensuring the quality and safety of the food supply in accordance with the ever increasing regulatory and consumer demands represents a significant analytical challenge. The focus of this presentation is to provide an overview of Waters recent technology developments designed to aid the work of the food analysis laboratory from the new Acquity QDa detector making MS accessibility a reality to ion mobility enabled QTof MS for non-targeted multi-residue screening in complex samples.

Informatics tools for streamlining the validation process

David Wayland

Waters Corporation

Introduction to UNIFI and NuGenesis capabilities showing the application of processing and data reporting tools and the industry perspectives using data generated as part of an independent validation study (SANCO 12495) of the pesticide screening solution.