A Q&A

Screening and Targeted Routine Quantitation of Pesticide Residues in Food Products

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The non-targeted screening and targeted routine quantitation of pesticide residues in food products are among the most important and demanding applications in food safety. Despite recent technological advancements in liquid chromatography–mass spectrometry (LC-MS), it is still challenging to detect and quantify hundreds of LC-amenable pesticides at low concentrations in different sample matrices. To assist pesticide residues chemists in addressing the challenge, Thermo Fisher Scientific has undertaken the development of the Thermo Scientific™ Pesticide Explorer Collection of comprehensive start-to-finish LC–MS workflows. These robust, sensitive, ready-to-go solutions, based on LC combined with triple-quadrupole MS/MS and high-resolution accurate mass (HRAM) MS/MS systems, have been validated in three matrices of differing complexity across four different laboratories. In addition, customized software used for data acquisition and processing allows the users to rapidly implement these methods to improve laboratory productivity. To find out more about the development, the detail, and recommended strategies for implementing targeted and non-targeted workflows, LCGC talked with Ed George, a Senior Applications Scientist with Thermo Fisher Scientific.

Michael Swartz: Why is LC-MS important in pesticide residue analysis?

Ed George: LC-triple quadrupole MS/MS is currently the preferred technique for targeted analysis of LC-amenable pesticide residue in food samples, primarily due to the combination of high specificity, high sensitivity, and multi-analyte capability. It is accepted by many regulatory authorities that good agreement between MS/MS ion ratios for pesticides in the sample compared to ratios in known standards will provide sufficient information to accurately identify the compound. Also, the specificity of ion ratios provides good discrimination between the pesticide of interest and matrix coextractives, reducing the potential for false positive and false negative results. Furthermore, the sensitivity of the instrument allows for dilution of the sample extract prior to analysis, helping to minimize matrix interferences. In addition, LC-MS provides the capability to consolidate legacy LC methods for specific analytes or compound classes into multi-residue, multi-class methods. It is not uncommon to analyze 300-400 pesticides in a single LC-MS analysis with good accuracy, precision, quantification and identification of the residues at very low concentrations, in compliance with regulatory requirements. At Thermo Fisher Scientific, we have developed a Pesticide Explorer Collection of start-to-finish workflows that allows an analyst to analyze over 270 pesticides in 15 minutes or 480 pesticides in 25 minutes, depending on the specific requirements of the laboratory in question.

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Michael Swartz: Can you give a brief overview of the analytical strategy for the use of Triple -Quadrupole mass spectrometry and high-resolution accurate mass spectrometry in pesticide analysis?

Ed George: The use of triple-quadrupole versus the high-resolution accurate mass approach depends on how pesticide residues are analyzed within a given laboratory workflow. For example, laboratories performing routine compliance testing will use triple-quadrupole systems with specific compound target lists, which will ignore other potential residues that are not included on this list. Therefore, if a pesticide is present in the sample, but not on the list, it will simply not be detected. Other labs may want to offer more capability to customers interested in other potential residues and contaminants in their samples. High-resolution accurate mass MS will not only provide excellent quantitation (in fullscan) and identification (MS/MS) of targeted analytes, but will also allow for non-targeted screening and retrospective data analysis. Advanced software tools and compound databases with accurate mass spectral libraries make the high-resolution accurate mass non-target screening workflow much easier for labs new to the technique. In fact, the accurate mass approach has the capability to provide simultaneous, targeted analysis and non-targeted screening analysis of not only pesticides, but also multiple classes of residues and contaminants in the same run.

Michael Swartz: What benefits do you think the Pesticide Explorer Collection of start-to-finish workflows brings to the pesticide community?

Ed George: The major benefit of the workflows is simply to help laboratories save time. The methods have already been tested, eliminating the need to optimize parameters for hundreds of compounds or build complex spectral libraries. This later point is really helping the analytical community adopt high-resolution accurate mass in recognition of the need to protect public health by screening food for other potentially harmful contaminants. The workflow package – whether it's triple-quadrupole or high-resolution accurate mass – includes the pre-configured instrumentation, the associated consumables, methods, and technical support, as well as the Thermo Scientific™ TraceFinder™ software method for efficient and automated data processing and reporting.

Michael Swartz: Data processing is the bottleneck in multi-analyte methods. How fast can you process and review the data using the Thermo Scientific TraceFinder software?

Ed George: Large data sets are easily processed using TraceFinder software, primarily because it uses a master method associated with a sample list and can process samples immediately after they are acquired, and during the analytical sequence. These methods are included with the Pesticide Explorer Collection kit. Data review has also been updated in TraceFinder so that all peak information can be custom displayed in a single-user-defined view, making data processing very rapid.

Michael Swartz: Robustness is extremely important to high throughput laboratories. What steps did you take to ensure your solution is robust?

Ed George: During method development we analyzed three matrix types, using the European citrate buffered version of the quick, easy, cheap, effective, rugged, and safe (QuEChERS) extraction method, but without cleanup. We evaluated strawberry, which has a high sugar and water content; leek, which is a complex green vegetable with high pigment content; and flour, which is a dry matrix with low water content. These matrices were analyzed at four different laboratory sites using different instruments to ensure consistent results in terms of calibration, linearity, method accuracy, limit of detection, and limit of quantitation. In addition, independent reference materials (FAPAS) were used to verify that the measured values obtained from the sample preparation and analysis protocols were within the limits specified by FAPAS.

Michael Swartz: How easy is it to modify the Pesticide Explorer Methods and for the user to add new compounds?

Ed George: The Pesticide Explorer Collection methods were designed to be flexible, and are therefore, very easy to edit in the TraceFinder software. Compounds can be added or removed individually, or if required, entire compound databases or methods can be exported into, and out of, Excel.

Michael Swartz: Do you consider this solution finalized or do you anticipate further development of the Pesticide Explorer Collection?

Ed George: The Pesticide Explorer Collection is definitely a work in progress. More pesticides are put into global use every year, so updates to the compound list and databases will continue. The high-resolution accurate mass spectral libraries will also grow, and the incorporation of new software tools will allow a user to easily expand the number of pesticides that can be used for screening workflows. Thermo Fisher Scientific and other collaborators are continually adding high-resolution accurate mass spectra to an advanced mass spectral database, known as mzCloud. To date, this database holds approximately 5,500 unique compounds and a wealth of associated metadata. It is highly curated to ensure spectral fidelity and is an ideal tool for high-resolution accurate mass unknown-screening workflows. In addition, the Pesticide Explorer Collection offers a software package known as Compound Discoverer 2.0. This unique software has built-in workflows that help users take a comprehensive look at their high-resolution accurate mass data for unknown compounds. It also has the ability to search against the mzCloud database and other commonly-used databases available on the web.