

Orbitrap GC-MS for Quantitative and Qualitative Multi-residue Analysis of Pesticides

A Q&A



Paul Silcock
Senior Marketing
Manager
Thermo Fisher Scientific

To learn more about the use of the Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system for quantitative and qualitative multi-residue analysis of pesticides, LC/GC Magazine talked with Paul Silcock, Senior Marketing Manager at Thermo Fisher Scientific. Paul leads the Orbitrap GC-MS Applications Team and has an extensive background in organic compound analysis, including 15 years' experience working for regulatory and contract testing organizations, as well as the analytical instruments industry. During this time he has developed expertise in the application of a number of different hyphenated MS techniques for the determination of trace level contaminants in food and environmental samples. Paul's focus has recently switched to working with leading scientists to explore the application of Orbitrap GC-MS full scan techniques to both targeted and non-targeted analysis in a diverse range of application areas. One area of particular interest has been pesticides.

LC/GC Magazine: Why is it important to monitor pesticide residues in food?

Paul Silcock: The use of pesticides on a global scale is an understandable necessity to generate a sufficient supply of food to feed the world's growing population. However, to ensure that we protect consumers and the environment, it is critical that pesticides applied to crops are regulated. Especially since residues of these chemicals can appear in our food and have the potential to pose risks to human health. The regulatory monitoring of pesticide residues in foods therefore aims to ensure dietary exposure remains at negligible levels to protect the world's population from harm.

LC/GC Magazine: What are the main challenges with respect to the analysis of pesticides?

Paul Silcock: From an analytical point of view the main challenge is addressing the requirement to quantitatively analyze a large number of residues at low concentrations in a very large number of different sample types. The European Commission MRL Database, for example, contains around 600 pesticides in almost 400 different products. The analytical methods need to be selective, sensitive and reproducible to be able to reach low part per billion target concentrations while meeting recognized guidelines for method validation and analytical quality control. Also, any testing approach needs to have a broad scope with the capability to analyze a large number of pesticides in a single analysis, and at an acceptable cost. The strategy of the past to simply divide and conquer by segmenting all of the different compound classes into a number of separate methods is less efficient and no longer an option for the vast majority of laboratories today. What is really needed is to be able to handle all compound classes and sample diversity with as few methods and techniques as possible.

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LC/GC Magazine: How has the analytical technology evolved over the years to support this application?

Paul Silcock: In general, technology has evolved to address the diversity in the application and the need to consolidate analysis into as few methods and techniques as possible. There's a strong trend towards having the selectivity in an analytical method come mainly from the chromatography and detection system as opposed to the sample preparation step. In pesticide analysis broad scope, low-cost, generic sample extraction with optional dispersive solid phase extraction clean-up has emerged as the approach of choice. Generic sample preparation such as QuEChERS is relatively fast, but poor selectivity often results in an extract that can contain high concentrations of co-extractives, thus putting more strain on the chromatography and detection system to provide the required selectivity. These generic extraction procedures are becoming ever-more popular and effective because of the increased instrument selectivity resulting from the move from traditional single quadrupole instruments to triple quadrupole instruments, and also from low to high-resolution accurate mass instruments.

LC/GC Magazine: Why are high-resolution accurate mass full scan techniques important for pesticide analysis?

Paul Silcock: Triple Quadrupole LC-MS/MS and GC-MS/MS systems are the gold standard for pesticide analysis because they offer a high level of selectivity and sensitivity for this application. They do however have some limitations; mainly that selectivity is achieved by targeting analytes during data acquisition with the consequence of the narrowing the scope of the analysis method. While it is possible to monitor larger numbers of compounds with this approach only those pesticides included in the acquisition method will be detected; thus pesticides which are present in the sample but not included in the method will not be detected. Compared to full scan methods, the setting up, optimization and management of triple quadrupole acquisition methods can be cumbersome and complex from a practical point of view. High-resolution systems have the advantage of being able to operate in full scan mode with high selectivity resulting in a simple experimental set-up. In full scan acquisition methods all of the pesticides that are chromatographed and ionized are monitored all of the time, so that the scope is virtually unlimited compared to targeted methods. Targeted data processing of the raw data acquired is usually done by screening the data against user defined databases or against much larger commercial libraries containing hundreds of pesticides. Another advantage of full scan methods is the capability to detect residues and contaminants from multiple chemical classes, in the same analysis,

as well as the ability to interrogate the data retrospectively in response to the emergence of new information.

LC/GC Magazine: What benefits do you think Orbitrap GC-MS brings to the pesticide community?

Paul Silcock: I'm very lucky to have the opportunity to work on Orbitrap GC-MS with some of the top experts in the pesticide analysis community. For example, Hans Mol from RIKILT and Richard Fussell, formerly of the Food and Environment Research Agency (FERA), UK. I was present for their first experiences with the Orbitrap GC-MS system. Richard and I were in Austin (TX) in the United States in the summer of 2014 working with a colleague of mine, Jason Cole, analyzing pesticides in complex samples; cold pressed orange oil and green tea samples. We were amazed by the quality of data obtained in terms of selectivity, excellent mass stability, sensitivity, the wide linear dynamic range, the low mass error and the absence of chemical interference when analyzing samples at an incredible 60,000 resolving power, especially when considering the ease of use of the system. Aside from some of this initial cooperative work, Hans Mol has had the opportunity to study the Orbitrap GC-MS instrument for a longer period of time. His assessment has confirmed the suitability of this technology for pesticide analysis. The utility of using full scan high-resolution accurate mass GC-MS instruments for this application has not been widely reported before. It has become apparent that the Orbitrap GC-MS operated in full scan offers the first real opportunity to perform broad scope pesticide screening, and simultaneous quantitation and identification in a single analytical run.

LC/GC Magazine: Do you think that the introduction of Orbitrap GC/MS will accelerate the move to qualitative screening methods in more laboratories?

Paul Silcock: Yes. I believe there's a real appetite from the community for high-resolution mass spectrometry coupled to GC. Not least because this need is currently being satisfied from an LC perspective, especially with the development of the Thermo Scientific™ Q Exactive™ Focus Hybrid Quadrupole-Orbitrap™ mass spectrometer that has been specifically designed for the analysis of LC amenable pesticides. Full adoption of these types of workflows makes more sense when you have a full coverage of both LC and GC amenable pesticides. The GC-MS part of this story has been missing until now, especially as time-of-flight technology has fallen short with respect to some of the analytical requirements. Orbitrap GC-MS joining Orbitrap LC-MS is the first real opportunity for laboratories to have the capability for truly broad scope analysis in pesticide residues. As Hans Mol said, "Orbitrap GC-MS completes the picture".