A Q&A

# GC-Orbitrap™ MS Technology for Pesticides Analysis

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Comprehensive testing for the presence of pesticide residues in food requires the application of both liquid chromatography (LC) and gas chromatography (GC) coupled to mass spectrometry. In particular, interest is growing in the use of full-scan High-Resolution Accurate Mass (HRAM) mass spectrometry (MS) such as the Thermo Scientific™ GC Orbitrap™ MS system for both the quantitation of target pesticides and non-targeted screening of unexpected pesticides, simultaneously in a single workflow. Historically, developments in GC-HRAM-MS have lagged behind those in LC-HRAM-MS, but the adoption of GC-HRAM-MS has been increasing recently. *LCGC* spoke with Prof. Amadeo R. Fernández-Alba, PhD, professor at the University of Almería in Spain, to share his thoughts on developments in GC-HRAM-MS technology and the prospects for the use of these powerful instruments for routine analysis in the future.

**LCGC: Can you give us a brief overview of your experience with GC-HRAM-MS technology for pesticides analysis?**

**Fernández-Alba:** We started working with time-of-flight high-resolution mass spectrometry (ToF-HRMS) instruments about 17 years ago. Around that time, in addition to teaching analytical chemistry, I founded the Agroalimentación (AGR) research group at the University of Almería in 1996 with the goal of facilitating the commercialization of fruits and vegetables in Europe. While the quality of ToF-HRMS data was good, retrieving and evaluating the information was time consuming and labor intensive. In addition, the mass accuracies at that time were much lower than those that can be achieved today. Since then, mass spectrometry platforms have evolved tremendously, especially with the development of the Thermo Scientific™ GC-Orbitrap™ technology enabling GC-High Resolution Accurate Mass (HRAM) mass spectrometry (MS). Important upgrades have improved systems' sensitivity, selectivity, the quantitation capabilities, and offered more comprehensive and faster software for data treatment. All these improvements allow HRMS and HRAM technologies to work with similar workflows as triple-quadrupole mass spectrometry (triple-quad MS) while offering several advantages.

**LCGC: What do you consider to be the main benefits of modern GC-HRAM-MS technology?**

**Fernández-Alba:** The first advantage is that it works in full scan every time. This capability means that we cannot only detect or identify targeted compounds, but we can also determine extra components that we did not predict we would find in our sample.

The second advantage, which is very important for routine labs, is that we can include new components within the scope of the method more easily than with triple-quad MS. In the case of triple-quad MS, we must target preselected ions to determine the voltage needed to get transitions. With GC-Orbitrap MS systems, we can work in full scan with electron ionization, which means that the inclusion of new components in the analysis is very fast and easy.

It's also important to consider that in the last year, companies have introduced new instruments that are even more sensitive than others previously available. The sensitivity that we can achieve with GC-Orbitrap MS technology is now similar to that of triple-quads.

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**LCGC: Please describe some specific applications of modern GC-HRAM-MS technology that you are most excited about.**

**Fernández-Alba:** Pesticide residue analysis is one for sure important because full-scan analysis is always a benefit for identification and management of the analytical scope.

What is probably the most impressive of all new applications are those related to situations where the target list of analytes is very extensive and a non-target analysis approach is necessary. Also, laboratories can use the technology to improve the overall scope of their analytical capabilities. For instance, this might be useful for analyzing food contact materials or investigating food fraud.

One must also consider the accurate mass aspect of GC-Orbitrap MS technology. Electron ionization (EI) makes analysis with this technology possible without having to obtain $MS^2$ (MS/MS) data. This makes the analysis simpler and easier with identification criteria based on mass accuracy and ion ratio of the EI fragment ions.

**LCGC: Are you aware of any limitations with using GC-HRAM-MS?**

**Fernández-Alba:** I don't see any disadvantages at the moment. GC-HRAM-MS is a new technology for many routine labs, and it takes time to become proficient in different types of instrumentation. At the moment, the gold standard is triple-quad MS instruments. As I mentioned earlier, the sensitivity that is now possible with new GC-Orbitrap MS technology is on par with that of triple-quads, which will help speed the introduction of this new technology into laboratories.

It's only a matter of time before lab personnel will be trained in GC-HRAM-MS, and I don't anticipate difficulties with analysts adopting this new technology.

**LCGC: Do you know the percentage of laboratories currently using full-scan GC-HRAM-MS and LC-HRAM-MS for pesticides analysis in Europe and the rest of the world?**

**Fernández-Alba:** In Europe, about 20 percent of pesticide residue control laboratories are currently working with HRAM and HRMS, and these groups are primarily using it for LC.

The introduction of HRAM-MS for GC has not happened at the same rate, so the percentage of labs working with GC-HRAM-MS is much lower than LC-HRAM-MS.

Some labs may be under the outdated impression that GC-HRAM-MS is too expensive or too limited to warrant its investment. One point to consider is that typically all new technology is more expensive in the first few years after its launch because of the large R&D efforts required to advance the market in a new direction. After the initial thrust, costs are often dramatically reduced. This is also the case for HRAM-MS. Investment in this technology was once quite high in comparison to TQ. Recently, we have seen the introduction of more affordable GC-HRAM-MS instrumentation, the Thermo Scientific™ Exactive™ GC Orbitrap GC-MS system, designed specially for routine anlysis. As more laboratories become interested in using all the benefits of this new technology, the costs will hopefully be reduced even more.

In non-European countries, I don't have a clear idea of the percentage of laboratories that have adopted HRMS and HRAM-MS. I recently returned from visiting several countries in Latin America, and I would guess that the level of adoption is much lower there—around two or three percent. It is clear, however, that laboratories are very interested in taking advantage of this new full-scan technology, so I believe that the adoption of the technique in the rest of the world will soon be like that of Europe.

**LCGC: Do you think GC-HRAM-MS technology will become as popular as triple-quadrupole technology for pesticides analysis?**

**Fernández-Alba:** The analytical performance of these instruments is comparable to triple-quad technology, and GC-Orbitrap MS technology has several advantages derived from the combination of its high resolution and excellent mass accuracy. It's important to note that high resolution and high mass accuracy do not automatically go hand in hand for all technologies. This is an important consideration for laboratories because high resolution is only useful if the instrument also offers accurate mass, which is the case with GC-Orbitrap MS systems. If these two characteristics are not present in combination, one may not be able to achieve the desired results. So, yes, I believe GC-HRAM-MS will achieve similar popularity to that of triple-quad technology in routine laboratories.

**LCGC: Laboratory guidelines relating to HRAM-MS are not harmonized worldwide. Do you have any thoughts on prospects for harmonization?**

**Fernández-Alba:** In the area of pesticide residue analysis, we work with especially strict controls and guidelines for the identification of components. But, it's important to note that both HRAM-MS and triple-quad MS provide data that comply with regulatory guidelines. In the case of quantitation, the requirements are the same for both technologies. New GC-Orbitrap MS platforms completely fulfill regulatory identification criteria satisfied by triple-quad MS.

Unfortunately, laboratories do not have a clear understanding about this issue, which relates to the fact that HRAM-MS is a relatively new platform for routine laboratories. Furthermore, there is currently no clear harmonization among guidelines worldwide, which some may see as a limiting factor in the acceptance of this new platform. We are working to improve this. In general, several international guidelines are very similar, so it's only a matter of producing more information and more data to adjust and harmonize the guidelines for everyone.