

GC Orbitrap MS/MS system addresses an expanding set of compounds of concern to health and the environment

“Our analyses must cover more than 50,000 compounds, so we need an instrument that can be used for many purposes. Our choice was the Q Exactive GC Orbitrap system.”

—Dr. Flavio Ciesa, Safety chemicals (REACH) and chromatographic analysis,
Agenzia Provinciale per l'ambiente





Photo courtesy of the Provincial Agency for the Environment

“If we find something that doesn’t look correct with a sample, or if we want to check a sample later for other contaminants, with the Q Exactive GC Orbitrap GC-MS/MS system we can go back to the full-scan data to determine with good sensitivity what is there, which is impossible with a single quadrupole system in SIM mode or a triple quadrupole in SRM mode.”

—Dr. Flavio Ciesa

Protecting human health and the environment against the risks of chemicals

Human health is not only affected by contaminants in foods and the environment, it is also influenced by the products—clothes, toys, cosmetics, and detergents—used daily. These are the concerns of the Agenzia Provinciale per l’ambiente (the Provincial Agency for the Environment) of Bolzano, Italy. In collaboration with private and public groups, its laboratories perform chemical and biological analyses of foods, beverages, feed, textiles, toys, cosmetics, detergents, jewelry, and more.

Using the Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system, the Agency is able to analyze a large and expanding list of compounds of interest to human health and the environment, with greater certainty and ease.

Food Analysis Laboratory interests extend beyond food and environmental samples

- Determination of phthalates (plasticizers) in toys
- Control of aromatic amines and carcinogenic dyes in textile products
- Testing for carcinogenic chemicals such as aromatic amines in inks used for tattoos and permanent makeup

European Union regulations increase the scope of compounds monitored

Recent European Union (EU) chemical safety, REACH, and CLP regulation is driving need for methods able to analyze a large and growing number of substances of interest. REACH (Registration, Evaluation, Authorization of Chemicals) aims to improve the protection of human health and the environment against the risks of chemicals, increase the competitiveness of the European chemical industry, and reduce the number of tests carried out on animals by promoting alternative methods for assessing substances. CLP (Classification, Labeling and Packaging) regulates the classification, labeling and packaging of substances and mixtures.

“When we have complex sample matrices, the Q Exactive GC Orbitrap GC-MS/MS system makes it a lot easier because we can prepare samples using a general method.”

—Dr. Flavio Ciesa

The Q Exactive Orbitrap GC-MS/MS system addresses expanding diversity of targeted and non-targeted analyses

With a broad analytical charter expected to continue to expand due to emerging health concerns and regulations, the laboratory needed an instrument that can be used to confidently detect and quantify a wide variety compounds in complex sample matrices. When unknown peaks are found, the laboratory often performs untargeted analyses to determine their identities.

With full-scan high-resolution accurate-mass (HRAM) capability, and the ability to perform MS/MS experiments and check isotopic abundance patterns, the Q Exactive GC Orbitrap GC-MS/MS system delivers more than high-capacity high-confidence screening and quantification. Using the Q Exactive GC Orbitrap GC-MS/MS system, the laboratory can also perform retrospective data analysis to identify compounds not detected using traditional targeted analyses, and to go back through data months or even years later to check for substances not previously targeted.

According to Dr. Flavio Ciesa of the REACH Analysis Laboratory, “When you work in full-scan you have a complete set of data that you can go back to. That’s been a good thing to have because, for example, after analyzing some fish samples for PCBs we were able to go back to the data without rerunning samples and find tetra-, penta-, and hexachlorobenzenes.”

High-resolution reduces interferences

Complex sample matrices present significant challenges to selectivity and detection limits, demanding that laboratories spend more time on sample preparation. With HRAM capability, the Q Exactive GC Orbitrap GC-MS/MS system provides excellent sensitivity, quantitative accuracy, precision, and linearity, even when a general method is used to prepare complex sample matrices.

Polychlorinated biphenyls (PCBs) are among the most widespread persistent organic pollutants and are identified in every compartment of the global ecosystem.

Chromatographic separation is complex and no single GC-column can completely separate all of the 209 possible congeners. Interferences such as co-elution of higher homologues can make MS detection difficult. The high-resolution capability of the Q Exactive GC Orbitrap GC-MS/MS system is powerful in minimizing interferences when analyzing complex matrices for PCB contamination (Figure 1).

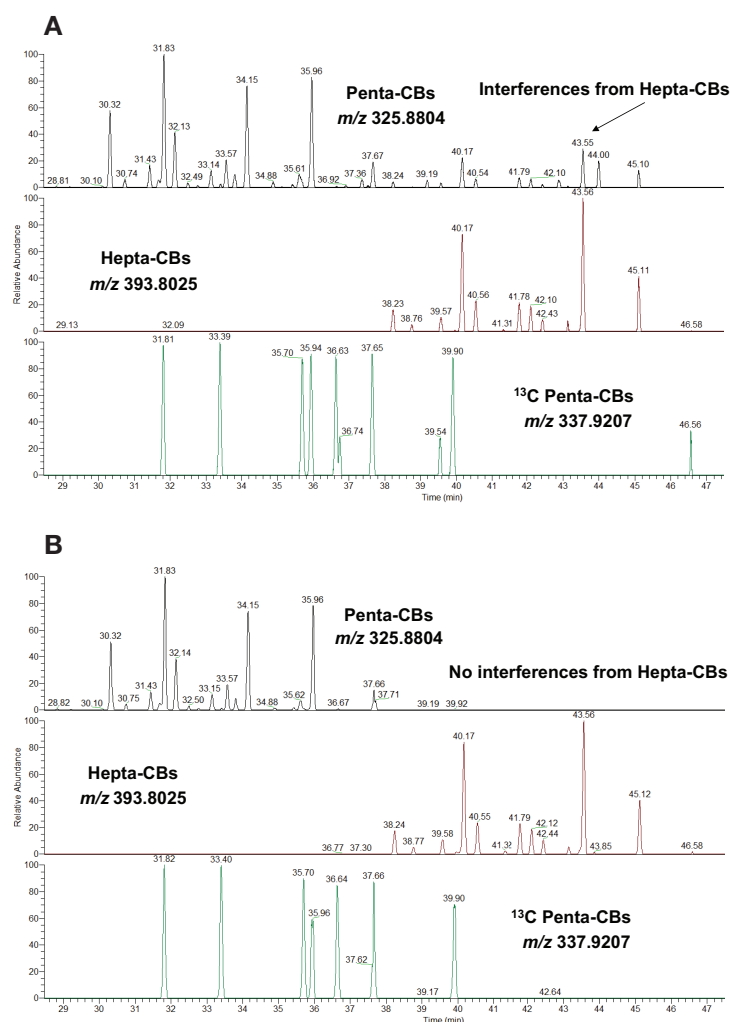


Figure 1. Resolving interferences when analyzing PCBs using the Q Exactive GC Orbitrap GC-MS/MS system. A. An ion chromatogram of a fish sample at 10,000 mass resolution shows interferences from hepta-chlorinated biphenyls (hepta-CBs). B. At 60,000 mass resolution, the hepta-CB interferences are eliminated. Courtesy of Ciesa, F. and D’Ambrosio, L. of the Laboratorio analisi alimenti; and Basso, A., Mair, K., Fellin, V., and Tirler, W. of Eco-Research, Bolzano, Italy.



Photo courtesy of the Provincial Agency for the Environment

“For multi-component applications I prefer Thermo Scientific™ TraceFinder™ software because the software is intuitive and time-saving and because it automatically performs complex calculations such as ion ratios.”

—Dr. Flavio Ciesa

HRAM data ensure high-confidence results that withstand challenge

Since a product could be recalled if a contaminant is detected above safe levels, laboratory results must be of highest quality and certainty, able to withstand any scrutiny. As Dr. Ciesa explains, “The results of our experiments are very important, so we have to be sure the data we obtain are correct. Whether we have a standard to use or not, when we work at $\geq 60K$ resolution and obtain an exact mass, we can perform MS/MS experiments and can control the isotopic abundance pattern so the results are the best any lab could provide.”

Conclusion

The Q Exactive GC Orbitrap GC-MS/MS system brings together the power of GC and HRAM Orbitrap MS to provide high-capacity targeted and untargeted component detection, even in extremely complex samples. Full-scan data acquisition makes it simple to perform targeted and non-targeted methods, and

allows for a potentially unlimited number of compounds to be monitored a single sample injection. Unlike SRM acquisition on a triple quadrupole instrument, high-resolution, full-scan data acquisition enables retrospective interrogation of data to search for emerging contaminants that were not screened for when the data were originally acquired.

About Flavio Ciesa

Flavio Ciesa studied chemistry at the University of Parma, and obtained his Ph.D. in Innovative Material Science. In 2008, Dr. Ciesa joined the Laimburg Research Centre as a postdoctoral researcher where he was involved in untargeted metabolomics analysis using different techniques. From 2010 to 2014, he headed various different projects covering analyses of apples and wines. In 2014, he joined the provincial environment agency in Bolzano, where he currently works to address the safety of toys, textile, tattoo inks, chemicals, and other areas of importance to public health.



Provincial Palace in Via Amba Alagi 5, Bolzano.
Photo courtesy of the Provincial Agency for the Environment.

About the Agenzia Provinciale per l'ambiente

<http://ambiente.provincia.bz.it/appa-bolzano.asp>

The Agenzia Provinciale per l'ambiente (Provincial Agency for the Environment) is the largest South Tyrolean institution of experts in the technical protection of the environment, climate, and resources. "We work for the respectful use of natural resources and for their long-term preservation on the provincial territory," explains Flavio Ruffini, director of the provincial Environmental Agency, "in order to promote, today and in the future, a sustainable development of the territory and a better quality of life for its population." To achieve these goals, the Agency provides advice to municipalities and institutions, follows the requests of citizens, finances measures and initiatives, and develops measures for protection, prevention, verification and control. For the Agency, the protection of the environment and climate and environmental sustainability are also cultural tasks, for which it is active, sensitizing and informing, in the areas of sustainable development, food safety and climate protection.

Find out more at thermofisher.com/OrbitrapGCMS

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