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SMART NOTE 10732

Orbitrap Exploris GC-MS



Can the Orbitrap Exploris GC drive profitability in analytical testing laboratories?

Expands analytical power through simplicity

For analytical testing laboratories, the efficiency of operations from sample receipt to report is what drives profitability. Every step in the process is critical and every instrument needs to make a return on investment. The Thermo Scientific[™] Orbitrap Exploris[™] GC mass spectrometer delivers new possibilities for analytical services to boost productivity and ultimately profitability. With outstanding real-world performance and analytical flexibility, the system can reduce the costs but increase the quality of results.

Analytical testing laboratories can explore new business opportunities, keep pace with changing regulations, and streamline processes through simplified, consolidated multi-class methods and secure the very highest confidence in compound detections.

Maximum system uptime is delivered through robust performance and automation, and with a compact footprint, the instrument conserves laboratory bench space.



Transforms efficiency

Lab managers in analytical testing laboratories are faced with unique challenges. Such challenges include an evergrowing list of target compounds to be analyzed with faster turnaround times and at a competitive cost. Essentially it comes down to the efficiency of operations to increase sample throughput and minimize instrument downtime.

The Orbitrap Exploris GC mass spectrometer brings new opportunities and data certainty to laboratories performing analyses in applications such as food safety, environmental, industrial, forensics, and anti-doping. The system enables highly selective screening and quantitation of both targeted and non-targeted compounds in complex matrices with minimal method development to ensure confident analysis and increasing lab productivity.

In this smart note a closer look at the key benefits of deploying Orbitrap Exploris GC is taken to answer how this system allows for unique advantages to drive profitability in analytical testing.

Provides high confidence in results

The Orbitrap Exploris GC mass spectrometers provide the capability to acquire accurate mass data in full scan, overcoming the limitations of triple quadrupoles without compromising quantitative performance. Additionally, due to its high and ultra-high resolutions, from 60,000 up to 240,000 (FWHM at m/z 200), the Orbitrap Exploris GC systems can resolve almost any matrix interference from analytes of interest, as well as determine fine isotopes (³⁴S, ¹⁸O, ¹⁵N, etc.) for easier and faster identification. High resolving power together with excellent mass accuracy increases analytical selectivity, which means less time is spent on data interpretation and sample results can be guickly reviewed and reported. The consequence of reporting a false positive or negative result can have serious implications. From full scan data, multiple points of identification can be used to quickly confirm or reject detections to give peace of mind. In addition to the retention time of target accurate mass ions, compound detection can be confirmed using spectral matching (Figure 1), isotope pattern, retention indices, and elemental compositions to provide detection certainty and deal with the tentative identifications that exist today with other technology.1-5

Maximizes return on investment

To comprehensively screen a sample for a wide range of chemical classes, multiple methods are often required. In a high-throughput environment this can involve multiple GC-MS/MS systems to address each of the compound classes, for example, PAHs, PBDEs, OCPs, SCCPs, etc. Having multiple instruments is costly as they require their own maintenance programs, service arrangements, consumables, and operators. These all increase the cost of analysis and impact efficiency.

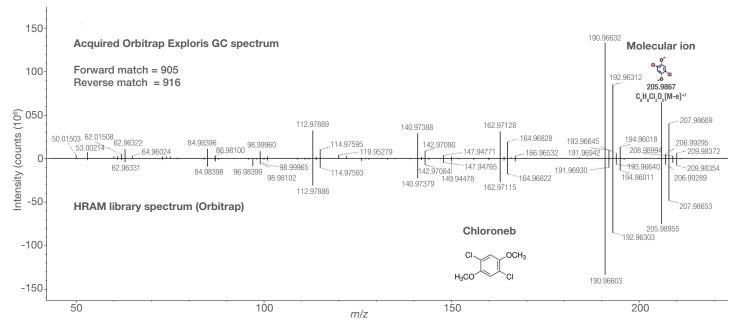


Figure 1. Full scan allows multiple compound identification points, such as multiple accurate mass ions, spectral matching, isotope pattern comparison (measured versus theoretical), and ion ratio confirmation. Example spectrum library match for chloroneb in a mixed pesticide standard using an Orbitrap Exploris GC 240 system operated in full scan at 240,000 resolution (FWHM at *m/z* 200).

This approach of multiple systems has developed through extraction and instrument capability, rather than by design. Through high resolution mass spectrometry, it is possible to take advantage of a full scan untargeted acquisition, but with the required selectivity and sensitivity that is demanded by quantitative applications (Figure 2). This enables a single data file to be acquired and processing methods then customized to extract the requested target compounds or even expand to a wider scope of analysis.

Operating one instrument instead of multiple single or tandem quadrupole systems, there is less time spent on routine daily maintenance and system set up. In addition, there is a significantly reduced bench space and instrument consumable requirements. The result is a much simpler operation that is efficient and flexible to adapt to changing laboratory needs. Furthermore, with fewer systems to maintain, instrument uptime is much higher and potentially all analytical personnel are able to process compounds from any chemical class.

Reduces method setup time

The Orbitrap Exploris GC system is designed to reduce training needs, while empowering staff of all skill levels through easy to use operation software and pre-defined method templates. The intuitive and standardized instrument control of the Orbitrap Exploris GC system guarantees that it is always performing at its best for both expert and non-expert users alike. It is now possible to initiate, tune and calibrate in under five minutes with full confidence that the system is at optimal performance. With full scan data across the entire chromatographic run, there is no need to spend time verifying that SRM windows are correct, as is the case with GC-MS/MS. This untargeted acquisition also enables the system to be quickly set up so that analysts can focus on results and not setup.

Increases the scope of analysis

Ever-changing regulations mean that analytical testing laboratories face an expanding list of analytes to be included in their scope of analysis, and they must also have the ability to respond to emerging food and environmental safety matters. Currently most laboratories rely on targeted analytical approaches using triple quadrupole mass spectrometry (MS) instrumentation to analyze a

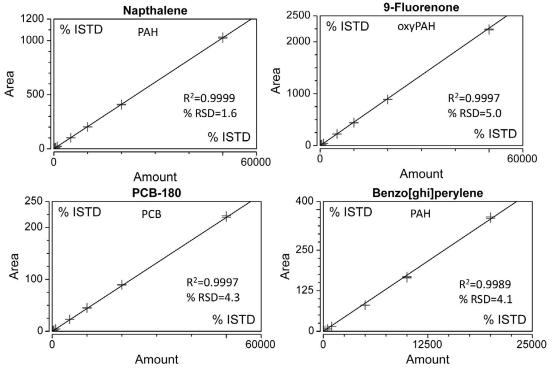


Figure 2. Quantitative capability for example PAHs and PCBs using solvent-based calibration curves ranging from 0.1 to 500 pg/µL (corresponding to 0.1–500 µg/kg in soil sample). Average calibration factor function (AvCF) was used in Chromeleon CDS and three replicate injections at each concentration with internal standard adjustment were performed.

target list of compounds. This technology covers a wide range of chemical classes and provides the required level of sensitivity and selectivity. However, they are limited to only detect those compounds in the method acquisition list. When new compounds are to be added, they require careful optimization of acquisition parameters and the checking of acquisition time windows to ensure detection of the target analyte. With an untargeted full scan acquisition, it is simply a case of updating the processing method with the appropriate ions of interest and retention time. With accurate mass selectivity, it is possible to extract target compound from a complex chemical background, and retrospective analysis of data allows the lab to investigate the presence of contaminants in samples collected and analyzed years ago.

Supports expansion into emerging applications and services

Food fraud and emerging environmental contamination is predicted to increase, and this is likely to raise concern for global regulatory authorities and consumers alike. This presents an opportunity for analytical testing laboratories to explore new services such as sample profiling and fingerprinting to observe what is normal and what is different. This is enabled through comprehensive data to allow additional questions to be asked of a sample, such as what is in my sample beyond a target list, when did it start appearing, what's different between sample groups, is my sample similar to others, and is there a marker of authenticity? You have the data, just ask the question.

Summary

Orbitrap mass analyzer technology has been successfully used to drive productivity gains in a wide range of environmental analysis, food testing applications, clinical, and anti-doping applications. The popularity of performing quantitative, qualitative, and screening analyses in a single injection is growing rapidly and provides a solution to ever-changing demands in analytical science. This is due to the Orbitrap mass analyzer's unique ability to provide high resolution accurate mass and both quantitation and gualification (accurate screening) data in a single analytical run. The quality and flexibility of data produced provides ultimate confidence in the results obtained. High resolving power increases analytical selectivity for compounds in complex matrices and thus reduces the uncertainty associated with the misassignment of positive results. The unique ability to capture all relevant data using full scan allows retrospective data analysis, reducing the need for additional sample injections.

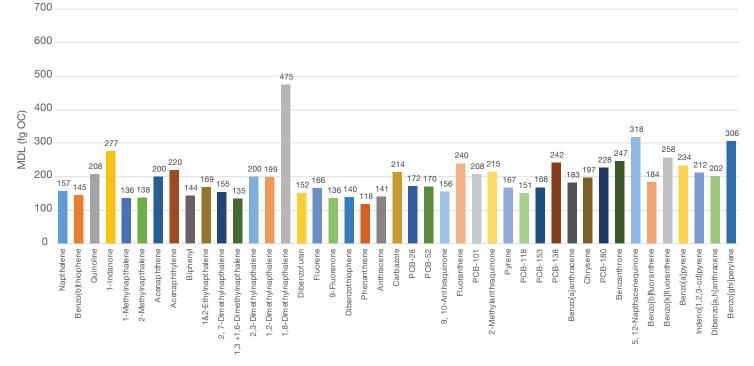


Figure 3. Sensitivity is a key factor in trace contaminant analysis. Graph showing individual method detection limit (MDLs) (as detectable fg on column) for 45 native PCB, PAH, methyl PAH, oxyPAH, and NSO-PAHs calculated from n=18 replicate injections of the lowest serially diluted matrix-matched standards.

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Furthermore, Orbitrap mass analyzers are enabling analytical scientists to raise their productivity and profitability to new levels. Compared to triple quadrupole MS-based quantitation methods that involve time consuming optimization of hundreds of SIM or SRM transitions in numerous time windows, Orbitrap mass analyzer methods enable the quantitation of virtually unlimited numbers of compounds that is fast and easy to set up. The Orbitrap Exploris GC provides unmatched versatility to meet the needs of analytical testing laboratories today and into the future.

References

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- 5. Technical Note 10728: Robust analysis of PAHs and PCBs in soil with over 500 repeat injections using Orbitrap Exploris GC. Thermo Fisher Scientific.

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