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MINIATURIZED ANALYTICAL EQUIPMENT SOLVES KEY CHALLENGES FOR LABORATORIES

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INTRODUCTION

As laboratories are increasingly called upon to do more with less resources, managers (and instrument suppliers) are getting creative about how to solve the problem in the most efficient way possible. This *LCGC* ebook highlights one interesting strategy: to do more with less instrument square footage.

Miniaturized Analytical Equipment Solves Key Challenges for Laboratories (sponsored by Agilent Technologies) is a collection of articles highlighting the important role that miniaturized instruments play in addressing challenges faced by laboratories such as the need for:

- more instruments in the same bench space
- fast, robust analyses
- less instrument downtime
- increased efficiency
- more intuitive software for analysts of various skill and experience levels

First, Badr Astiphan, marketing manager of quadrupole mass spectrometry at Agilent Technologies, talks with *LCGC* about the technical challenges of reducing an instrument's footprint and how his team of engineers tackles that problem. He then offers a white paper about the top challenges faced by analytical laboratories today and how new technologies may offer solutions.

Last, Patrick M. Jeanville, Agilent's triple quad LC/MS product manager, and Terri Sosienski, LC/MS marketing applications scientist at Agilent, talk about how a breakthrough in product and software design led to Agilent's Ultivo Triple Quad LC/MS, a fit-for-purpose" triplequad LC/MS designed to maximize laboratory efficiency, productivity, and results.

These papers show how sometimes, great solutions come in small packages.

TOC
Table of contents

MINIATURIZED ANALYTICAL EQUIPMENT SOLVES KEY CHALLENGES FOR LABORATORIES

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Novel Solutions for Achieving Instrument Miniaturization

An interview with Badr Astiphan

Miniaturized laboratory instrumentation is an important tool for laboratories looking to increase efficiency in numerous ways. But, reducing the footprint of complex analytical tools is a major challenge for engineers and scientists, and few instrument makers have created smaller instruments that do not sacrifice robustness. *LCGC* recently spoke with Badr Astiphan, marketing manager of quadrupole mass spectrometry at Agilent Technologies, about these challenges and how his firm addressed them with its newly launched Ultivo Triple Quadrupole LC/MS system.

What challenges do engineers face when they're looking to reduce an instrument size?

There are several challenges that come to mind. The first is how to design the miniaturized components that make up the instrument without sacrificing the instrument's performance. When you're dealing with smaller components, you have to engineer them in a way that they can still generate equivalent or improved ion flux and ensure efficient ion transmission throughout the device. You're dealing with the forces of physics, electronics, and chemistry, and you have to be able to handle it at a much smaller scale, using much smaller components.

The second piece to consider is how precise the manufacturing of those components must be for it to occur reproducibly.

How did Agilent address both of those issues with its new Ultivo system?

Agilent has been a manufacturing powerhouse for many decades. Our deep experience over the years—designing and developing GC/MS instruments, LC/MS instruments, as well as GC, LC, and ICP-MS systems—has made our manufacturing group world-class. It gave us the ability to manufacture to the precision and tolerances necessary to assemble a miniaturized instrument like the Ultivo without compromising robustness or performance.

The Cyclone Ion Guide, for instance, uses an innovative twisted and tapered

dual-hexapole, which focuses the ion beam down into a much smaller space. We used that same design—a twisted and tapered set of rods—in the Vortex Collision Cell as well. The tapered design maximizes ion collection from the entrance of the devices, while producing a tightly focused beam of ions at the exit aperture.

To significantly minimize the footprint of the Ultivo's pre- and post-filters, we used wafer-thin filters that do not use RF fields. Essentially, this provides faster MRMs in multi-analyte methods and "flat-tuning" of the device, extending the performance of the device over longer periods of time. This design maximizes ion transmission in a small amount of space. In the end, the filters have a much shorter optics length than what you'll find on legacy instruments.

These three components allowed us to miniaturize without sacrificing performance. In fact, the Ultivo system delivers unexpected levels of power and performance. The instrument exceeded our expectations on that front.

Could you talk about some of the testing that your team did to ensure that the Ultivo system is as robust as some of the larger legacy instruments that labs are using right now?

We hold ourselves to a really high standard when it comes to quality testing. We engage in two types of testing. One is design-phase quality testing and the second is application testing by our scientists to mimic real-life laboratory environments.

In terms of quality testing during the design phase, we put all our instruments through a rigorous test regime, which includes everything from temperature and atmospheric testing to how the instrument will perform after it is transported on a cargo flight. We do rigorous drop testing to simulate the instrument falling off a bench during an earthquake, falling off a FedEx truck, or rolling down a set of stairs. We also do thorough shake and vibe testing to simulate an instrument being transported in the back of a truck going cross-country over rough roads.

After all these tests, the instrument goes back on a bench, gets pumped down, and has to turn on and operate. So, from a robustness quality perspective, we want to ensure our instruments can withstand unexpected levels of stress.

And then, to ensure that the instrument performs as well as our prior instruments do in real-world environments, we have a suite of application notes testing the instrument in the food analysis space and the environmental analysis space, and we are looking at extending those applications as well. These application notes showcase areas like limits of detection, sensitivity levels, how an instrument performs with an application, and more.

We are also working on a robustness technical overview. We injected over 1,500 samples consecutively, and we've

seen a very stable response in terms of reproducibility, accuracy, and robustness. We're continuing that experiment and plan to significantly increase the number of samples that we aim to inject.

For labs that are concerned about maximizing efficiency and their bottom lines, how do you feel that smaller instruments are helpful?

The benefits of smaller instruments are particularly amplified for laboratories where the real estate is very expensive or where there is no room for expansion. Smaller instruments allow a laboratory to expand the number of samples it can analyze on a daily basis. More instruments will fit on a bench, which provides a higher throughput within the same laboratory space.

What about the embedded software? Could you talk about how that helps to increase efficiency and maximize economic outcomes?

There are a couple of aspects to consider. We believe that smart instrumentation must have a positive and direct business outcome. We have software on the instrument that is constantly monitoring the state of the instrument to let the user know whether the instrument is ready for use or whether it needs maintenance before analysts load a valuable batch of samples and let it run overnight. This constant real-time monitoring helps ensure that the first time a sample or batch is run will be the last time it is run. We want to minimize the need for reruns, which are very, very expensive both in terms of time and when sample material is scarce. Sometimes, it is just impossible to obtain more sample.

The other piece is on the method development side. We've looked at ways to streamline how an end-user that develops and runs methodologies will acquire the data. The Ultivo uses Quant-My-Way data analysis software to give them the ability to personalize their experience. They can hide features they don't need for their specific workflow and highlight the features they do need as they're analyzing the data that they've acquired on Ultivo. This provides significant time savings.

What kind of skill level is required for an analyst to use the Ultivo?

We're getting feedback from many of our customers that the technicians and analysts that they're hiring now are not necessarily PhD trained mass spectrometrists. And so, we were very sensitive to that when designing the instrument to ensure that we are minimizing a technician's interaction with the actual hardware itself. For instance, we created the VacShield to allow end-users to do front-end source maintenance without having to vent and disassemble the instrument.

On the software side, some of the areas I mentioned earlier are helpful to new and veteran analysts alike. In the past, a customer would have had to know which

signs to look for to determine whether the system was stable and ready to run a sample. Today, the Ultivo is doing that for the customers with its embedded diagnostics (early maintenance feedback), which monitor system status in real time and proactively alert the user if an issue arises, so that's a significant step forward. It is allowing for less-experienced technicians to get meaningful data out of the instrument in a straightforward way.

Finally, Quant-My-Way allows users to personalize their software experience. By allowing for personalization of that experience—and only highlighting the feature set that any specific workflow would require—we're not distracting a technician from having to wade through a lot of calculations or functions in order to find the calculation that he or she needs.

We are very consciously moving our instruments toward being more accessible to more people, and the Ultivo is a major step in that direction.

Addressing Challenges and Maximizing Resources in High-Throughput Laboratories

Badr Astiphan

New miniaturized instrumentation increases productivity and offers fast return on investment.

Fast and accurate analysis is an absolute "must" for any high-throughput analytical laboratory, and demands are only increasing every year from both regulators and customers. Food and environmental labs have especially large volumes of samples to analyze with shortening deadlines for report delivery. As laboratories take on new contracts, capacity becomes even more strained. How can labs address this issue?

Though it is not an ideal solution from a business perspective, third-party laboratories are often contracted to fill the excess demand. Such outsourcing not only increases turnaround time, but also sacrifices some profit margin.

Another option is for laboratories to invest in laboratory expansion by acquiring real estate to make room for additional instruments. This strategy, of course, cannot be deployed quickly and requires a significant capital investment. Finding qualified technicians and scientists to operate the expanded laboratory places even more stress on laboratory managers.

Hardware is only part of the story. The software used to acquire and process the data to generate the final results are a key component of the overall user experience and directly impacts the productivity of the laboratory. Streamlining software design with an acutely user-centric focus to increase accessibility to the software and to shorten time-to-report offers immediate productivity, and hence business, payback to the lab manager.

As laboratories are forced to do more with less, those that optimize the tools that technicians use every day to amplify productivity without sacrificing the quality of the delivered results will give laboratories a competitive edge. What follows is a discussion of the top four pain points faced by analytical lab managers, as well as an overview of how new instrumentation helps address these needs.

Top Four Challenges Faces by Analytical Laboratories

1. Too much instrument downtime.

It is not uncommon for typical liquid chromatography/mass spectrometry (LC/MS) systems to require routine maintenance, which sometimes requires venting the instrument to perform. The time required to shut down a system for upkeep and return it to a fully functional state can be substantial. Depending on the type of maintenance, such work displaces up to a half-day of analytical work.

Since time is money, there is a huge business advantage in deploying a fleet of analytical instruments that minimize the downtime for set-up and maintenance. The more systems that are up and running, the more samples that can be analyzed—and the better the business proposition.

The Agilent Ultivo Triple Quad LC/MS was intended to address this problem and other pain points felt by the food and environmental testing laboratory managers that use triple-quad LC/MS systems for quantitative analyses. Ultivo minimizes instrument downtime as well as maximizes productivity in the laboratory in several ways. For instance, VacShield allows users to conduct rapid routine front-end ion source cleaning and maintenance without the need to vent the instrument. This feature reduces wear and tear on the vacuum systems and saves hours of lost operational time.

Ultivo also has features that streamline more involved, non-routine maintenance tasks, like preventative maintenance and detector replacement. In one example, Ultivo was designed with an easily accessible and exchangeable detector assembly that can be accessed without unstacking the HPLC and without disassembling the LC/MS. This keeps the instrument running longer and generating data needed to keep operations moving smoothly.

2. Unexpected downtime.

A second major frustration among analytical laboratory managers is the need for more intelligence and predictive diagnostics from instruments. They are looking for smart systems that actively monitor and proactively communicate maintenance work required for an analysis to run smoothly. It is extremely wasteful in terms of time, energy, and resources to start running an expensive batch only to discover that it cannot be completed properly due to required ion source cleaning or an approaching end-of-life of the electron multiplier. Lab managers and technicians would like the confidence to know that their batches will run to completion before they start the analysis, and would like to know how to resolve issues if the instrument is not ready. Eliminating the need to re-run batches of samples flows straight to a laboratory's bottom line.

Ultivo was engineered with intelligent diagnostic tools to provide users with the

information necessary to understand the state of the instrument *before* running samples. Just like a car's diagnostics system is equipped with sensors that actively monitor status and proactively alert the driver when the brakes need maintenance or an oil change is needed, Ultivo monitors itself in real time and then proactively alerts the user when an issue is detected that requires attention. With Ultivo's intelligent diagnostics features, the instrument gives technicians the confidence that they can run a sample batch without having to discontinue their work for unplanned maintenance and reruns.

3. Large, cumbersome instrumentation. To address capacity challenges, many laboratory managers are actively seeking out instruments with space-saving designs. Standard LC/MS systems and gas chromatography/mass spectrometry (GC/MS) instruments occupy significant space on the bench. As the number of those instruments installed in the laboratory increases to deal with an uptick in demand, available square footage becomes harder and harder to find—and is nonexistent in many laboratories. Therefore, it is becoming an increasingly important strategic decision for laboratories to invest in LC/MS systems that have been engineered with a small footprint.

It takes both significant technological and engineering innovations on the part of an instrument provider to drive down a system's size. Miniaturization of the components that make up an instrument within the constraints of the laws of physics that govern handling of ions required creative thinking. Creatively designed components must be engineered and manufactured to exacting specifications and tolerances. The components must be built into a small, rugged, well-ventilated enclosure and operate in close proximity to each other without negative impact. Ultimately, the instruments must deliver trusted answers under a wide variety of operating conditions. A world class R&D, engineering and manufacturing organization, like Agilent, is required to deliver on the vision of the designers, engineers, and the scientists that created Ultivo.

Agilent is very experienced at miniaturizing analytical instruments. For example, when the 6470 Triple Quad LC/MS was launched, the instrument's footprint decreased by 30% when compared to the 6460 Triple Quad LC/MS. A 30% space savings is significant for laboratories with a large deployment of a Triple-Quad LC/MS systems. Ultivo's goal was to free up even more bench space while delivering at least the same level of sensitivity performance and analytical power as a 6460. Ultivo's revolutionary design met that lofty goal and features an instrument footprint that is 70% smaller than previous instruments. When you consider the Ultivo as a direct replacement for older instruments, three

or four instruments could fit into the same bench space that older mass specs currently occupy, which could triple or even quadruple a lab's capacity within increasing their physical real estate.

One example of the creatively designed and precision-engineered components in Ultivo is the Cyclone Ion Guide, which represents a revolution in miniaturized ion optics. The twisted and tapered design of the ion guide allows it to tightly focus and columnate the ion beam over a very short path and through a significant pressure drop. Another example is the revolutionary manufacturing technique that allows quadrupoles to be manufactured with the tolerances required to enable the space-saving design without compromising the performance levels that can be achieved with larger quadrupoles. Also, the Vortex Collision Cell is a miniaturized collision cell that delivers all the power of a full-sized collision cell with no cross talk and with consistent ion fragmentation patterns.

4. Data Analysis Challenges

In addition to the instrument size being a challenge for labs, technicians also find the data analysis software tools to be cumbersome. Laboratory managers want to purchase instruments that can be used by technicians and analysts of various skill and experience levels. While it is important for instrument hardware to be accessible to a broader group of analysts, who are often called upon to handle increased loads with diverse sample types, software usability and accessibility is just as critical. In fact, improving the usability of the data acquisition and data analysis software was as important to Agilent's software engineers as decreasing the size of Ultivo.

Quant-My-Way is a key new feature of MassHunter that allows for significantly streamlined data analysis workflows. Quant-My-Way enables the lab manager to personalize data analysis workflows by creating and using customized views. MassHunter Quantitative Analysis software is extremely feature rich, with many calculations and data visualization options available to the user. For workflows that do not require the use of all the features, the lab manager can create an assay-specific custom view that only shows data analysis features that the analysis will use in that specific circumstance. Custom views reduce human-induced errors by hiding features that are not needed. Quant-My-Way can save analysists hours per week of sample processing time. From a lab manager perspective, reducing the number of errors introduced by their technicians increases productivity while maintaining data quality, which, in turn, reduces laboratory costs.

Summary

All told, laboratories face significant challenges as they prepare to handle increasing sample capacity. Whether time and profit are lost when sending samples out to a third-party laboratory

to fill overflow demand, or productivity is sacrificed due to planned—or unplanned—maintenance, labs need new options to help them meet today's unique challenges. Given the increase in productivity that the instrument provides, Agilent's Ultivo Triple Quad LC/MS is an excellent fit for high-throughput contract laboratories that are under significant regulatory and business pressure to analyze an increasing sample load per day.

Badr Astiphan *is the marketing manager of quadrupole mass spectrometry at Agilent Technologies.*

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Evolution of Liquid Chromatography Triple-Quadrupole Mass Spectrometry for Low-Level Residue Analyses in Food and Environmental Matrices

Patrick M. Jeanville and Terri Sosienski

Triple-quadrupole liquid chromatography/mass spectrometry (LC/MS) is the current standard for routinely identifying and quantifying trace levels of target compounds in difficult matrices. Deployment and use of triple-quad LC/MS instrumentation has increased significantly, especially in commercial analytical laboratories that require the ability to confidently process and deliver high-quality data quickly and routinely. As the technology entered widespread use by organic chemists, biologists, food and environmental scientists, among others, demand for improvements in usability and accessibility intensified. Improvements in hardware and software design, coupled with the development of workflow-specific tools helped triple-quad LC/MS instrumentation become accessible to more laboratories. Today, with the rise of global regulatory demands in the food and environmental sectors, and the challenges associated with global development become more acute, it is paramount to ensure that the tools scientists use are designed to quickly, easily, and seamlessly answer the questions that the scientists are asking.

A breakthrough in product and software design led to the Ultivo Triple Quad LC/MS, the ultimate partner for productivity. Ultivo is a "fit-for-purpose" triple-quad LC/MS designed with a specific goal in mind: to maximize laboratory efficiency, productivity, and results in a remarkably small package. The applications shown below demonstrate Ultivo's ability to provide effective analysis of trace organic compounds and per/polyfluoroalkyl substances in water, as well as the sensitive and robust analysis of mycotoxins and pesticides in foods.

Special Features

Overview

The Ultivo triple-quadrupole LC/MS is designed for the environmental and food safety markets, which comprise more than one-third of the total LC/MS market. Growth in these segments is projected to rise at double-digit rates and is accelerated by the need to perform high-throughput quantitation with precision

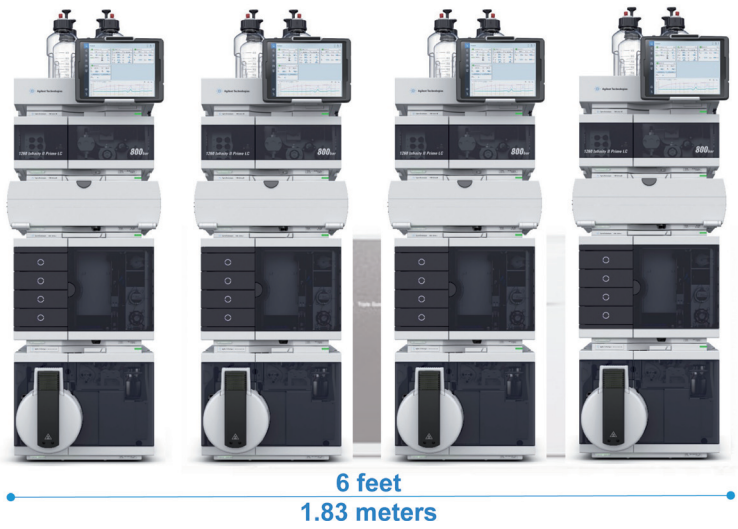


Figure 1: Stacked configuration of Agilent's Ultivo triple-quad LC/MS systems.

and accuracy at low-cost. Because Ultivo is a fit-for-purpose instrument that is designed for their specific applications, it has several features that directly address the needs of those laboratories.

In the early days of triple-quad LC/MS technology, instruments were mainly operated by PhD scientists. Today, many operators lack this level of training and may be seeing these instruments for the first time on the job. With this shift in the user-base and the need to increase overall productivity, software is a critical component for triple-quad LC/MS systems in the applied markets. Ultivo software, therefore, is designed to simplify operation and provide efficient operation with smooth workflow, thereby maximizing a business' return on investment (ROI).

The instrument's footprint is extremely small, at 15.4 in (39 cm) wide x 31.1 in (79 cm) deep x 12.6 in (32 cm) high, yet it still achieves the accuracy and sensitivity that environmental and food applications demand. As seen in **Figure 1,** LC components can be stacked on top of the Ultivo, and four complete Ultivo triple-quad LC/MS systems take up the same amount of room as one traditional triple-quad LC/MS. In addition, Ultivo features next-generation ion optics, precision-made hyperbolic quadrupole rods and a robust high-energy detector. The instrument's diagnostics provide "real-time" information to the operator regarding system status and guide the operator to take appropriate corrective action. Overall, the Ultivo is robust, reliable, and easy to maintain.

Hardware

The innovations incorporated within the Ultivo system were specifically designed to meet the challenging requirements that LC/MS operators face on a daily basis. **Figure 2** illustrates these hardware advancements, including VacShield, Cyclone Ion Guide, Vortex Collision Cell, Hyperbolic Quadrupoles, and the High-Energy Dynode Detector. Apart from the Jet Stream technology ion source

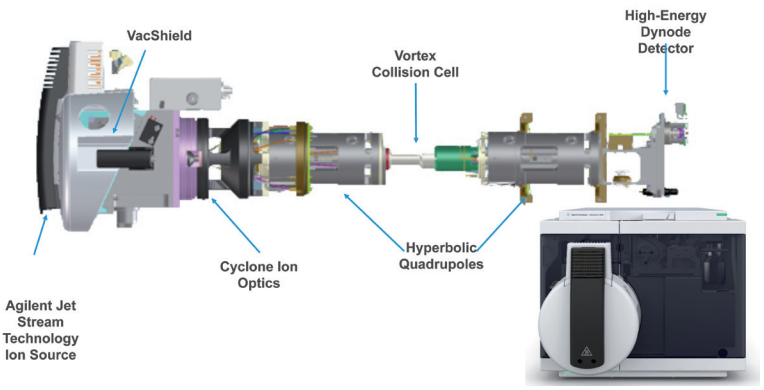


Figure 2: Ultivo: designed for robust performance.

on the front end, everything has been completely reformatted and redesigned for the utmost in performance and robustness.

Agilent's Jet Stream Technology uses super-heated sheath gas, which collimates the nebulizer spray, creating an entrenched ion beam, thus enhancing signal intensity and improving robustness. VacShield allows convenient insertion and removal of the ion injector without venting the instrument. This reduces downtime for this maintenance task to just a few minutes.

After ions are transferred from the ion source into the vacuum system using a resistive ion injector and skimmer, they are collected using our patented dodecapole cyclone ion guide. The heart of the cyclone ion guide is a tapered and twisted hexapole that passes through multiple vacuum stages. The taper enables efficient ion collection at the front, while yielding a tightly collimated ion beam at the exit. Since the pressure drops by more than 10,000-fold through the cyclone, the twist enables a greater pressure drop over a shorter length by allowing openings between the vacuum stages and minimizing the gas flow. A resistive coating on the rods allows the use of a DC bias to gently pull the ions to prevent ion stalling. Finally, a second set of rods surrounding the inner rods improves high mass transmission efficiency by providing additional confinement at the entrance of the device. Thus, the cyclone ion guide ensures smooth transition between regions of high and low pressures and facilitates compression of the ion beam, leading to higher transmission efficiencies.

Like the cyclone ion guide, the vortex collision cell is made of a twisted and tapered dual-hexapole. The taper allows efficient ion collection from the first scanning quadrupole (Q1) while yielding a tightly collimated beam for injection into the second resolving quadrupole (Q2). The twist enables optimal pressure and fragmentation of the ions, as well as reduced gas flow out of the collision cell. Ion stalling is prevented by applying a DC bias to the resistively coated rods. Special

openings at the exit of the collision cell enable a fast pressure drop while the ions are still confined, which prevents scattering at the entrance of Q2. The construction of the vortex collision cell yields consistent mass fragmentation and optimum ion transmission efficiency and therefore better MS/MS performance.

Traditional Brubaker pre-filters enhance instrument sensitivity by improving the quadrupole transmission efficiency. They suppress ion instability in the fringe field region of the quadrupole using RF voltages applied to electrodes adjacent to the quadrupole. Unfortunately, they require a significant amount of space, which disqualifies them for use in a small yet sensitive instrument. The approach devised for the Ultivo is to cancel the DC field in the fringe field region in order to enhance the quadrupole transmission efficiency. This can be done by applying cancelling DC voltages to a small quadrupole lens placed next to the filtering quadrupole. This virtual pre-filter strategy prevents quadrupole fringe field instability from reducing instrument sensitivity while keeping a small instrument footprint.

A quadrupole's performance is defined by the shape of the electrodes, radius, length, frequency and voltage. The Ultivo's Next Generation Hyperbolic Quadrupoles operate at a higher frequency and voltage, which allows a smaller sized quadrupole to achieve exceptional performance. The patented manufacturing process produces high precision, reproducible quadrupole electrodes that promote higher ion transmission and improved peak shapes for better quantitative results.

Increased surface area of the high-energy dynode detector horn collects ions over wide energy spreads, allowing for maximum sensitivity of the detection system and lower limits of detection and quantitation. To simplify replacement, the detector assembly is mounted on a removable card on the back side of the instrument.

Software

Operators of the Ultivo may use the traditional MassHunter Quantitative Analysis interface or may choose to use the new Quant-My-Way interface, which is a subset of functionalities designed within MassHunter. Quant-My-Way is built around the Microsoft Office concept of ribbon customization. Settings are saved as "flavors." Flavors enable the administrator to create user specific views with user specific features creating a customized look and workflow. Once created, flavors can be deployed to all workstations running the latest version of MassHunter Quantitative Analysis. **Figure 3** shows the vanilla flavor of MassHunter Quant-My-Way. Note its simplicity: add samples, create a batch, load the method, analyze the samples, and generate a report. This new software feature significantly reduces the time spent setting up a run.

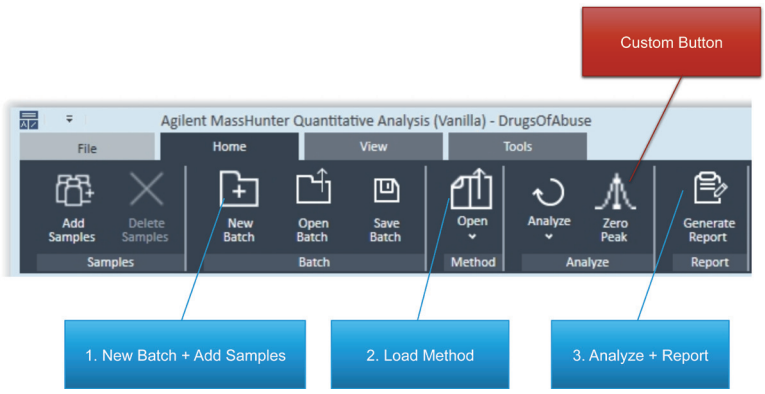


Figure 3: MassHunter Quant "vanilla" flavor.

Applications

Food Safety: Mycotoxin Analysis

Mycotoxins result from fungi that can occur on foods during growth and while in storage. They are found on all kinds of foods, and because of their toxicity, they are regulated by government agencies around the world. They typically have a very broad maximum residue limit (MRL) range, from less than 1 ppb to over 1000 ppb. Because they are so widely regulated, screening for regulated mycotoxins is a common analysis done in food testing laboratories.

Figure 4 shows the results of a conventional mycotoxin analysis in three commonly regulated matrices: corn, peanut, and black pepper. Twelve regulated mycotoxins in corn and peanuts, and five mycotoxins in black pepper were analyzed with European regulatory measures as a guideline. This analysis was completed using an Agilent 1290 Infinity II HPLC and the new Ultivo triple-quad MS system. The figure shows that the Ultivo achieved excellent sensitivity, with the majority of the compounds for each matrix having a quantitation limit 20x lower than the designated MRL, even in the more difficult matrices, peanut, and black pepper. The instrument also achieved excellent precision, with a relative standard deviation less than 10% for all compounds in each matrix at the limit of quantitation.

Food Safety: Pesticide Analysis

Because there are hundreds of different pesticide compounds used in modern agriculture, high-throughput labs need to screen for all of them as quickly as possible. In this example, 246 pesticides and their metabolites with MRLs of 10 ng/g were analyzed in three very different matrices: black tea, orange, and avocado. They were extracted with Agilent EN QuEChERs (with different clean-up for each matrix) and analyzed using a 1290 Infinity II HPLC coupled to Ultivo in a quick 20-minute method.

The graphs in **Figure 5** showcase the excellent sensitivity and precision that was achieved. The majority of the compounds for avocado and orange have a quantitation limit two times lower than the MRL, and most of the compounds in black tea were detected at two times lower than the MRL.

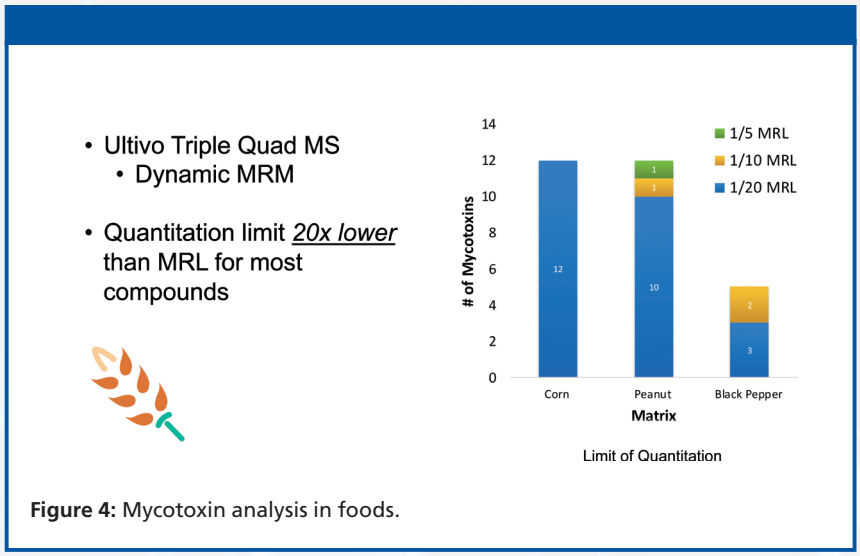


Figure 4: Mycotoxin analysis in foods.

entire method was only 16 minutes long.

The analysis achieved high linearity with an R^2 greater than 0.99 for the quantitation range of 0.5–200 ng/L. The majority of compounds were accurately quantified down to 0.5 ng/L or 0.5 ppt. No complex sample preparation was needed to achieve these low quantitation levels.

Environmental: Trace Organic Compounds in Drinking Water

Trace organic compounds (TOrCs), sourced from industrial and household waste, are not completely removed from wastewater and drinking water treatment. Thirty-one representative TOrCs were analyzed using the Ultivo triple-quad MS instrument, including pharmaceuticals such as ibuprofen and carbamazepine (an anti-seizure drug), personal care products such as benzophenone (a component of sunscreen) and DEET (the insect repellent), and industrial compounds like benzotriazole (a corrosion inhibitor) and BPA (the plasticizer). Sample preparation was automated using the Agilent Flex Cube Online SPE, which was interfaced with a 1260 Infinity II HPLC. Online SPE requires no bench-top sample pretreatment, which saved a considerable amount of time. The

Environmental: Per/Poly Fluoroalkyl Substances in Water

Per/poly fluoroalkyl substances (PFAS) are ubiquitous in the environment. Sourced primarily from fire-fighting foams, non-stick cookware and food packaging, they do not degrade easily. The US EPA drinking water health advisories for perfluorooctanoic acid (PFOA) and perfluorooctanesulfonic acid (PFOS) are 70 ng/L in drinking water.

Seventeen PFAS in drinking water, which included all 14 from the US EPA 537 method, were analyzed using a 1290 Infinity II HPLC and the Ultivo triple-quad MS instrument. **Figure 6** shows the results of the 19-minute run. Recoveries of 70–120% were achieved for all compounds at both the 1 µg/L and 5 µg/L spiking levels. Excellent sensitivity and linearity at a range of 0.1–20 µg/L were observed, along with relative standard deviations

- Outstanding sensitivity
  - LOQ 1ng/g and 5ng/g for most compounds
- Excellent Precision
  - RSD% below 20% for >98% of the compounds

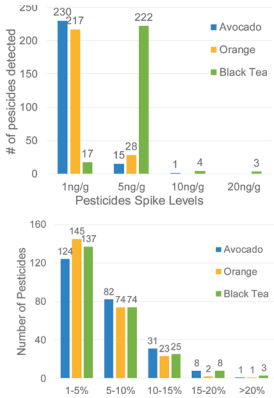
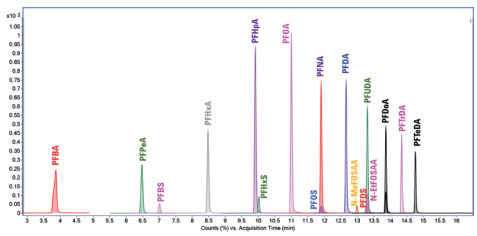


Figure 5: Pesticide analysis in foods.

- 17 PFASs in drinking water.
  - All 14 from USEPA 537 method.
- 250mL water samples.
  - Extracted with Agilent Weak Anion Exchange (WAX) cartridges.
- 1290 Infinity II LC
  - Delay Column: Zorbax Eclipse plus C18 4.6x50mm, 3.5µm
  - Analytical Column: Zorbax Eclipse plus C18 3.0x50mm, 1.8µm
  - Mobile Phase: H_2O and 95:5 MeOH/H_2O, 5mM Ammonium Acetate
  - Flow Rate: 0.4 ml/min
  - Runtime: 19 minutes



Ultivo Triple Quad MS in negative ionization mode.

Figure 6: Per/poly fluoroalkyl substances (PFAS) in water.

(RSD) between 0.3 and 10.8% for all compounds in the method.

Conclusion

The Ultivo instrument transcends the existing size-performance paradigm, opening new avenues for scientists to extract more revenue out of their available lab space. Innovations within the Ultivo facilitate faster setup and scanning, which relates to increased throughput. Greater ion transmission efficiency in the Ultivo leads to greater sensitivity, better and more reproducible peak shapes, and improved quantitation. Fast and easy maintenance, combined with an intelligent way of monitoring the system to quickly pinpoint issues, reduces downtime.

Thus, Ultivo reflects a transformative approach in LC/MS, and ushers in a new generation of fit-for-purpose liquid chromatography triple-quadrupole mass spectrometry.

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