Triple Quad™ 3500 System Compendium Volume 1

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SCIEX Triple Quad 3500 System Compendium Volume 1

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Introduction

SCIEX Triple Quad 3500 System Compendium Volume 1

Liquid chromatography coupled with mass spectrometry (LC-MS) is sometimes viewed as beyond the technology budget of many start-ups and routine testing labs. It is also perceived to require specialized operator training with constant maintenance needed to enable the uptime demanded for high sample throughput.

However, for challenging applications requiring identification and quantification of known and unknown analytes at low concentrations, the power of LC-MS is undisputable. The SCIEX Triple Quad 3500 System provides all the advantages of advanced LC-MS technology for labs operating on a tight budget, and its simplicity of operation is on par with gas chromatography.

Mass spec technology allows busy labs to improve efficiencies, drastically increasing their throughput by condensing multiple sample analyses into a single run. The Triple Quad 3500 System is designed for ultra-fast detection and high sensitivity for comprehensive multi-component analysis. This capability is delivered by advanced eQ™ electronics and the curved LINAC® collision cell. This introductory MS system also provides exceptional robustness and ruggedness owing to the proven design of a Turbo V™ source and Curtain Gas™ interface, enabling routine analysis of complex samples, day in and day out. With the Triple Quad 3500 System, SCIEX makes its legendary power, speed, and accuracy more affordable than ever – empowering routine testing labs in their important role as monitors of food and the environment.

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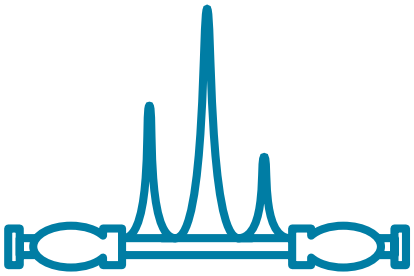

What is LC-MS/MS?

Liquid chromatography (LC) enables the analysis of a wide array of analytes by separating a sample into its many components, which can then be ionized and sent through a mass spectrometer for identification and quantitation.

Many compounds that are difficult to analyze by GC-MS, such as thermally labile and chemically unstable analytes, amines, and semi-volatile compounds, are ideal candidates for LC-MS/MS. The strength of this technique lies in the separation power of LC for a wide range of compounds combined with the capability of MS to quantify compounds with a high degree of sensitivity and selectivity based on the unique mass/charge (m/z) transitions of each compound of interest.

Liquid chromatography is an analytical chromatographic technique that separates ions or molecules, which are dissolved in a solvent, over a column. If the sample solution is in contact with a second phase, solid or liquid, the differences in adsorption, ion-exchange, partitioning, or size will allow the mixture components to be separated from each other as they pass through the column at different rates. Most routine LC methods require minimal sample handling preparation steps, reducing the risk of user error and saving valuable time in labs aiming for high-throughput analysis.

LC-MS/MS experiments frequently employ soft ionization methods not available in GC-MS, such as electrospray ionization. This prevents analyte degradation and allows for more controlled fragmentation. In tandem mass spectrometry (MS/MS), a molecule of interest is isolated within the mass spec instrument and fragmented into multiple subunits. These subunits then undergo ionization in order to help elucidate the parent molecules composition. This is accomplished by having mass spectrometers in series. Through a process in tandem MS termed multiple reaction monitoring (MRM), analyte precursor ions are selected in the first stage of analysis, dissociated into fragment ions within the second stage, and selectively filtered and detected within the third stage of analysis. By sequentially selecting and fragmenting each analyte so that only analyte-specific product ions are detected, the specificity and sensitivity of the assay can be improved exponentially. The co-eluting analytes and samples within complex matrices, which may have been problematic for other assays, can greatly benefit from the additive power that MS/MS provides.

LC-MS/MS with electrospray ionization operating in MRM mode has become a standard technique for targeted quantitation because of its well-known selectivity and sensitivity. Furthermore, its popularity has increased due to the ability to screen for, quantify, and identify large panels of analytes across different compound classes in a single analysis. Mass spectrometers are typically considered to be expensive and complex instruments but advances in electronics have resulted in economical and robust benchtop LC-MS/MS instrumentation. In addition, recent software developments make LC-MS/MS as easy to use as standard GC instrumentation. The SCIEX Triple Quad 3500 System provides labs with robust and reliable mass spec technology and methodology, at an affordable price.

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Making the Leap
to LC-MS/MS from GC-MS

Historically, LC-MS/MS has been used as a complementary tool for the analysis of compounds that were difficult or impossible to analyze by GC.

GC-MS has traditionally been the preferred technique for the analysis of less polar and more volatile compounds and can offer exquisite separation, however the high temperatures used for vaporization prior to GC separation can cause degradation or modification of up to half the analytes in a sample.[1] This is a particular concern in life science research, as many biological molecules are relatively labile and break down easily at high temperatures. Time-consuming, labor-intensive sample preparation and long chromatographic run times further reduce the efficiency of GC-MS analysis.

These factors have led to the rapid adoption of LC-MS/MS in analytical and routine testing labs across a wide variety of applications. LC-MS/MS offers specific advantages over GC-MS, such as the ability to identify and measure a wider range of compounds with minimal sample preparation. The technology is broadly compatible with both polar and nonpolar compounds, and offers exceptionally high selectivity and sensitivity, which typically results in radically improved limits of detection and quantitation accuracy over GC-MS. The transition from a niche tool for analytical chemists to standard equipment in life science labs has been further aided by greatly simplified sample preparation. Many analyses throughout industry are now being transferred from GC-MS to LC-MS/MS, enabling labs to reduce costs and minimize the potential for errors or contamination.

GC is commonly interfaced to single MS, providing constraints on the types of workflows that can be carried out and the types of samples that can be successfully quantitated. Part of the enhanced sensitivity and selectivity of LC-MS/MS comes from the coupling to tandem MS, which allows experiments such as multiple reaction monitoring (MRM). LC-MS/MS with MRM can be utilized to analyze multiple drug classes in a single assay for quantitation/confirmation, as well as comprehensive drug screening. These workflows also allow quantitation of trace levels of analytes (parts per trillion) in complex samples such as food, tissues and soil. The simplified sample preparation and handling is delivered by the versatility of LC-MS/MS instrumentation. In GC-MS experiments, samples must be in an organic injection solvent and derivatization is often necessary to improve peak shape, ionization, and volatility. LC-MS/MS typically does not have these requirements, and furthermore has become more robust and reliable with every iteration of new technology, allowing it to handle dirtier samples and a wider variety of underivatized analytes. While LC-MS/MS sample preparation methods can include solid-phase extraction or liquid-liquid extraction, they are often as simple as direct injection, dilution, or protein precipitation.

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The SCIEX Triple Quad 3500 System offers enhanced results for low level residue testing, and modern performance for labs on a budget – quantitation without compromise. The system enables the analysis of multiple compounds in every injection with excellent accuracy, along with large sample volumes, greatly improving throughput and overall productivity over conventional LC or GC workflows. The system has been developed to give labs of all skill levels or budget constraints access to the best technology for success.

1. Reference: Fang, Mingliang, et al. "Thermal degradation of small molecules: a global metabolomic investigation." Analytical chemistry 87.21 (2015): 10935-10941.

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Expand Your Lab's Potential

Governments, companies and the general public rely on testing labs to fulfill regulations, illicit drug analysis and protect the integrity of food and the environment. A laboratory aiming to deliver reliable data, while also offering value for money, must have an instrument that can deliver premium performance at the right cost of ownership. For any lab currently running assays using GC, GC-MS, or HPLC, a bold new world awaits.

The SCIEX 3500 Triple Quad System can consolidate current assays, dramatically increasing data quality, and vastly expanding the repertoire of possible assays – without breaking the budget. With the Triple Quad 3500 System, modern hardware, powerful software, and robust engineering combine to enable lower levels of detection and quantitation than conventional GC and LC workflows, and across a wider range of analytes. This allows for expert level performance at an entry level price.

SCIEX has numerous systems in place to ensure that LC-MS/MS methodology can be implemented rapidly, delivering added value to new and existing customers with uninterrupted operation. Specialist engineers from SCIEX provide onsite training to fully understand the unique needs of every lab and ease onboarding. Intuitive software from SCIEX streamlines workflows and ensures that researchers can quickly get the answers they need. Ongoing training is provided by SCIEX University™, which adopts unique learning models to ensure maximum knowledge retention for less experienced users. The industry-leading SCIEX service and support organization are primed to help labs, especially those new to mass spec, to develop their methods and transition from their existing methodologies.

LC-MS/MS simplifies routine testing and allows cost-savings and increased throughput via simplified or minimal sample preparation. In addition, LC-MS/MS helps to ensure no data becomes lost in matrix interference, as the technology offers highly accurate results, injection after injection with maximum uptime. This allows more to be seen, more to be tested and subsequently more return on investment. The Triple Quad 3500 System package includes MultiQuant™ Software, which simplifies data processing, review, and reporting, and is easy to adopt for new users. By leveraging the power of LC-MS/MS analysis, testing labs can grow, offer more services, and stay ahead of competition

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SCIEX has built its reputation on developing high quality, robust, and reliable instrumentation supported by vast technical expertise and highly accessible servicing. In-house research scientists have a long track record of innovating and advancing mass spectrometry technology for novel and routine applications. Evolved from an industry-leading legacy and customer feedback, the budget-friendly SCIEX Triple Quad 3500 System contains all of the robust quality engineering expected from the SCIEX portfolio. This technology can open your organization to a new world of unrivalled data accuracy accompanied by an enormous return of investment potential. With little spend, the SCIEX 3500 Triple Quad System achieves productivity, reliability, and robustness for routine mass spec analyses with a modern entry-level mass spec system designed for today's analytical laboratories.

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Intuitive Software from SCIEX

For busy testing labs, every second counts, and it is important that data processing is as efficient and intuitive as possible. The software offering provided by SCIEX streamlines the interpretation of data from high-throughput analysis, quickly providing meaningful and reliable results.

Two key pieces of software for the Triple Quad 3500 System are Analyst® Software and MultiQuant Software. These programs are easy to implement into lab workflows, and quick to master. Each has been specifically designed to enable all users, regardless of mass spec expertise, to have complete control over their experiment parameters and also to easily understand the acquired data.

Analyst Software is an integral part of all SCIEX Triple Quad Systems, serving as a single point of control for auto-samplers, HPLC pumps and ion sources. It is created to give maximum control in experimental design with minimal user intervention, enabling researchers to acquire precisely the data they need. This flagship software is constantly evolving to meet industry demands, with broad functionality increases lab productivity. Powered by advanced algorithms, Analyst Software can monitor up to 4000 MRM transitions when needed, allowing a vast library of compounds to be monitored in a single run. The software also features smart background removal with the Dynamic Background Subtraction™ algorithm. This means that analyte peaks can be uncovered even in noisy data from complex samples with high matrix interference. One of the most important features for high-throughput labs is Scheduled Ionization. Scheduling the formation of ions controls the build-up of instrument contamination and maximizes the time between instrument cleanings, ensuring sufficient uptime for high capacity data acquisition. Finally, Analyst Software is designed to ease regulatory compliance. It is GxP compliant with electronic audit trails and complete role-based security.

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SCIEX software is fully integrated with the Triple Quad 3500 System, reducing user frustration and further easing the implementation of LC-MS/MS workflows into labs. High-throughput, reliable quantitation of multiple analytes has never been easier, and SCIEX software ensures that researchers will always be able to find the answers they need.

MultiQuant Software is a powerful tool for processing data acquired with the Triple Quad 3500 System. Regardless of user expertise, it allows accurate analyte quantitation in large batches of data within minutes. The software is designed to reduce data processing bottlenecks by being as intuitive as possible, with minimal mouse clicks required to set up a new method and access saved data. When a sample is selected, only a single click is required to view quantitation results of all or specific analytes. Several tools are also provided to help assess peak shape and MRM transitions in order to optimize performance. Time-consuming manual tasks can be reduced through utilization of the powerful and robust integration algorithms built into the software, such as MQ4 and advanced SignalFinder™ algorithm. These are able to generate reliable integration results faster with less user intervention than ever before, helping researchers maximize productivity and minimize human error. Like other tools from SCIEX, MultiQuant Software supports companies with regulatory compliance, through electronic audit trails and a seamless link to the most widely used LIMS system.

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Triple Quad 3500 System Compendium: Application Note Summary

Simultaneous Analysis of Chloramphenicol and Tetracycline Antibiotics in Food Samples Using the SCIEX Triple Quad 3500 System

The use of antibiotics in agriculture is an issue of growing public concern. Not only can it contribute to the prevalence of antibiotic resistance, it can also lead to severe health effects in allergic individuals. It is therefore important that food products are routinely monitored for antibiotic residues, in order to protect consumers from mislabeling and prevent adverse health issues. Maximum residue limits (MRLs) have been set by many regulatory agencies around the world, and food testing labs require robust techniques to ensure they can keep pace with regulatory demands.

Here, SCIEX outlines a method for the simultaneous detection of four common antibiotics, chloramphenicol and three tetracyclines, in milk, meat and honey samples. The method utilizes the speed and accuracy of the SCIEX Triple Quad 3500 System in multiple reaction monitoring (MRM) mode, providing high resolution and excellent peak shape. Prior to LC-MS/MS analysis, milk and meat samples underwent generic solid phase extraction procedures. For honey, samples could simply be diluted before direct injection onto the system. The detection limits for the assay were all well below regulatory limits, and displayed linearity across four orders of magnitude.

Simultaneous Analysis of 26 Mycotoxins in Grain on a SCIEX Triple Quad 3500 System

Mycotoxins are group of compounds produced by fungi that can cause considerable health issues and death if consumed through contaminated food and agricultural commodities. As a matter of public health, it is important to monitor the global food supply chain for their presence, and many countries have implemented strict regulations controlling mycotoxin concentrations. To ensure the highest accuracy and reliability, LC-MS/MS is rapidly becoming the method of choice for such analyses. The technology has the ability to analyze a wide range of compounds in a single analysis, and Multiple Reaction Monitoring (MRM) delivers high sensitivity and selectivity.

Previous LC-MS/MS methods have relied on different sample preparation techniques for each class of mycotoxin, introducing time-consuming and laborious steps. SCIEX researchers have therefore developed a simplified extraction procedure and an improved analysis method using the SCIEX Triple Quad 3500 System. The assay radically cuts the time needed for mycotoxin analysis, enabling 26 mycotoxins to be detected simultaneously in complex grain samples. The lower limits of quantitation (LLOQ) of all mycotoxins in the sample were found to be between 0.5 µg/kg and 20 µg/kg, well within the requirements of grain industry regulations.

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Analysis of Pesticides in Food Samples Using the SCIEX Triple Quad 3500 System

Pesticides are extensively used in agriculture to protect critical food sources and improve production efficiency. Feeding the world's rapidly growing population relies on the use of these chemicals, yet residual pesticide in consumer food products may present a significant threat to human health. It is imperative that food testing labs have access to techniques that can rapidly and accurately screen food samples for the hundreds of different pesticide residues that may contaminate the supply chain.

SCIEX has developed a robust and reliable method for the SCIEX Triple Quad 3500 System that uses simple, generic extraction procedures and multiple reaction monitoring (MRM) to screen food samples for catalogue of hundreds of pesticides in a single injection. Advanced software – the *Scheduled* MRM™ Pro Algorithm – was used to automatically optimize data quality using information on retention times to alter MRM dwell times. The method was validated using store-bought fruit and vegetables, demonstrating detection limits for all pesticides of 2 ng/mL or lower with good linearity across 4 orders of magnitude. LC-MS/MS on the SCIEX Triple Quad 3500 System delivers the sensitivity, selectivity, and speed, to meet the demands of routine testing of food samples and protect public health.

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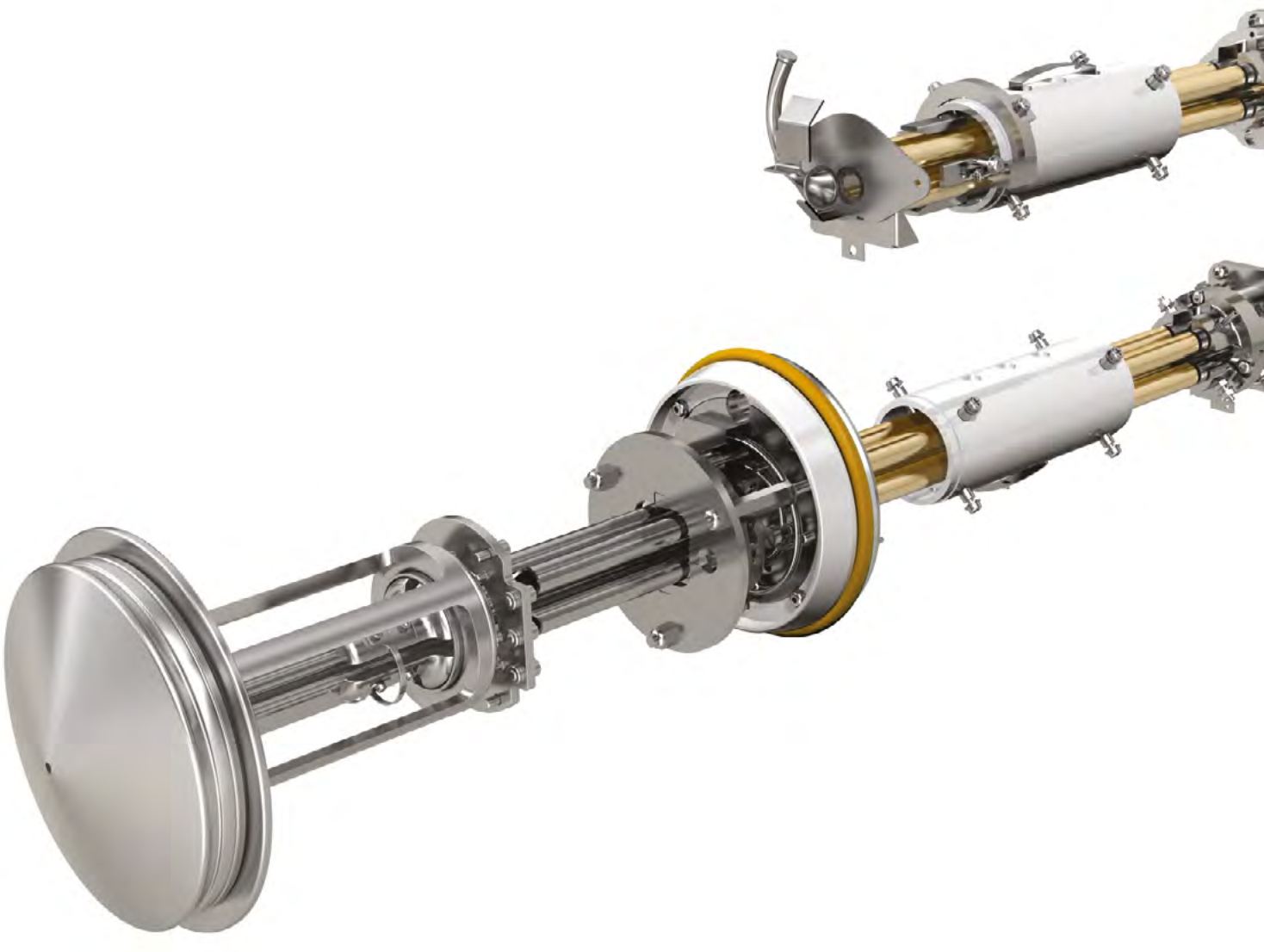
Application Notes



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Simultaneous Analysis of Chloramphenicol and Tetracycline Antibiotics in Food Samples Using the SCIEX Triple Quad 3500 System

André Schreiber
SCIEX Concord, Ontario (Canada)

Overview

Utilizing liquid chromatography with tandem mass spectrometry (LC-MS/MS) to analyze for antibiotic residues in a food samples offers many benefits to routine food testing labs, including the ability to screen for many compounds at once, the selectivity to meet regulatory guidelines, and the sensitivity to reduce sample preparation time to get to results faster. The SCIEX Triple Quad 3500 System enables labs performing antibiotic testing in foods to upgrade to LC-MS/MS and capitalize on its many benefits, at an affordable price.

Here we present a method using QuEChERS extraction (for the analysis of milk, meat and shrimp samples) with Phenomenex roQ kits and dilute-and-shoot (for honey samples), separation using a Kinetex Biphenyl 2.6u (50 x 2.1mm) column, and the SCIEX Triple Quad 3500 System for the detection of Chloramphenicol and Tetracyclines. The mass spectrometer was operated in highly selective and sensitive Multiple Reaction Monitoring (MRM) mode. Limits of detection (LOD) met regulatory limits. Compound identification and quantitation was achieved by monitoring two or three MRM transitions for each analyte. The MRM ratio was automatically evaluated in the MultiQuant Software.

Introduction

Antibiotics are widely used as growth promoting agents and therapeutics against microbial infections. The presence of antibiotics in food of animal origin is of concern due to the potential of increasing bacterial resistance and to hypersensitivity for some individuals. Tolerance limits and maximum residue limits (MRL) have been established around the world and agencies monitor the food supply to ensure that antibiotic residue concentrations do not exceed these levels.

LC-MS/MS based methods for single-residue and single-class residues are used to monitor veterinary drugs in food. Recently multi-class multi-residue methods have been introduced to further increase monitoring efficiency.[1-3]

Generic extraction procedures[4-5], ultra high performance LC systems combined with core-shell particles columns, providing good resolution and excellent peak shape, made it possible to detect a variety of antibiotics in a single method. The LC-MS/MS system is typically used in MRM mode because of its excellent sensitivity, selectivity, and speed.

The SCIEX Triple Quad 3500 System takes the best features of the API 3200™ System and enhances them with modern engineering and electronics. The proven design of Turbo V source and Curtain Gas interface provide exceptional robustness and ruggedness. The advanced eQ electronics and the curved LINAC collision cell were designed for ultra-fast speed of MRM detection and fast polarity switching for comprehensive multi-component analysis.

A triple quadrupole based method for the quantitation of Chloramphenicol and three selected tetracyclines was developed using selective Multiple Reaction Monitoring (MRM) with the *Scheduled* MRM Algorithm activated. The ratio of quantifier and qualifier transition was used for compound identification. Sensitivity of detection met existing regulatory requirements, such as Codex Alimentarius' Maximum Residue Limits (MRL) of 200 µg/kg (tissue) and 100 µg/L (milk) for tetracyclines, the MRL

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of 50 µg/kg set by Chinese government, and the Minimum Required Performance Limit (MRPL) for Chloramphenicol set by the European Union of 0.3 µg/kg.[6-8]

The method was successfully applied to the analysis of store-bought milk, meat, shrimp, and honey samples.

Experimental

- Store-bought food samples (milk, meat, shrimp) were extracted following the protocol of the European standard method 15662[5] using the Phenomenex roQ QuEChERS kit buffer-salt mix and the dSPE kit (#KS0-8913) containing 150 mg $MgSO_4$, 25 mg PSA, and 25 mg C18
- QuEChERS extracts were diluted 10 times with water to minimize possible matrix effects
- Honey samples were diluted with 5 times water and injected directly
- The injection volume was set to either 10 or 50 µL, depending on targeted LOQ
- LC separation was achieved using a Phenomenex Kinetex Biphenyl 2.6u (50 x 2.1mm) column and a fast gradient of water and acetonitrile with 0.1% formic acid at a flow rate of 0.5 mL/min (see Table 1 for the gradient profile)
- The SCIEX Triple Quad 3500 System was operated with Turbo V source and Electrospray Ionization (ESI) probe set to 500°C
- Two MRM transitions were monitored for Chloramphenicol and three transitions were monitored for each tetracycline (Table 2)
- The *Scheduled* MRM Algorithm was activated to achieve best data quality
- Fast polarity switching of 50 msec was used. The IS voltage was to -4000 V and +5000 V, respectively
- MultiQuant Software 3.0 was used for quantitative and qualitative data processing

Table 1. Gradient conditions used for the separation

Step	Time (min)	A (%)	B (%)
0	0.0	80	20
2	4.0	5	95
3	7.0	5	95
4	7.1	80	20
5	10.0	80	20

Table 2. MRM transitions and retention times (RT) used for the detection of Chloramphenicol and tetracyclines

Compound	Polarity	RT (min)	Q1 (amu)	Q3 (amu)
Chloramphenicol 1	negative	1.32	321	152
Chloramphenicol 2	negative	1.32	321	257
Chlortetracycline 1	positive	1.30	479	444
Chlortetracycline 2	positive	1.30	479	462
Chlortetracycline 3	positive	1.30	479	154
Oxytetracycline 1	positive	0.57	461	426
Oxytetracycline 2	positive	0.57	461	444
Oxytetracycline 3	positive	0.57	461	201
Tetracycline 1	positive	0.76	445	410
Tetracycline 2	positive	0.76	445	427
Tetracycline 3	positive	0.76	445	154

Results and Discussion

Sensitivity, Reproducibility, Linearity and Accuracy

The LC-MS/MS chromatogram of a 10 ng/mL solvent standard is shown in Figure 1 highlighting the excellent separation and peak shape achieved using the Phenomenex Kinetex Biphenyl with a fast gradient of water and acetonitrile containing 0.1% formic acid. Fast polarity switching was required to detect all compounds in a single method since Chloramphenicol (negative polarity) and Chlortetracycline (positive polarity) are not chromatographically separated by this method.

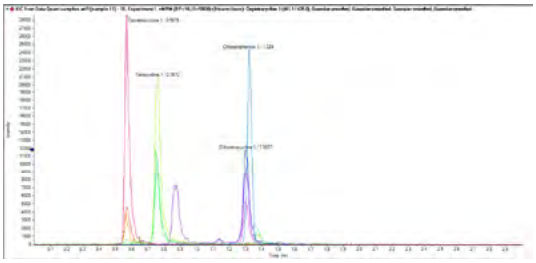

Figure 1. LC separation and detection in MRM mode of three tetracyclines and Chloramphenicol at 10 ng/mL

Figures 2 and 3 show the achieved sensitivity for all targeted antibiotics. Tetracyclines can be easily quantified at the target MRL using a small injection volume of 10 µL reducing the matrix

load for the mass spectrometer to increase robustness and to reduce potential ion suppression.

However, Chloramphenicol sometimes requires a larger injection volume to match the target MRPL while still allowing sufficient dilution to minimize potential matrix effects. In these cases, 50 µL injection volumes were utilized.

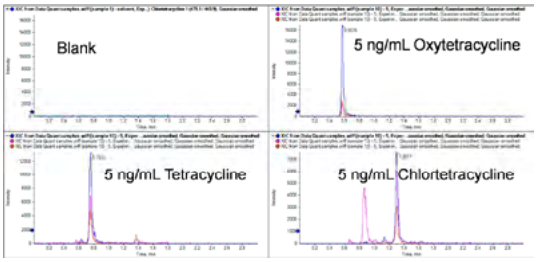

Figure 2. Sensitivity of a 5 ng/mL standard of tetracyclines (injection volume of 10 µL)

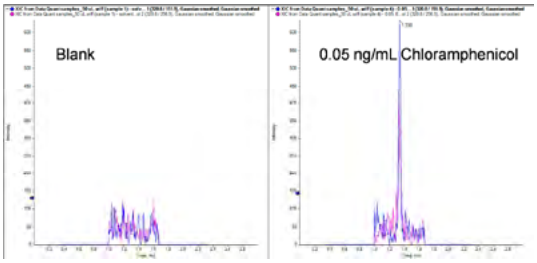

Figure 3. LOQ for Chloramphenicol of less than 0.05 ng/mL with an injection volume of 50 µL, allowing 10x dilution of matrix extracts

Calibration lines are shown in Figure 4, over the range of 0.05 to 100 ng/mL for Chloramphenicol and 0.1 to 100 ng/mL for tetracyclines, respectively, with a coefficient of regression > 0.997.

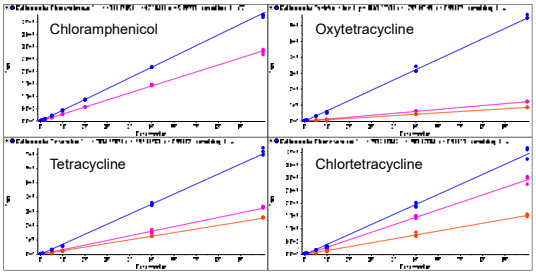

Figure 4. Calibration lines for all 4 compounds analyzed in this study

Accuracies for all calibration standards were between 80 and 120%, and repeatability was found to be better than 5% CV and 10% at the LOQ (n=3).

The achieved method performance allowed diluting sample extracts by a factor of 10 to reduce possible matrix effects. The additional use of isotope labeled internal standards is recommended to compensate matrix effects.

Findings in Food Samples

Figures 5 and 6 show matrix samples tested negative for Chloramphenicol and tetracyclines. The honey sample had a trace contamination with Chloramphenicol below the LOQ of 0.05 ng/mL (0.25 µg/kg in matrix after accounting for the 5x dilution during sample preparation).

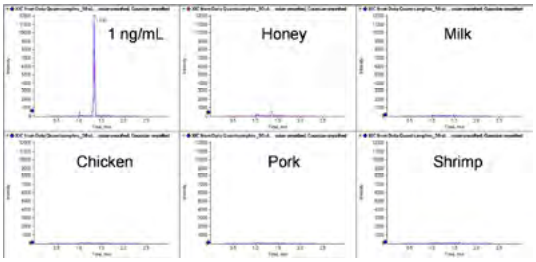

Figure 5. Blank matrices tested for Chloramphenicol (50 µL injection), the honey sample had a trace contamination with Chloramphenicol below the LOQ of 0.05 ng/mL (0.25 µg/kg in matrix after 5x dilution)

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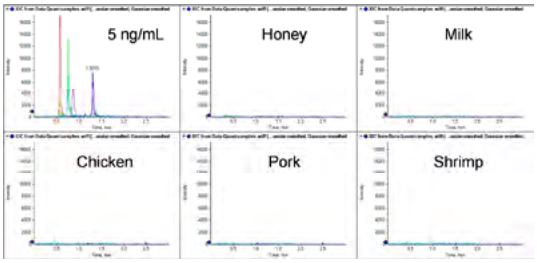

Figure 6. Blank matrices tested for tetracyclines (10 µL injection)

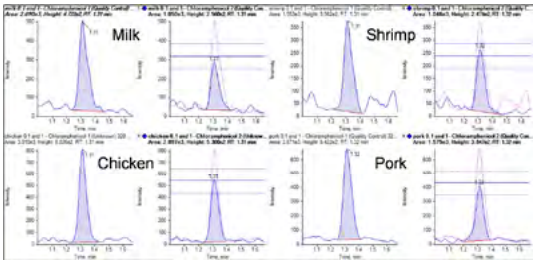

Figure 7. Different food extracts spiked with Chloramphenicol at 0.1 µg/kg (50 µL injection), the MRM ratio tolerances are displayed in the peak review window

Example chromatograms of different food samples spiked with antibiotics are presented in Figures 7 and 8. Compound identification was based on the criteria of directive 2002/657/EC[9] (retention time tolerance of ± 2.5% and maximum tolerances for ion ratios of ± 20 to 50% depending on the ratio). All quantitative and qualitative results were automatically calculated in MultiQuant Software (Figure 6).[10]

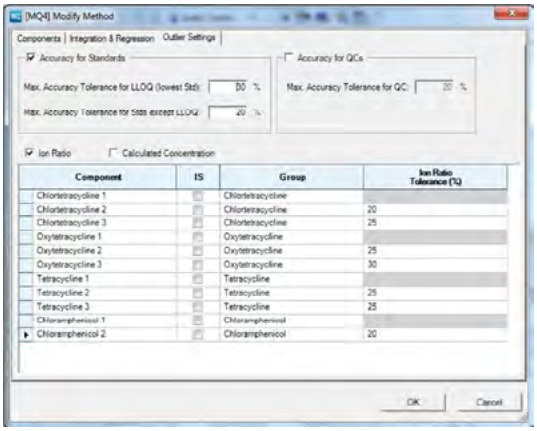

Figure 6. MRM ratio tolerances setup in the method editor of MultiQuant Software

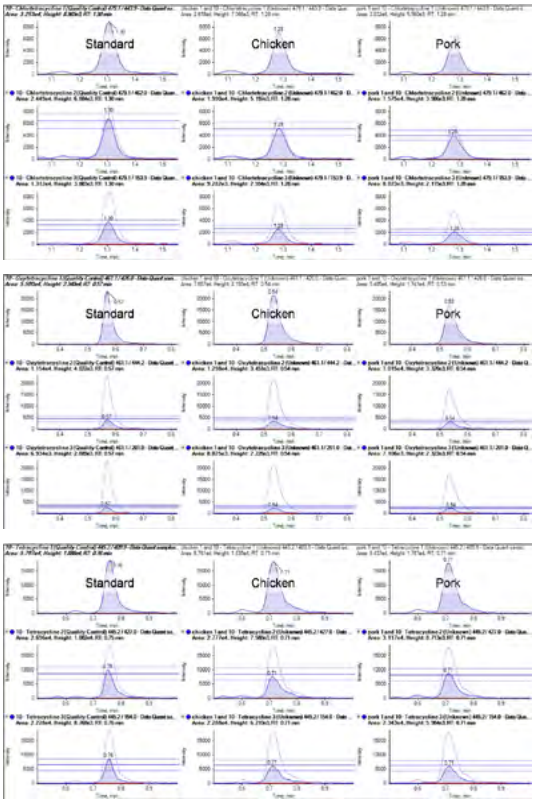

Figure 8. Side-by-side peak review of a standard injection (left) and spiked meat extracts (middle and right) with automatic calculation of MRM ratios, the MRM ratio tolerances are displayed in the peak review window

Summary

A new LC-MS/MS method for the identification and quantitation of antibiotics was developed and successfully applied to different food samples, including honey, milk, shrimp and meat.

The method consists of QuEChERS extraction followed by dilution to minimize possible ion suppression and a dilute and shoot approach for honey. The SCIEX Triple Quad 3500 System operated in MRM mode and utilizing the *Scheduled* MRM Algorithm was used for detection. Limits of detection (LOD) met regulatory requirements. Two to three MRM transitions were monitored for each analyte and the ratio of quantifier and qualifier transition was used for identification. Data processing was performed in MultiQuant Software. Identification criteria of directive 2002/657/EC were used for identification.

Acknowledgement

The author thanks Cheryl Stephenson (Eurofins Central Analytical Laboratories US) New Orleans, LA for providing standards.

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8 2003/181/EC: 'setting of minimum required performance limits (MRPLs) for certain residues in food of animal origin' (2003)

9 2002/657/EC: 'concerning the performance of analytical methods and the interpretation of results' (2002)

10 A. Schreiber: 'MultiQuant Software 3.0 - Improving Data Quality and Processing Throughput with Better Peak Integration, Quantitative and Qualitative Compound Review for the Analysis of Food, Drinking Water, and Environmental Samples' Application Note SCIEX (2013) #8160213-01

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Analysis of Pesticides in Food Samples Using the SCIEX Triple Quad 3500 System

André Schreiber
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Overview

Pesticides are widely used in agriculture to protect crops and to improve efficiency of production. Pesticide residues may pose a potential threat to human health. Modern analytical techniques, such as LC-MS/MS allow the screening for hundreds pesticide residues in food samples quickly, efficiently, and with excellent sensitivity and selectivity to meet global food trade guidelines and regulations.[1-3]

Mass spectrometers are typically considered to be expensive and complex instruments. However, the SCIEX Triple Quad 3500 System, combined with an extensive compound MRM catalog, provides labs with robust and reliable mass spec technology and method starting points, at an affordable price.

Here we present a method using QuEChERS extraction with Phenomenex roQ kits, filtration with Thomson filter vials, separation using a Kinetex Biphenyl 2.6u (50 x 2.1mm) column, and the SCIEX Triple Quad 3500 System. The mass spectrometer was operated in highly selective and sensitive Multiple Reaction Monitoring (MRM) mode. The *Scheduled* MRM Pro Algorithm was used to obtain the best data quality. Compound identification and quantitation was achieved by monitoring two MRM transitions for each pesticide. The MRM ratio was automatically evaluated in MultiQuant Software.

Introduction

LC-MS/MS is a powerful analytical tool capable of screening samples for numerous compounds. MRM is typically used because of its excellent sensitivity, selectivity, and speed.

Generic extraction procedures, like QuEChERS, ultra high performance LC systems combined with core-shell particle columns, providing good resolution and excellent peak shape, made it possible to detect pesticides of a wide variety of compound classes and chemical properties in each sample. State-of-the-art LC-MS/MS systems make it possible to detect hundreds of pesticides and other food residues in a single run.

The SCIEX Triple Quad 3500 System takes the best features of the API 3200 System and enhances them with

modern engineering and electronics. The proven design of Turbo V source and Curtain Gas interface provide exceptional robustness and ruggedness. The advanced eQ electronics and the curved LINAC collision cell were designed for ultra-fast speed of MRM detection and fast polarity switching for comprehensive multi-component analysis.

Advanced software tools like the *Scheduled* MRM Pro Algorithm intelligently uses information of retention times to automatically optimize MRM dwell time of each transition and total cycle time of the experiment resulting in best data quality. Two MRM transitions were monitored for each pesticide to use the ratio of quantifier and qualifier ion for compound identification.

Experimental

- The SCIEX iDQ*uant*™ standards kit for pesticide analysis was used for method setup and preparation of calibration standards[4]
- Store-bought fruit and vegetable samples were extracted using Phenomenex roQ QuEChERS kit buffer-salt mix and dSPE kits following the European standard method 15662[5]
- Extracts were diluted 5 times with water in Thomson filter vials, filtered using the 0.45 µm PVDF membrane and directly

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placed into the autosampler for LC-MS/MS analysis. The injection volume was set to 2 µL

- LC separation was achieved using a Phenomenex Kinetex Biphenyl 2.6u (50 x 2.1mm) column and a fast gradient of water and methanol with 5 mM ammonium formate buffer at a flow rate of 0.5 mL/min (see Table 1 for the gradient profile)

Table 1. Gradient conditions used for the separation of pesticides

Step	Time (min)	A (%)	B (%)
0	0.0	90	10
1	0.5	90	10
2	2.0	70	30
3	9.0	40	60
4	11.0	20	80
5	12.0	5	95
6	15.0	5	95
7	16.0	90	10
8	20.0	90	10

- The SCIEX Triple Quad 3500 System was operated with Turbo V source and Electrospray Ionization (ESI) probe set to 400°C
- Approximately 400 MRM transitions were monitored in positive polarity. Optimized transitions for all compounds were obtained through the MRM catalogue of the iMethod™ application for Pesticide Screening version 2.1
- The *Scheduled* MRM Pro Algorithm was used with a target cycle time of 0.5 sec and compound dependent detection windows and thresholds (Figure 1)

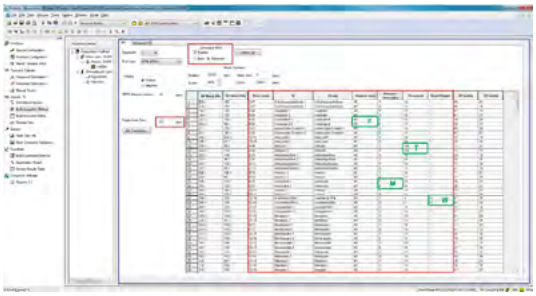

Figure 1. *Scheduled* MRM Pro Algorithm allowing: Flexible Window Width (F), Dynamic Window Extension (T), MRM-triggered MRM (M, T), Dwell Time Weighting (W)

- MultiQuant Software 3.0 was used for quantitative and qualitative data processing

Results and Discussion

Sensitivity, Reproducibility, Linearity and Accuracy

Chromatograms of a solvent standard at 10 ng/mL analyzed using the API 3200 System and SCIEX Triple Quad 3500 System are shown in Figure 2. An average gain in sensitivity of 3x was observed.

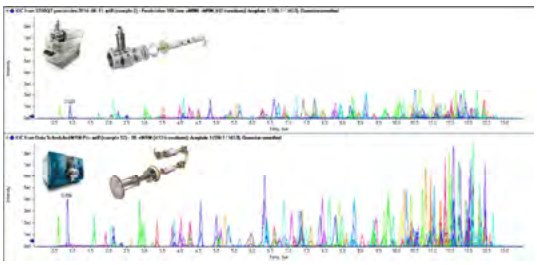

Figure 2. Sensitivity comparison of a 10 ng/mL standard analyzed using the API 3200 System (top) and SCIEX Triple Quad 3500 System (bottom) with an average sensitivity gain of 3x

Most pesticides were detectable at a concentration below 1ng/mL and all pesticides had a limit of detection (LOD) of 2 ng/mL or lower. Example chromatograms at a concentration of 5 ng/mL are shown in Figure 3. The achieved sensitivity allows sample extract dilution by 5x to minimize possible matrix effects.

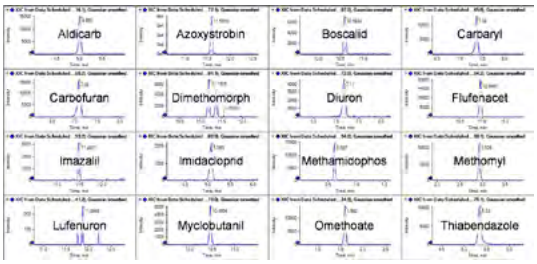

Figure 3. Sensitivity of selected pesticides detected at a concentration of 5 ng/mL using the Triple Quad 3500 System

Linearity was obtained over 3 to 4 orders of magnitude for most pesticides with accuracies between 80 and 120%. Data points of

the lowest or highest standards were excluded for a few pesticides with weak or strong ionization, respectively. Repeatability was studied at 1 and 10 ng/mL (n=5). The coefficient of variation (%CV) was typically below 10%.

An example calibration line of Acephate is shown in Figure 4. Both MRM transitions had a regression coefficient of > 0.998 and excellent repeatability of 2.9 and 3.2% at 1 and 10 ng/mL respectively (n=5).

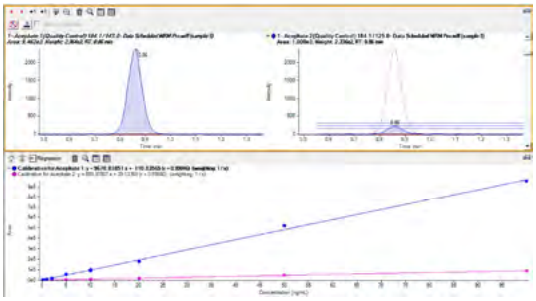

Figure 4. Peak review quantifier-qualifier ratio of Acephate at 1 ng/mL and calibration line from 0.1 to 100 ng/mL with %CV of 2.9% and 3.2% at 1 and 10 ng/mL, respectively

Findings in Fruit and Vegetable Samples

The developed method was applied to the quantitation and identification of pesticides in real food extracts. Different dispersive SPE kits of Phenomenex (roQ KS0-8913, 8914, 8915, 8916) were used for sample cleanup depending on the type of matrix following the European standard method 15662. Extracts were diluted 5 times with water to minimize possible matrix effects. The diluted extracts were filtered using the Thompson 0.45 µm PVDF membrane and directly placed into the autosampler for LC-MS/MS analysis.

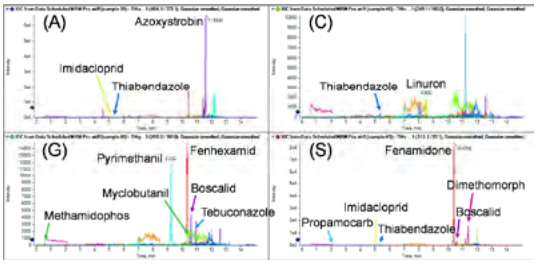

Figure 5. Detection of pesticides in filtered QuEChERS extracts of avocado (A), carrot (C), grapes (G), and spinach (S)

Example chromatograms of different type of food samples with detected compounds are presented in Figure 5. Qualitative and quantitative results are summarized in Table 2. Compound identification was based on the criteria of SANCO/12571/2013 (retention time tolerance of ± 0.02 min and maximum tolerances for ion ratios ± 30%). All quantitative and qualitative results were automatically calculated in MultiQuant Software (Figure 6).[6]

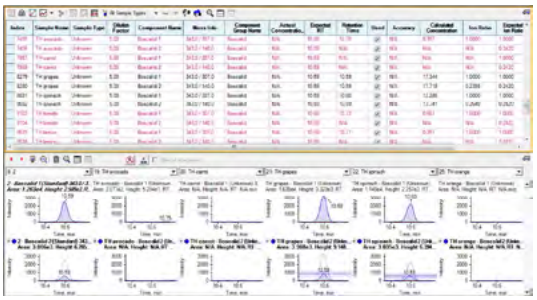

Figure 6. Quantitation and identification based on MRM ratios in MultiQuant Software, the example shows the side-by-side peak review for Boscalid with positive findings in grapes and spinach samples

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Table 2. Summary of pesticide findings in store bought food above a concentration of 1 µg/kg

Sample	Pesticide	Concentration (µg/kg)	RT Error (min)	MRM Ratio (Expected)
Avocado	Azoxystrobin	55.0	0.01	0.146 (0.126)
	Imidacloprid	6.2	0.03	0.823 (0.818)
	Thiabendazole	2.9	0.06	1.035 (0.820)
Carrot	Linuron	14.3	0.00	0.613 (0.742)
	Thiabendazole	5.3	0.04	0.995 (0.820)
Grapes	Boscalid	17.3	0.00	0.240 (0.242)
	Fenhexamid	363	0.04	0.973 (1.053)
	Methamidophos	1.2	0.01	0.873 (0.698)
	Myclobutanil	14.2	0.02	0.811 (0.830)
	Pyrimethanil	687	0.05	0.482 (0.435)
	Tebuconazole	7.1	0.03	0.030 (0.261)
Grapefruit	Imazalil	899	0.07	0.410 (0.348)
	Imidacloprid	1.3	0.03	1.052 (0.993)
	Thiabendazole	7.6	0.03	0.812 (0.820)
Lemon	Imazalil	981	0.06	0.266 (0.348)
	Thiabendazole	7.6	0.04	0.782 (0.820)
Orange	Imazalil	1830	0.06	0.282 (0.348)
	Thiabendazole	>3000	0.04	0.812 (0.820)
Spinach	Boscalid	12.3	0.00	0.264 (0.242)
	Dimethomorph	53.7	0.08	0.537 (0.541)
	Fenamidone	755	0.01	0.749 (0.672)
	Imidacloprid	217	0.03	0.907 (0.993)
	Propamocarb	3.1	0.06	0.260 (0.336)
	Thiabendazole	3.6	0.05	0.917 (0.820)

Improving data acquisition quality with *Scheduled* MRM Pro Algorithm

Figures 7 and 8 show results of pesticides detected in food samples to explain different features of *Scheduled* MRM Pro Algorithm.

The detection window can be set differently for each compound depending on LC peak width and potential retention time shifts. This allows a more effective scheduling of MRM transitions resulting in better data quality. The example in Figure 7 shows Boscalid detected with a window of 45 sec, while the window of Dimethomorph was set to 120 sec to detect both isomers together.

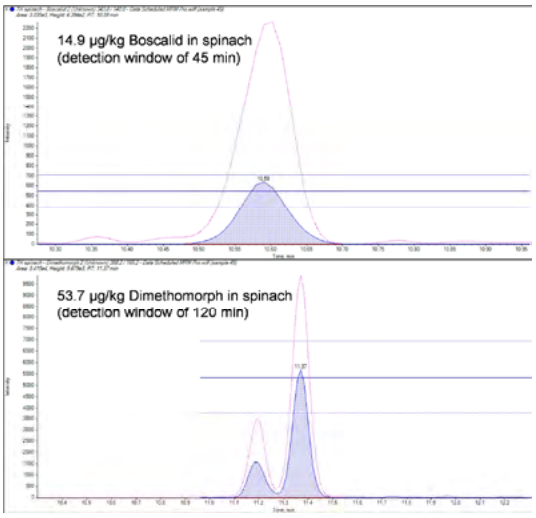

Figure 7. Examples of using the Flexible Window Width in a *Scheduled* MRM Pro Algorithm: the window for Boscalid was set to 45 sec and Dimethomorph was detected using a wider window to detect both isomers together

The *Scheduled* MRM Pro Algorithm also allows automatic triggering of qualifier MRM transitions when a quantifier transitions is present (Figure 8). This feature further optimizes the MRM scheduling. The threshold is also used to automatically extend the detection window if an MRM signal is still present at the end of the default detection window.

Figure 8 shows an example of dynamic window extension for the detection of Thiabendazole in an orange sample. The sample contained Thiabendazole at more than 3000 µg/kg resulting in peak tailing. The automatic extension of the detection window enabled to capture the complete peak area for accurate quantitation and identification based on the MRM ratio.

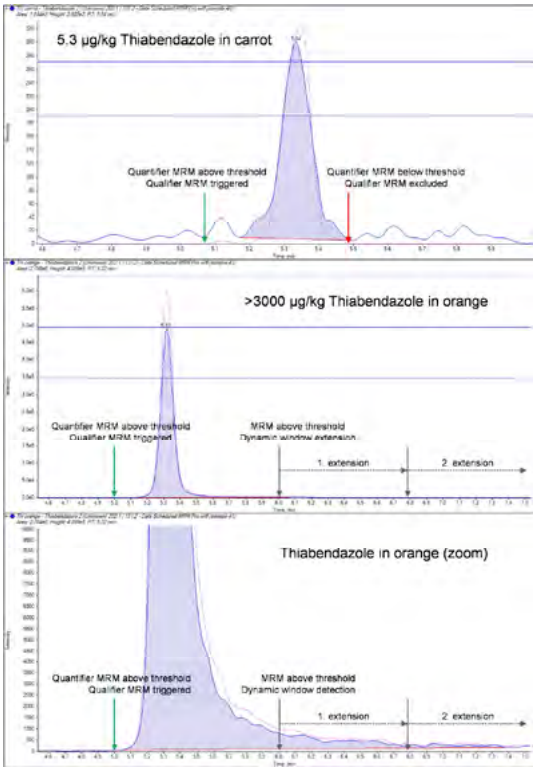

Figure 8. Examples of MRM-triggered MRM and Dynamic Window Extension: the qualifier MRM transition is automatically triggered when the quantifier MRM transitions exceeds the threshold set in the *Scheduled* MRM Pro Algorithm, the detection window is automatically extended if the MRM signal is above the threshold at the end of the detection window

Summary

A new LC-MS/MS method for the identification and quantitation of pesticides was developed and successfully applied to fruit and vegetable samples.

Samples were extracted using a QuEChERS protocol following the European standard method 15662 with Phenomenex roQ kits. Sample extracts were diluted 5x to minimize potential matrix effects and filtered using Thomson filter vials. The SCIEX Triple Quad 3500 System operated in MRM mode and utilizing the *Scheduled* MRM Pro Algorithm was used for detection. Two MRM transitions were monitored for each analyte and the ratio of quantifier and qualifier transition was used for identification.

Qualitative and quantitative data processing was performed in MultiQuant Software. Criteria of SANCO/12571/2013 were used for identification. All pesticides had an LOD of 2 ng/mL or lower and good linearity of 3-4 orders of magnitude with repeatability well below 10%.

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Simultaneous Analysis of 26 Mycotoxins in Grain on a SCIEX Triple Quad 3500 System

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Mycotoxins are secondary metabolites produced by a wide range of fungi known to contaminate a variety of food and agricultural commodities worldwide and have been recognized as a potential health threat to humans and animals. Many countries have regulations in place for mycotoxin detection and identification and their permissible limits. In China, the limits of mycotoxins in certain products are regulated by GB 2761 and in EU, mycotoxin limits are harmonized in the regulation for contaminants in foodstuffs EC 1881/2006 and the amended regulation EC 1126/2007. Regulations on food and environmental analysis require the analysis of contaminants using confirmatory techniques. Thus, there is a demand for powerful and rapid analytical methods that can detect very low concentrations of mycotoxins in a variety of sample matrices. In recent years, LC-MS/MS has gained popularity, becoming the method of choice, leveraging its ability to analyze a wider range of compounds in a single analysis coupled together with the high selectivity and sensitivity of Multiple Reaction Monitoring (MRM).

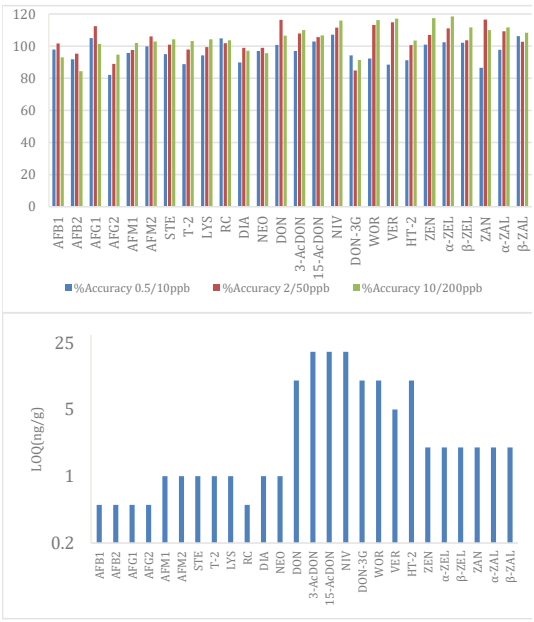

Figure 1. Accuracy and LOQ Values Shown for the Panel of Mycotoxins. Limits of Quantitation (LOQ) of all mycotoxins were found between 0.5 ng/g and 20ng/g. Accuracy assessed over three concentrations ranged from 80% to 120%. These measurements of performance demonstrate excellent sensitivity and accuracy for this assay

Traditionally, different classes of mycotoxins required different sample preparation techniques, making the process laborious and time consuming. Presented here is a single workflow to analyze 26 compounds simultaneously. This workflow consists of a simplified extraction procedure that does away with additional clean-up steps by immunoaffinity columns and couples it to high resolution LC separation and high sensitivity MS detection.

Key Assay Attributes

- A fully integrated LC-MS/MS solution is presented to analyze 26 common mycotoxin residues simultaneously in relevant grain samples. Polarity switching ensures best coverage of relevant analytes
- Simplified extraction procedure is described which does away with additional clean-up steps, saving time and labor at the front end of analysis
- The method was validated for performance including sensitivity and robustness in different grain matrices
- Limits of Quantitation (LOQ) of all mycotoxins were found between 0.5µg/kg and 20µg/kg. All LOQ meet the requirements of the grain Industry standard

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Experimental

Sample Preparation: Sample preparation was carried out in accordance to the vMethod SOP (P/N 5060674). Grain samples (corn, rice, wheat etc.) were first homogenized and 2.5g of sample was extracted using a mixture of acetonitrile and water. Once sonicated and centrifuged, the supernatant was passed through a Cleanert MC SPE Cartridge (Agela Technologies, P/N ZS-MYT10-B) which contains a sorbent chemistry specially optimized for mycotoxins. The filtrate was then dried down and reconstituted for LC-MS analysis.

LC Conditions: Liquid chromatography analysis was performed using a SCIEX ExionLC™ AD UHPLC system. 20µL was injected onto a Phenomenex Kinetex C_{18} column (100mm X 2.1 mm, 1.7µm, P/N 00D-4475-AN). Mobile phase A contained water with 0.1% formic acid and mobile phase B contained methanol with 0.1%.

Table 1. LC Gradient Time Program. Flow rate at all steps was 0.3 mL/min, and the total run time was 13 minutes including re-equilibration

Time (min)	%B
1.0	*3*
2.0	*10*
4.0	*50*
9.0	*80*
9.1	*99*
11.0	*99*
11.1	*3*
13.0	*3*

MS/MS Conditions: Electrospray ionization was carried out on SCIEX Triple Quad 3500 System with fast polarity switching. The Turbo V source was kept at a temperature of 550°C and the *Scheduled* MRM Algorithm was used to analyze grain samples for 26 mycotoxins in a single injection by multiplexing the detection of multiple MRM transitions for signature fragments

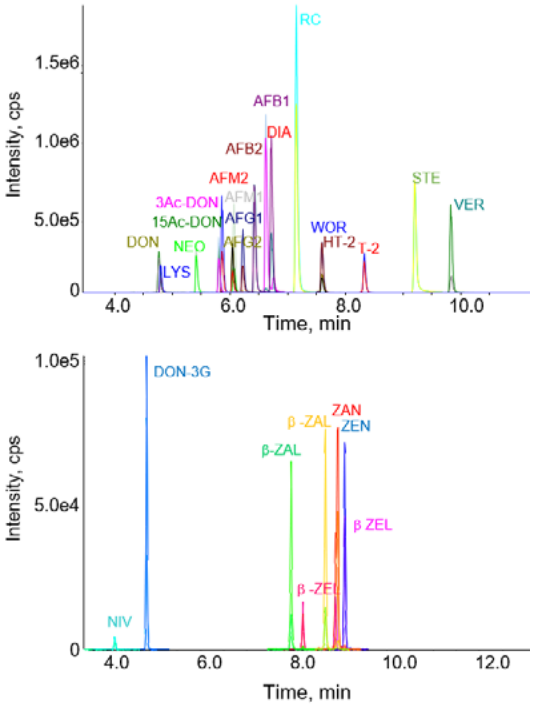

Figure 2. Chromatographic Profile for 26 Mycotoxins. Both positive and negative modes were analyzed simultaneously during a single sample injection, allowing all 26 mycotoxins to be analyzed in one data acquisition method. (Top) 18 mycotoxins were collected in ESI positive mode (top) and 8 mycotoxins were collected in ESI negative mode (bottom)

Results and Discussions

For each analyte, two signature MRM transitions were chosen to ensure confidence in the identification of each mycotoxin (Table 2). To monitor many MRM transitions during a single injection, the *Scheduled* MRM Algorithm was employed, where individual MRM transitions were monitored for a short time window during their expected retention time. Thus, at any one point in time, the number of concurrent MRM transitions were significantly reduced resulting in much higher duty cycles for each analyte. Combining with fast polarity switching further allowed extending the target list of mycotoxins, thus maintaining sample throughput by eliminating need for multiple injections. Typical chromatograms of solvent standard were shown in Figure 2. The total target cycle time of 0.6 sec ensured the collection of at least 12 data points across the LC peak resulting in excellent accuracy and reproducibility. The system suitability was tested with the

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concentration of 5/50 ng/mL standards and the standard solution was injected three times. The %CV of each analyte peak was calculated to less than 15%.

For sample preparation, a simplified sample clean-up method was developed. Instead of immunoaffinity columns, a special solid phase extraction (SPE) column (Cleanert MC, Agela) with optimized sorbent chemistry for mycotoxin extraction was used. This column proved advantageous in that it doesn't need to be activated, washed, and eluted. It not only shortened the sample preparation time, but also saved cost. Figure 3 shows the comparison of the sample clean-up step before and after.

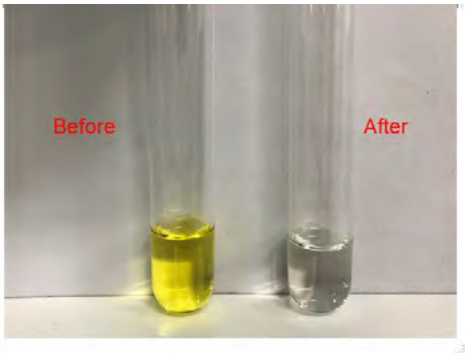

Figure 3. Sample Preparation and Clean Up. Visual comparison of a grain sample before and after the Cleanert SPE column clean-up step. Cleaning up the sample can provide reduction of matrix interferences as well as help in maintaining instrument performance

The limit of quantitation and matrix matched linearity were evaluated. Because of the matrix inhibitory effects, the matrix matched curves were used to quantify the unknown samples. For AflatoxinB1 (AFB1) and Deoxynivalenol (DON) as example, the method was found to have good reproducibility and the linear regression coefficient was found to be greater than 0.99 (Figure 4). According to the different sensitivity levels of each compound on the instrument, the LOQ of all targeted mycotoxins were from 0.5 ng/g to 20 ng/g. The accuracy of low, medium and high concentration spiked sample was between 80% and 120% (Figure 1).

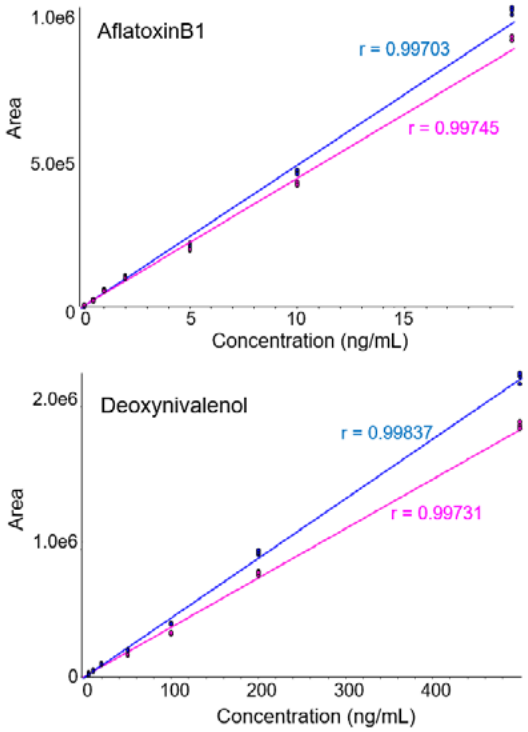

Figure 4. Calibration Curves for AflatoxinB1 and Deoxynivalenol. Calibration curves were generated from 5 to 500 ng/mL. Two MRM transitions were monitored: fragment 1 (blue) and fragment 2 (pink). R-values shown for both transitions for both representative analytes are >0.99, demonstrating excellent linear range and response for the assay

Conclusions

A fast, robust, and reliable method for the detection 26 mycotoxins in the matrix grain was developed and validated. A fast purification method was used to cover the 26 kinds of mycotoxins. High resolution LC using a small particle size column was combined with high sensitivity detection using a SCIEX Triple Quad 3500 System. Multiple Reaction Monitoring (MRM) was used because of its high selectivity and sensitivity. The *Scheduled* MRM Algorithm used to obtain optimized dwell times and cycle times for best sensitivity and reproducibility. The method was validated in different grain matrices. Limits of Quantitation (LOQ) of all mycotoxins were found between 0.5µg/kg and 20µg/kg. All LOQ meet the requirements of the grain Industry standard.

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Table 2. MRM Transitions and Retention Times are Provided for Two Transitions for each Mycotoxin in the 26 Analyte Panel

Compounds name	RT (min)	MRM (Primary, Quantifier)	MRM (Secondary, Qualifier)
AflatoxinB1 (AFB1)	*6.62*	*313.1>285.1*	*313.1>241.1*
AflatoxinB2 (AFB2)	*6.43*	*315.1>287.1*	*315.1>259.1*
AflatoxinG1 (AFG1)	*6.22*	*329.1>243.2*	*329.1>214.9*
AflatoxinG2 (AFG2)	*6.05*	*331.1>245.1*	*331.1>189.1*
AflatoxinM1 (AFM1)	*6.07*	*329.0>273.1*	*329.0>268.9*
AflatoxinM2 (AFM2)	*5.86*	*331.1>273.1*	*331.1>285.1*
T-2 toxin (T-2)	*8.32*	*484.2>305.3*	*484.2>185.1*
Verruculogen (VER)	*9.84*	*534.3>392.3*	*534.3>191.1*
Neosolaniol (NEO)	*5.41*	*400.2>185.1*	*400.2>305.2*
Wortmannin (WOR)	*7.59*	*447.2>345.2*	*447.2>285.2*
Roquefortine C (RC)	*7.13*	*390.3>193.1*	*390.3>322.2*
Sterigmatocysin (STE)	*9.19*	*325.1>310.1*	*325.1>281.0*
Lysergol (LYS)	*4.80*	*255.3>240.2*	*255.3>197.2*
Diacetoxyscirpenol (DIA)	*6.70*	*384.2>307.2*	*384.2>105.1*
HT-2 Toxin (HT-2)	*7.59*	*442.1>263.1*	*442.1>215.0*
Deoxynivalenol (DON)	*4.76*	*296.9>249.1*	*296.9>231.1*
3-Acetyl Deoxynivalenol (3-AcDON)	*5.80*	*339.0>231.0*	*339.0>203.0*
15-Acetyl Deoxynivalenol (15-AcDON)	*5.80*	*339.1>321.3*	*339.1>137.2*
Deoxynivalenol-3-Glucoside (DON-3G)	*4.83*	*503.1>427.1*	*503.1>457.1*

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LC-MS/MS enables you to combine laborious workflows associated with HPLC and put them into one suite without compromising data quality or expensive staffing. By employing LC-MS/MS you can grow your lab, offer more services and stay ahead of your competition.

4 Get more data even in tough matrix

See what your HPLC assay can't

With LC-MS/MS the matrix doesn't get in the way of the data. Our mass spectrometers are engineered to handle the most complex food matrices, you get highly accurate results, injection after injection with maximum uptime. See more, test more and earn more.

SCIEX Mass Spectrometry
Better accuracy. Superior confidence. Unrivalled speed.

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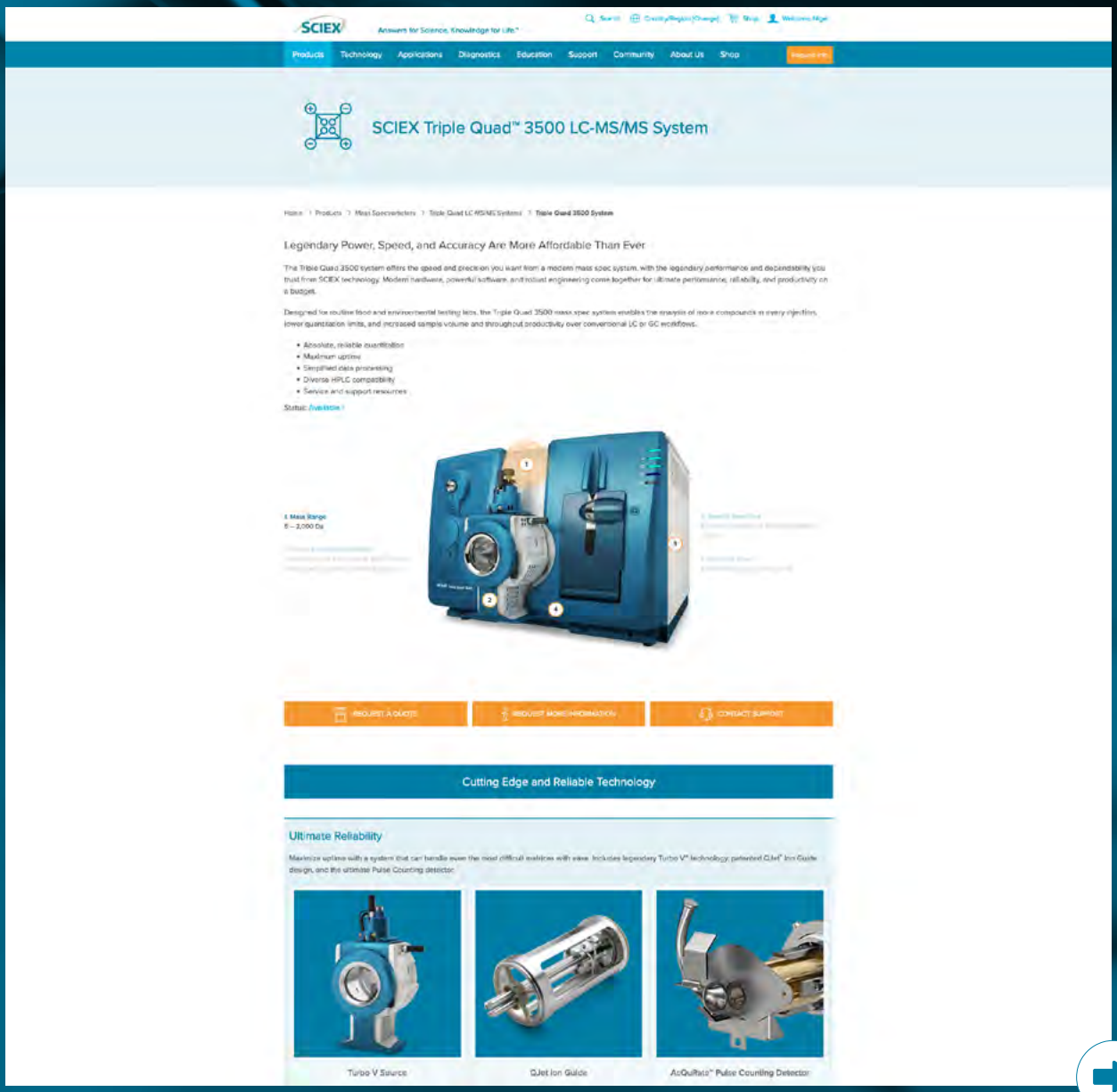
References & Links

SCIEX Triple Quad 3500 System Compendium Volume 1

Visit the website for more information



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