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SMART NOTE

Transitioning to confident quantitation—in search of a better tomorrow

What is quantitation and why do we need it?

For one to identify and understand any unknown substance, the first step is always characterization. Hence, from identifying the nature of pesticides used to keep insects and pests away from crops to the chemicals that result in a life-saving drug; from drugs found in an athlete's urine to chemicals that can potentially turn our drinking water into a toxic waste—identification is always the first step. However, identification of the nature and type of a chemical in a fruit or a medicine, urine of an athlete or drinking water is only half the work. For many labs, the next question is "How much?" The ability to provide the total amount of chemicals and beyond requires the development and validation of quantitation assays agreed upon by a group of scientists and regulatory governing organizations. Quantitation allows a food to be labeled as "inedible", a drug as "unusable", an athlete as "someone who tested positive" or water as "unsuitable for human use".

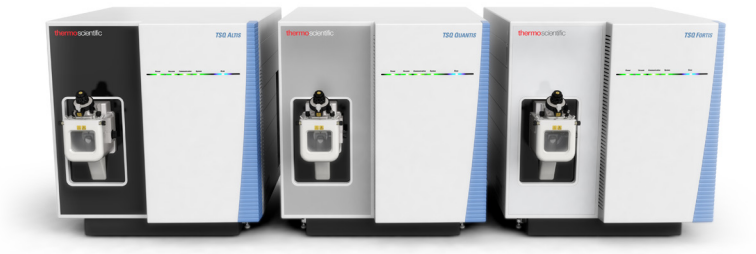


Figure 1. Thermo Scientific™ TSQ™ triple-stage quadrupole mass spectrometers.

ThermoFisher SCIENTIFIC

Both qualitative and quantitative analyses are critical to the analytical process that ensures the quality of a product—whether it is food or something that we use every day. Focusing on the quantitative analytical processes—there are challenges faced by every analytical scientist in the world of quantitation. Some of these challenges include:

1. **Certainty of your target:** It is critical to confirm every analyte that needs to be quantified. In certain situations, a by-product or a metabolite from a target analyte can pose some serious threats. It is important to have the qualitative analyses done properly and accurately before deciding on the levels that would be needed for quantitation.

2. **Right method:** For any quantitation assay to work, the quantitation method has to be robust, reliable, fast, and reproducible. From choosing the right technology to the protocol that has to be followed, the workflow solution to optimizing critical parameters to maximize your assets—it is important that you understand what is needed and what has to be done.

3. **Better confidence:** Are you certain that you have quality data that can offer you the confidence that you aspire for? The method should not only be robust and reliable, but also needs to be sensitive and offer increased selectivity and specificity. These features allow you to identify and quantify your target analyte(s) from other components of the mixture.

4. **Optimal support:** Choose technology based on your testing goals and what needs to be achieved, not on your analytical scientist's or lab technician's expertise. This will ensure the most appropriate technology is selected and matches your business requirements. Select the most appropriate technology and one that is easy to implement with optimal support for achieving the desired result within the proposed timeline.

5. **Addressing goals:** Whether you are a scientist or an executive, from your scientific goals to your organization's profitability goals—it is important that you address them with ease, speed, and confidence. The technology, platform, workflow solution—should all combine to cater to these demands.

6. **Address critical concerns:** From your customer's requirements to the regulatory demands—quantitation assays have to abide by the rules, regardless of the technology you choose.

LC-MS: path to confident quantitation

What is LC-MS?

Advancements in liquid chromatography (LC) coupled to mass spectrometry (MS) technologies have led to widespread implementation of LC-MS in analysis, identification, and quantitation of analytes across a wide range of applications. This combined technology offers the ability to deliver high sensitivity and selectivity to ensure isolation of target analyte from what could be a sample containing thousands of other different molecules. Typically, MS or LC alone are unable to meet this need as they can only differentiate compounds by their mass-to-charge ratio (*m/z*) or retention time on the column, respectively, which is often less efficient in most practical applications. Therefore, there is a strong requirement for a technique (LC-MS in this case) that utilizes an ideal separation platform and an efficient selective-and sensitive platform for detection, analysis, and quantitation.

LC-MS is the combination of two selective techniques that allows isolation and quantitation of target analyte(s) in complex mixtures across all application areas.[1-3] As indicated above, LC differentiates compounds by their physicochemical properties and MS differentiates compounds by their *m/z* ratio. It is the dual selectivity that makes LC-MS such a powerful analytical tool.

Why use LC-MS for quantitation?

Before going into the pros and cons of why LC-MS should be used for quantitation, it is important to understand the features and benefits offered by mass spectrometry, especially, triple quadrupoles.[4,5] LC-MS platforms are capable of performing electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), or photo ionization (APPI) which ionize various semi-volatile, thermally labile, and polar-to-nonpolar compounds, such as pharmaceuticals, pesticides, personal care products, steroids, explosives, drugs of abuse, etc., in trace levels. Ions generated after ionization are transferred through a vacuum interface into the mass analyzer.

Quadrupoles are mass analyzers that consist of four rods with DC and RF voltages applied (Figure 2). An ion of a specific mass-to-charge ratio (*m/z*) will be stable and can pass through the quadrupole only when a specific DC/RF voltage combination is applied. Quadrupoles are therefore called mass filters.[6]

LC-MS has become a popular technique owing to several advantages that it offers (Table 1).

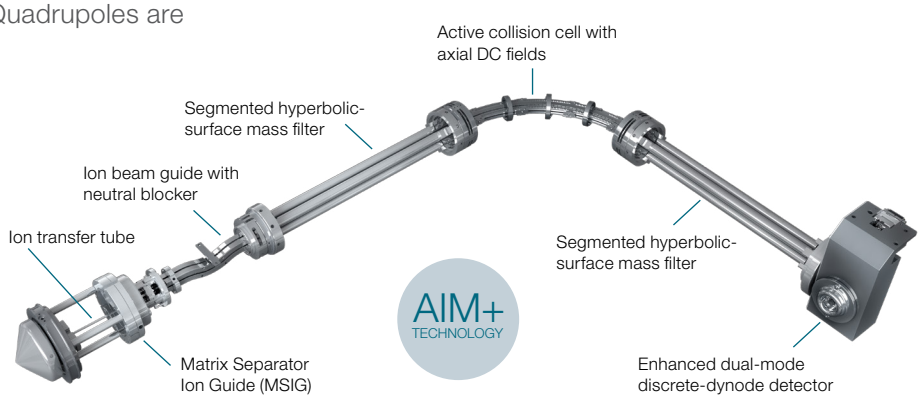


Figure 2. Ion path of TSQ Fortis.

Table 1. The "pros and cons" of LC-MS technology.

Pros	
Selectivity	Combining two separation mechanisms of LC and MS allows the analysis of complex mixtures. The resulting selectivity allows a particular analyte(s) to be isolated from the mixture offering you confidence that the correct component is measured. Since analytes are separated by their *m/z* ratio, the technique allows for the use of isotopically labeled internal standards, which may not be separated by LC but can be separated by their mass difference. The use of internal standards can help control variability in a quantitative assay.[7,8]
Speed	Since the mass spectrometer will distinguish compounds based on mass, the chromatographic method does not have to separate every single component in the sample, so coelution of non-isobaric analytes is possible. This allows fast LC analysis times and reduced sample preparation, which helps with method development and high-throughput sample analysis.
Sensitivity	Mass spectrometers are inherently sensitive. Good selectivity also leads to reduced noise, allowing easy development of highly sensitive assays.[7-11]
Cons	
Expense	Compared to other widely used technologies, LC-MS can turn out to be more expensive, potentially affecting organization's cost/sample goals.
Complexity	Individually, either LC or MS can be difficult to optimize so optimizing the two together requires even more complex co-dependent synergy. The ionization mechanism can be especially complicated—often several charged species are formed in the ionization source and multiple charging of ions can occur. Care must be taken to choose conditions for optimum sensitivity and reproducibility. Sufficient training is also needed to allow analysts to run the systems effectively.
Dynamic range	Compared to other quantitative techniques, LC-MS can have a limited range where the response is linear with respect to concentration.
Excessive selectivity	In quantitative analysis, it is usual that the mass spectrometer is set to only detect specific analytes. This results in a very "clean" looking chromatogram, and it may be easy to forget that there can be many components still present, but not seen. These components can cause challenges in achieving reproducible quantitation and can be difficult to trace if they are not being looked for.

Table 2. Benefits and ideal applications for QqQs and HRAMs.

Triple quadrupole MS (QqQ) productivity—Fast acquisition modes with MS/MS sensitivity offers excellent reproducibility for quantitative analysis at the limit of detection (LOD) or quantitation (LOQ)	**High-resolution accurate mass (HRAM) productivity**—Outstanding resolution offers clarity of the analytes in environments not seeking ultimate in high-throughput
Robustness and reproducibility in targeted quantitation—highly demanded in a targeted quantitation environment for quantitation of one to hundreds of analyte(s) in complex matrices	HRAM provides information concerning the elemental composition and molecular weight of an analyte. Accurate mass of fragments is not sufficient to ellucidate the structure. The confirmation of analyte structure is done by NMR.
Ultimate sensitivity—for a host of molecule types in complicated biological matrices	**Sensitivity is not the driving force**—Full Scan MS is not as sensitive as a targeted acquisition mode
Cost/sample reduction—robust, reproducible workflows for sample analysis, every day	**Retrospective search**—Full Scan MS is an information rich mode that can be analyzed post acquisition
Address regulatory requirements—from regulated environments to established methods; easy method development for all molecule types	**Growing footprint**—while some laboratories are validating HRAM to perform studies in a regulated environment, they are mostly used in upstream discovery work
Selectivity—offers high-resolution selected reaction monitoring (SRM) capabilities; records nominal mass	**Excellent resolution**—obtain better information about your sample with the ability to distinguish between two peaks with similar ion-to-charge ratio

Types of LC-MS: which one is right for you?

While the LC-MS technique has gained widespread popularity, there are some significant differences between technologies. There are primarily two types of mass spectrometers (MS) that are used: high-resolution accurate mass (HRAM) or triple quadrupole mass spectrometers (QqQ) (Figures 1A and 1B). Both HRAM and QqQs have their unique set of advantages, and a decision to use one over the other will be based on your requirements, sample preparation capabilities, analyte and matrix complexity, user requirements, throughput requirements, etc. Table 2 highlights the benefits and ideal applications for QqQs and HRAMs, which can enable you to decide the right MS platform for your laboratory.

Change is in the air

The world around us is evolving quite rapidly. A lot of changes can be observed in the world of analytical sciences as well. For quantitative analyses, it is absolutely crucial to develop robust, reliable, reproducible, and sensitive quantitative methods that can address regulatory requirements while reducing cost/sample. Hence, if you are addressing your quantitation requirements via any technology and find the process difficult, perhaps it is time to consider a different approach. The following section will highlight the pros and cons of moving from your existing technology of choice to LC-MS/MS for your quantitation assays—a technique that offers robust, reliable, reproducible, sensitive quantitative assays for any molecule type, in any matrix, and for any user.

Are you considering a move from single quadrupole MS-oriented workflows?

Both single and triple quadrupole MS allow quantitation of analytes. However, single quadrupole MS contain only one mass filtering quadrupole while triple quadrupole MS consist of three quadrupoles. Selected Reaction Monitoring (SRM) is the most common mode of using a triple quadrupole MS/MS for quantitative analysis, allowing enhanced sensitivity and selectivity. Triple quadrupole MS (often shown as MS/MS) offers some significant benefits when compared to a single quadrupole MS (Table 3).

As highlighted in Table 3, detection in SRM mode using a triple quadrupole MS/MS has a number of advantages in comparison to SIM mode with a single quadrupole MS. Triple quadrupoles offer much higher selectivity with less interference of coeluting compounds and matrix components, resulting in less time-consuming method development and faster analysis times. Better signal-to-noise ratio allows quantitation with lower limits of quantitation (LOQ). Fewer ions have to be detected per compound with MS/MS in comparison to MS for confirmatory analysis resulting in significant difference in performance. Finally, a wider linear range, higher accuracy, and reproducibility can be obtained on triple quadrupole MS/MS (Figure 3).

Table 3. Triple quadrupole MS compared to a single quadrupole MS.

Features	Single quadrupole MS	Triple quadrupole MS
Mass filtering capabilities	Only one mass filtering quadrupole	Three quadrupoles: Q1 and Q3 are mass filters while Q2 is a collision cell
Selectivity mode	A fixed set of DC and RF voltages is applied to the quadrupole and only a single *m/z* can pass. Ions with different *m/z* are filtered out. Selectivity is achieved via Selected Ion Monitoring (SIM)	Selectivity is offered by Selected Reaction Monitoring (SRM). The first quadrupole filters a specific precursor ion of interest. Ions generated in the ion source that have a different *m/z* cannot pass Q1. The collision cell is optimized to produce a characteristic product ion by collision of the precursor ion with a neutral collision gas, such as nitrogen. Generated product ions are transferred into the third quadrupole where only a specific *m/z* is allowed to pass. All other product ions are filtered out in Q3. SRM works like a double mass filter that reduces noise and increases selectivity significantly.
Selectivity	Low	Higher—results in reduced interference of coeluting compounds and matrix. Easier to detect and quantify, and also reduced requirement of an ideal LC separation.
Detection	Single mass filtering mode is often found to have limitations for samples in complex matrices, as well as complicated sample mixtures	Double mass filtering allows MS/MS to offer higher selectivity with less interference of coeluting compound and matrix components, resulting in less time-consuming method development and faster analysis times
Sensitivity	Typically low owing to use of one set of quadrupoles	Higher—better signal-to-noise (S/N) ratio allowing quantitation with lower limits of quantitation. Fewer ions have to be detected per compound on MS/MS in comparison to MS for confirmatory analysis.
Reliability	SIM mode has limitations that increase variability especially for complicated analytes or analyte mixtures in complex matrices	Higher—in identification of detected analytes using SRM in comparison to SIM
Linear dynamic range	Limited, with at least two orders of magnitude less than triple quadrupoles	Higher compared to the single quadrupole MS
Accuracy and reproducibility	Limited, and often requires high sample concentration	Higher, especially beneficial for sample limited situations or low concentrations

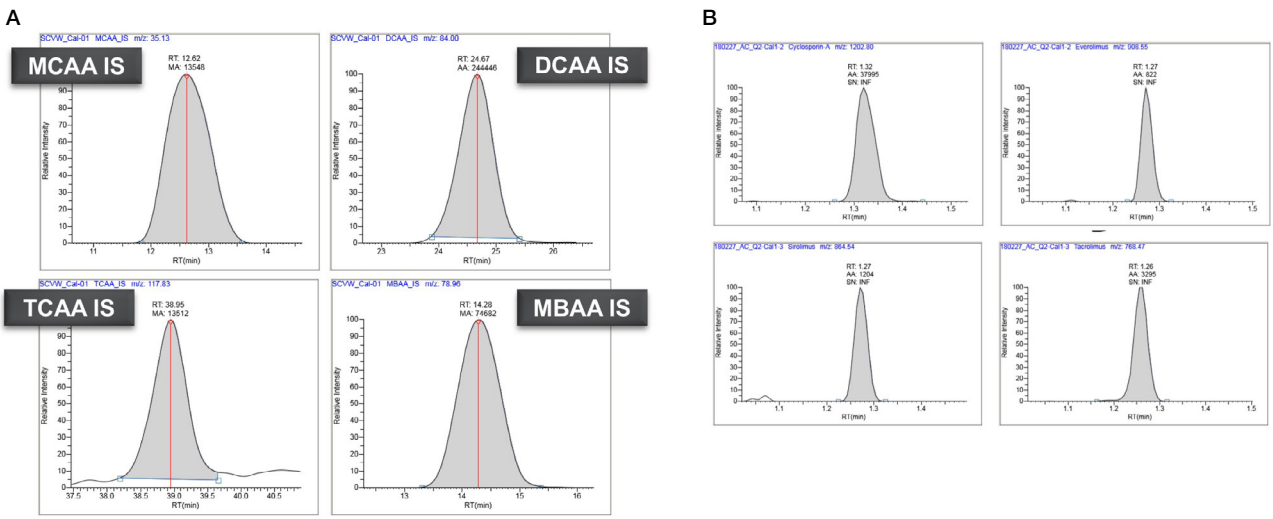


Figure 3. Comparison of sensitivity between full scan and SRM for any analyte with TSQ Fortis MS. Exemplary linearity and class leading sensitivity for polar contaminants in water (A), address demands for quantitation of immunosuppressants (B).

Quantifying with other technologies

Ligand-binding assays (LBAs) have been used for quantitation (mainly bioanalytical assays) of small and large molecules since the late 1950s. The widespread usage of LBAs in biomarker analysis is attributed to their inherent high sensitivity and throughput, especially for large molecules presenting at femtomolar to attomolar levels in biological matrices. Enzyme-linked immunosorbent assay (ELISA) is a typical format of LBAs, which is performed using a primary capture antibody immobilized to the surface, while the concentration of the targeted analyte is detected through the binding of secondary antibody coupled to enzymes, and the detectable signal is produced by the enzymatic conversion of substrate molecules (Figure 4). ELISA is less suitable for multiplexed measurements because of a greater incidence of nonspecific signals. In LBA measurements, it is important to choose appropriate antibodies since LBAs rely heavily on the quality of assay reagents. Unfortunately, in some situations, LBAs may not have the required specificity to distinguish the original compound from its metabolites or distinguish intact proteins from its heterogeneous forms. Therefore, the assay specificity and accuracy can be questionable if the antibodies do not possess suitable quality.[12]

With the development of increasing sensitivity, mass spectrometers coupled with liquid chromatography (LC-MS) have become a useful alternative to LBAs for many bioanalytical applications. The success of LC-MS is mainly driven by its high specificity, broad dynamic range, fast method development, and the fact that it does not necessarily require immunochemical reagents. Among available LC-MS quantitative techniques, SRM, conducted with a triple quadrupole mass spectrometer, has been widely adopted as the "gold standard" for quantitative measurement. LC-SRM has evolved as a widely accepted, multiplex-capable method for the quantitative determination of both small and large molecules. Pros and cons of LBA and LC-MS for quantitation are summarized in the Table 4.

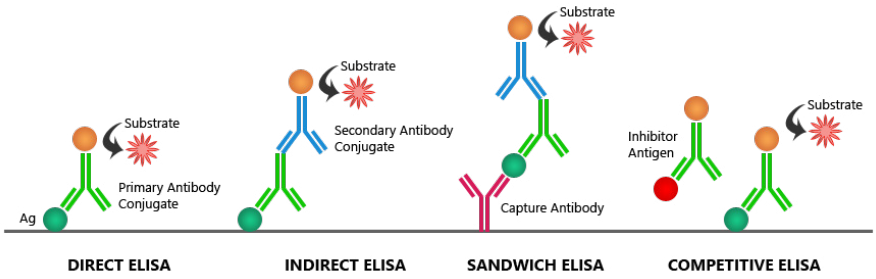


Figure 4. Different forms of ELISA.

Table 4. Triple quadrupole MS compared to LBA.

Attributes	LBA	Triple quadrupole MS
Throughput	High	High (with multiplexing); otherwise lower than LBA
Cost	High operating cost	High instrument cost; low operating cost
Method development	Slow	Fast
Dynamic range	<2 orders	>4 orders
Sample pretreatment	Simple	Simple to complex; depends on sensitivity requirements
Sensitivity	High	Offers a range; high with triple quadrupole MS high sensitivity
Specificity	Monospecific (antigen-antibody recognition), low	Multispecific (retention time, precursor *m/z*, product *m/z*), high
Precision	Moderate (CV<25%)	Great (CV<15%)
Validation	Can be difficult as it is dependent on quality of antibodies	Uniform and robust validation; offered as a service with the purchase of a triple quadrupole MS
Affinity dependent	Sensitive	Not relevant
Analyst dependent	Yes	No

LBAs and LC-MS generate complementary results, and both technologies are used during development and in routine analysis. However, liquid chromatography-tandem mass spectrometry (LC-MS/MS) technology plays an extremely important role in supporting clinical studies and mechanism-based researches. LBA and LC-MS techniques can be coupled to combine the selectivity of immunoaffinity extraction with the specificity of MS detection. It is extremely promising that integration of ligand binding and LC-MS assays will help provide more meaningful data for biomarker quantification. However, for most users who seek increasing specificity and selectivity while achieving the same level of sensitivity as that of LBAs, LC-MS/MS with a triple quadrupole MS is an ideal platform.

Considering moving from LC-only quantitation to LC-MS/MS?

For years, LC has been used as a primary technology for quantitation of analytes in matrices. From early-stage discovery to quality assurance and quality control (QA/QC) or operations, high-performance liquid chromatography (HPLC) or ultrahigh performing liquid chromatography (UHPLC), LC traditionally has been the technique of choice for performing quantitation assays. Typically, the high resolution and the ability to address both small and large molecules, as well as nonpolar and polar (often with derivatization) molecules, enables LC to be an automatic choice for quantitation. However, with the advancement in LC-MS technology, one can achieve significantly better quality results, and increased confidence in quantitation assays. As the analytes continue to become more complicated in terms of additional functional groups or structural features, there is the additional challenge of higher numbers of analytes to be identified and quantified in complex matrices, which can vary between different food types to biological samples. Hence, the specificity, selectivity, and sensitivity offered by MS combined with resolution (high-resolution SRM by triple quadrupole MS and high resolution offered by HRAM) enables better quality of quantitative data, increased confidence in data, and helps ensure higher product quality, with robust, reproducible, reliable, and sensitive assays. Some of the comparison features of the two technologies, LC only versus LC-MS, are summarized in Table 5.

Table 5. LC compared to LC-MS/MS.

Attributes	LC only	LC-MS/MS
Throughput	Low to High (with multiplexing capabilities)	High faster speed allows higher throughput (especially with multiplexing)
Instrument expense	Economical	Less economical
Speed	Slow	Fast
Dynamic range	<2 orders	>4 orders
Sample pre-treatment	Required (especially for complex matrices)	Required and is controlled by sensitivity requirement
Resolution	Moderate; analytes separated by retention time (e.g., polarity, column type)	High (LC's resolution combined with highly selective SRM (H-SRM))
Sensitivity	Moderate	Offers a range; high with high-end QqQs
Specificity	Limited; shorter run times or similar polarity of analytes result in signal overlap	Multispecific (retention time, precursor *m/z*, product *m/z*), high-resolution SRM allows additional specificity
Precision	Good (<25%)	Great (CV<15%)
Validation	Can be difficult as it is dependent on quality of antibodies	Uniform and robust validation; offered as services
Selectivity	Moderate	Excellent; LC selectivity combined with *m/z* selectivity
Usability	High	Growing because of increased specificity, selectivity, sensitivity

LC has traditionally been the technology of choice for performing qualitative and quantitative analyses of a host of molecule types in a variety of complex matrices. Their resolution, speed, and ability to address different molecule types contribute significantly to this technology being the first choice. However, when the strengths of LC are combined with those offered by triple quadrupole MS, it results in some significant gains. From additional specificity to selectivity, and sensitivity to robustness, LC-MS/MS technology is gaining popularity, and with the rise of affordable MS/MS, such robust quantitative workflows can now be implemented in day-to-day quantitation environments.

Setting up a new laboratory

When you are setting up a new laboratory, regardless of your application type, you face the following inherent challenges:

- **How much can you reduce your cost/sample?**
  This is critical for your organizational profitability and achieving other related business goals.

- **Do you know enough about your molecule of interest?**
  Knowing your analyte(s), and being able to quickly get to the quantitation assays is extremely important for faster turnaround of results, confidence in data, and also ensuring reduced cost/sample.

- **Which technology is right for you?**
  While a large collection of technologies allows you to have additional breadth and capabilities to offer, they also require consumption of your time and resources (technical and financial). If you need to choose between multiple platforms, you need to address the challenge and ensure that you have made the correct decision.

- **How difficult would it be to learn a new technology?**
  While the advantages of LC-MS/MS can offer significant benefits, should this be a new technology for your users? If so, how long would it take for your users to be comfortable with the technology and start producing results that address your commercial and scientific goals?

- **How much support can you expect from the vendor?**
  As a follow-up to the previous point; this is where the LC-MS/MS vendors can assist you, enabling your laboratory, and helping your scientists optimize the methods to ensure a faster uptime/turnaround time for high-quality, confident results.

- **Can you develop robust, reliable, and sensitive quantitative workflows?**
  Yes, if this is your goal, LC-MS/MS should be able to help you achieve this goal. However, the time required to be up and running, ease of implementation, expertise that can be transferred, and the knowledge of your analyte(s) and matrix (or matrices) are critical. This is where a partnership with the vendor becomes extremely important.

- **How do you protect your investment?**
  While your needs and requirements for LC-MS/MS can be imminent based on a certain project that you have, you need to protect your purchase by ensuring that the same system can help you address quantitation challenges of other classes of molecules in different matrices. From small to large molecules, your triple quadrupole mass spectrometer system should be able to address all scientific requirements, upcoming analytical challenges, and protect your investment for a longer period of time.

The challenges are critical and the answers can be complex. However, Table 6 offers a quick and comprehensive response to the questions these questions.

While being productive, addressing critical quantitation challenges, and ensuring prompt delivery of high-quality data remains the center of your attention—it is important that you also address your business and scientific goals with technologies that can offer you high-quality data with minimal downtime. Often, more accessible triple quadrupole LC-MS/MS technology can offer the quality you aspire to achieve with the ease you want and affordability you deserve.

Table 6. Benefits of LC-MS/MS technology.

Attributes	LC-MS/MS offerings	Benefits/impact
Throughput	Faster speed allows higher throughput (especially with multiplexing)	Address larger number of transitions or more samples/day to ensure higher profitability
Resolution	Excellent (LC's resolution combined with H-SRM)	Achieve better quality data for every molecule type, across different matrices
Sensitivity	Offers a range; higher with high-end triple quadrupole MS	Choose what is needed for your project
Selectivity	Excellent; retention time combined with *m/z* selectivity	Separate between overlapping signals, complex peptides; achieve confidence in data quality
Specificity	Multispecific (retention time, precursor *m/z*, product *m/z*), High resolution SRM allows additional specificity	Lower limits of detection enables increased confidence in data quality
Cost/sample	Depends on requirement	Robust workflows ensure lower cost/sample
Validation	Uniform and robust validation; offered as services	Enables you to address regulatory requirements
Usability	Growing because of increased specificity, selectivity, and sensitivity	Additional confidence in technology with more references
Workflow Solution	Offered for specific applications (e.g., Thermo Scientific™ Pesticide Explorer Collection)	Ensures short time before you are productive; higher profitability
Ease-of-use	Portability of methods; workflow oriented methods; universal operational guidelines	Enables robustness of data, ease-of-implementation and getting started fast and correctly
Support—service	Readily available in all regions	Ensures instrument uptime, which also reduces cost/sample
Support—application	Offered at multi-levels and depending on expertise needed	Enables confident quantitation regardless of user expertise; faster time to quality results
Faster turnaround	Robust workflows with easy-to-use software ensures faster turnaround of quality results	Enables confident quantitation regardless of user expertise; faster time to quality results

Is it time to replace older instruments or upgrade?

You have an established laboratory for performing screening, identification, and untargeted and targeted quantitation of analytes across multiple matrices, what you need to consider is an upgrade? What are the scientific and business values that you need to consider for an upgrade?

- **Ensure confident quantitation today and tomorrow**
  Many analyses call for triple-quadrupole MS, especially where the goal is to quantify sample analytes. Using two stages of mass analysis improves sensitivity compared to simpler forms of MS (or most other technologies). A key facet for using targeted quantitation workflows is to achieve high sensitivity and with today's advancements in LC-MS/MS technology, one can now easily monitor low levels of analyte(s) across all matrices.[15-18] While your level of affordability may not have increased, a more accessible triple quadrupole MS with an LC should be able to offer the sensitivity for your application requirements (Figure 5).

- **Ability to leverage new technologies to get better results, faster**
  Analyte(s) are becoming more complex and are likely to get even more complex in the future. Alternative technologies (use of dried blood[16], low-flow-rate devices, etc.) that preserve precious samples, use less solvent, and offer higher sensitivity, are becoming imminent. While your previous-generation LC-MS/MS platforms may not have the ability to work with all of the accessories that are popular in today's analytical laboratories, your new-generation LC-MS/MS (with low-end QqQ) can still deliver a varied range of capability with excellent sensitivity (Figure 6).

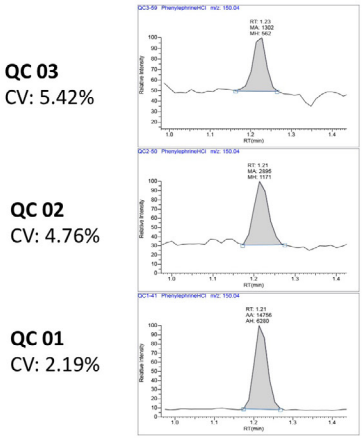
- **Achieve faster data and higher throughput to increase profitability**
  The speed of today's triple-quadrupole MS systems has broadened their use significantly without compromising performance. This is extremely important when monitoring hundreds of analytes simultaneously. Figure 7 illustrates the setup of a multi residue pesticide method, available as a method template in the Thermo Scientific™ TSQ™ triple quadrupole MS. Now it is easy for you to confidently quantify hundreds of compounds or analyze hundreds of samples independently of your experience with mass spectrometry.

- **Support when needed**
  If you plan to transition from your previous generation of LC-MS/MS platforms to a newer platform, some of the biggest requirements will be method development optimization, instrument control training, and ensuring instrument uptime. All of these features contribute significantly towards ensuring your organizational profitability, your business goals, as well as your scientific achievements. It is imperative that the vendor offers utmost support when needed—from ensuring instrument uptime (service) to helping maximize your new platform's potential (application support).

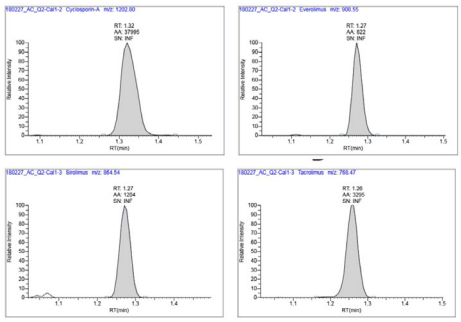
- **Robust, reliable, reproducible workflows with superior sensitivity**
  Your biggest challenge is to find out why you need to upgrade and update your LC-MS/MS to a new platform. You need to offer robust, reliable, reproducible workflows with excellent sensitivity for every analyte type, regardless of the matrix and user expertise. When you change your existing, older LC-MS/MS platforms to something new, regardless of your budget, you deserve a workflow that offers you high-quality data, faster than ever before, helping ensure that you achieve your business and scientific goals (Figure 8).

Conclusion

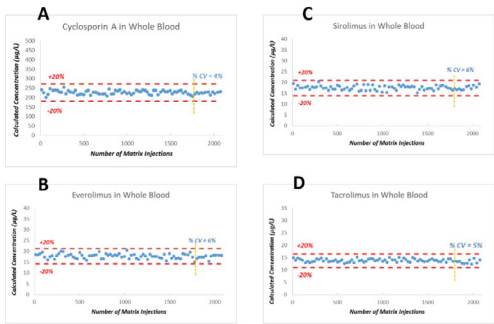
Triple quadrupole mass spectrometers are often used when higher sensitivity and specificity is required. They may also be used to generate additional fragmentation data from ions of interest. LC-MS/MS as a technology has evolved significantly in the last decade and is capable of delivering outstanding results. Comprehensive workflow solutions with Thermo Scientific™ Vanquish™ Flex UHPLC system and TSQ triple quadrupole mass spectrometers can enable robust, quantitative superiority for every quantitative environment that faces challenges in terms of developing robust, reliable, and reproducible quantitation workflows.



Increased confidence for QC analysis of Phenylephrine in water.



Address demands for quantitation of immunosuppressants.*



Proof of robustness for immunosuppressants for more than 2600 sample injections.*

Figure 5. Sensitivity data with %CV data.
* For Research Use Only. Not for use in diagnostic procedures.

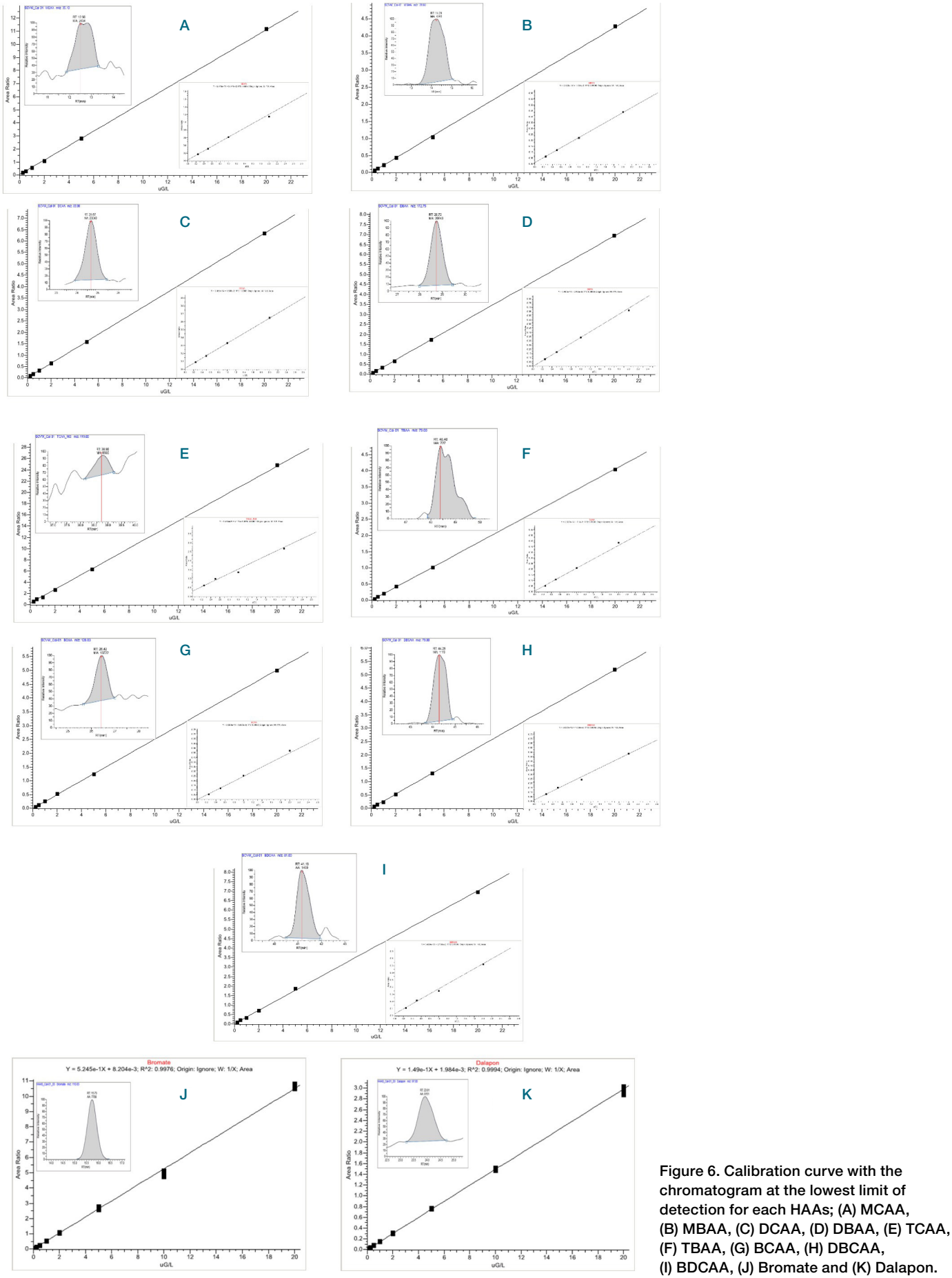


Figure 6. Calibration curve with the chromatogram at the lowest limit of detection for each HAAs; (A) MCAA, (B) MBAA, (C) DCAA, (D) DBAA, (E) TCAA, (F) TBAA, (G) BCAA, (H) DBCAA, (I) BDCAA, (J) Bromate and (K) Dalapon.

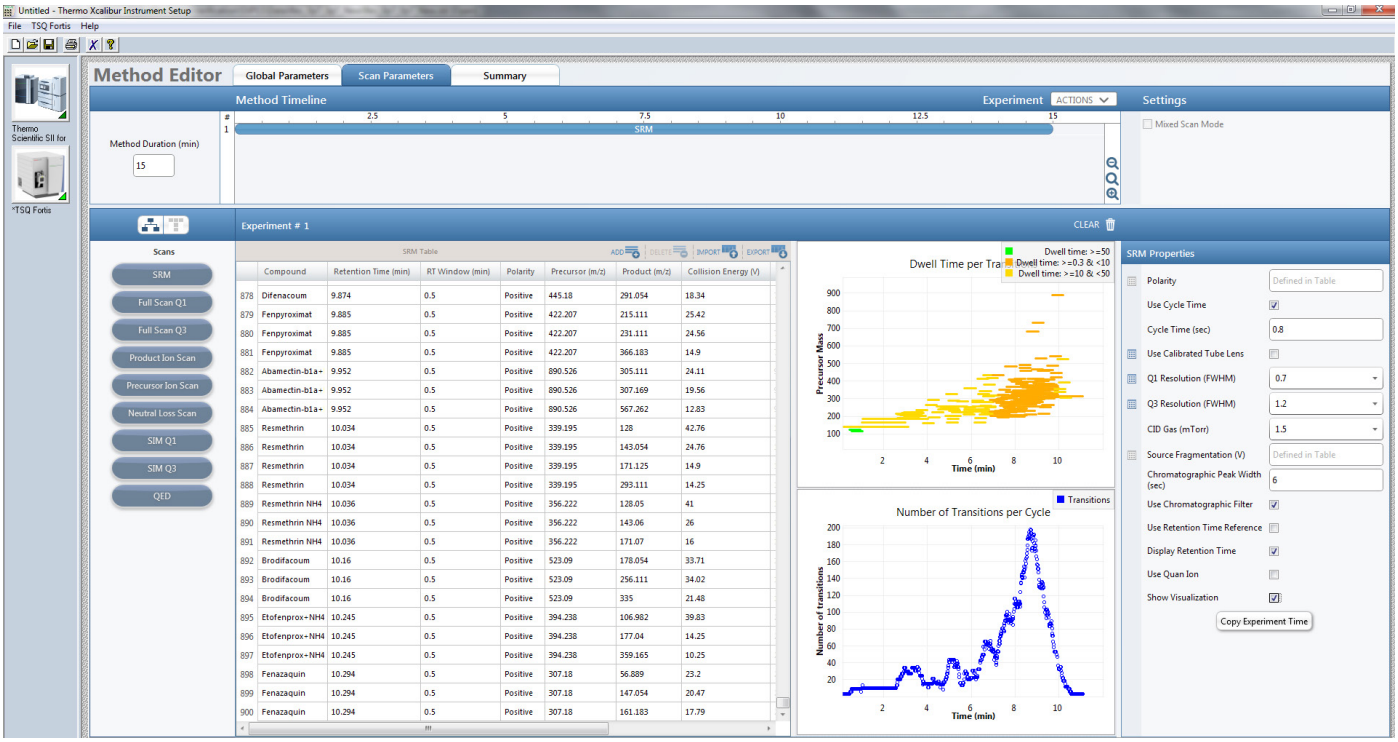


Figure 7. Instrument method template for multi residue pesticide analysis. Precursor and product masses, collision energies and general method settings have been optimized for the TSQ platform.

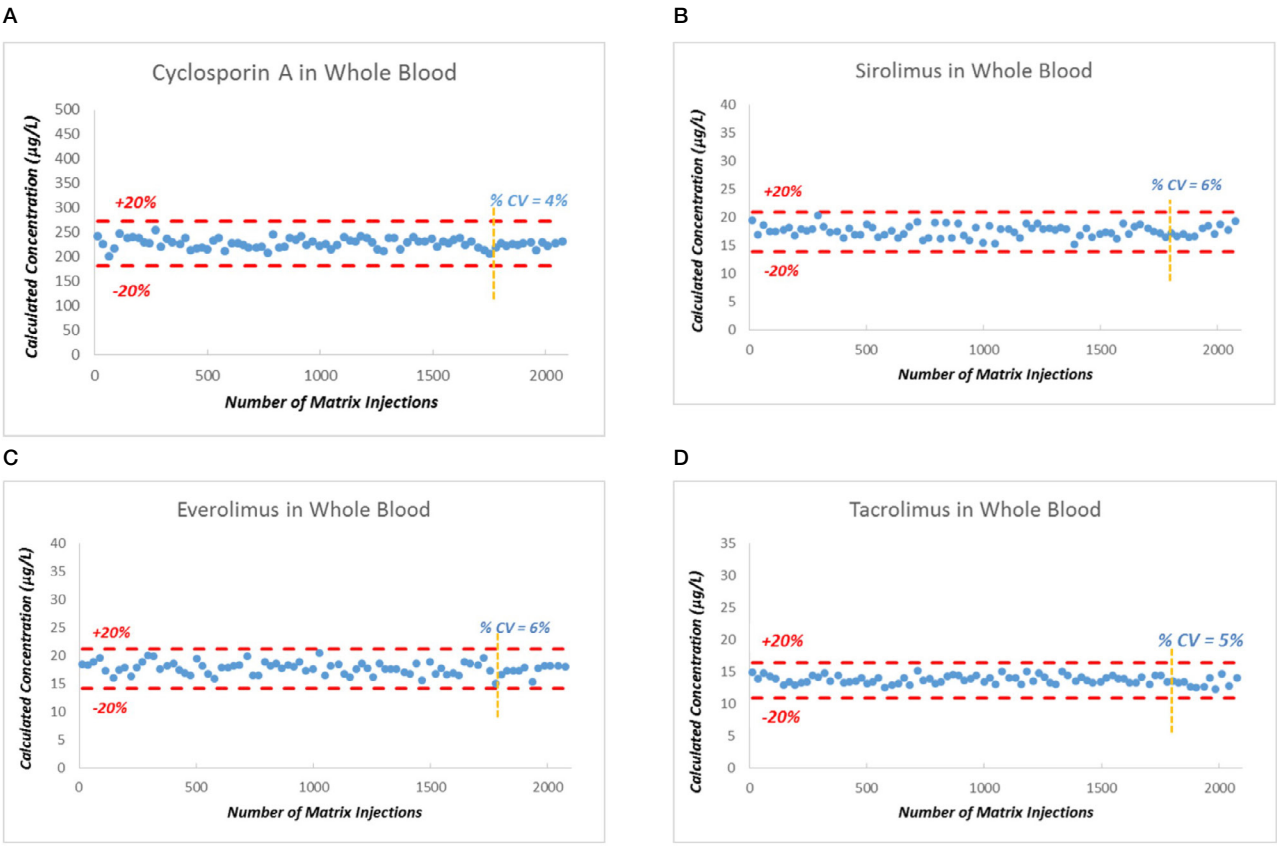


Figure 8. Robustness study of Immunosuppressants in whole blood using TSQ Fortis MS shows very low variability over ~2700 sample injections. For Research Use Only. Not for use in diagnostic procedures.

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