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Hints, tips, updates and advice for Triple Quadrupole Mass Spectrometers

Alan Atkins, Application Specialist
Quantitation.

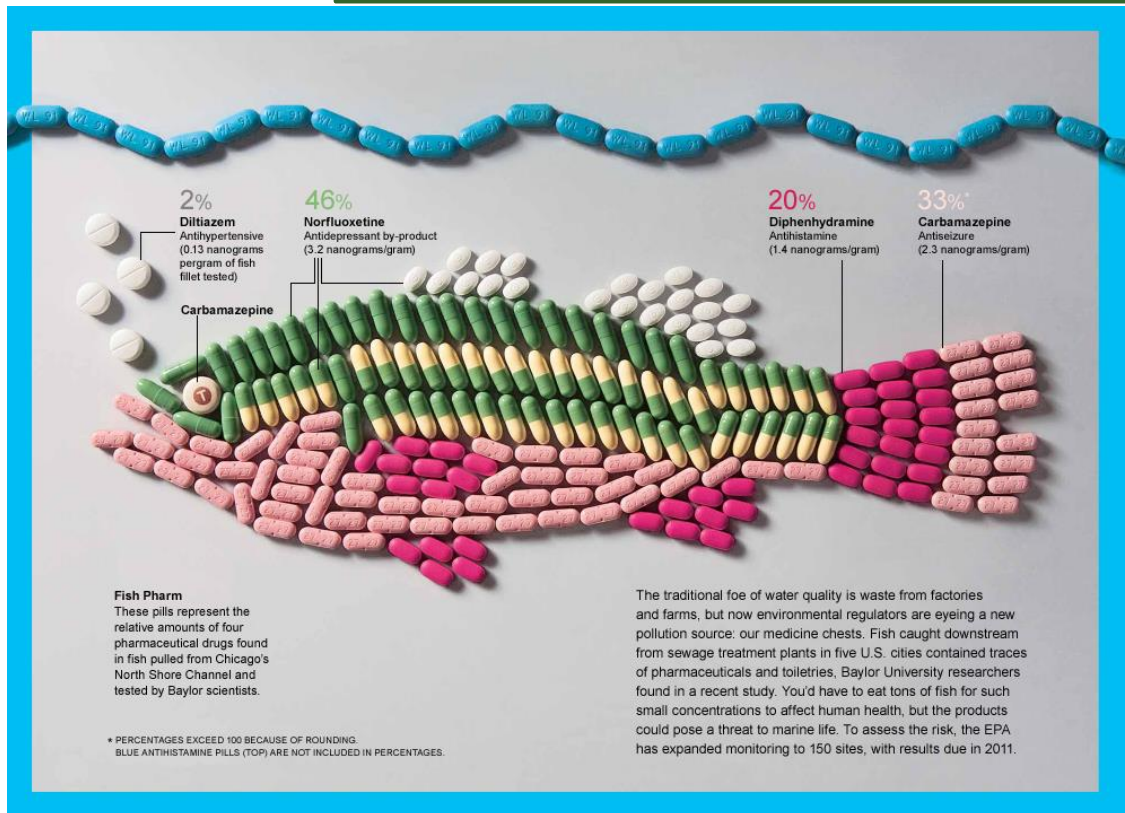
Hints, tips, updates and advice for Triple Quadrupole Mass Spectrometers



- What can a QQQ do for Environmental Analysis.
- What are the common constraints with Environmental analysis
- What is new for Thermo QQQs

Key features of LC-MS/MS Triple Quadrupole Mass Spectrometers.

Can detect wide range of analytes; Pesticides, Pharmaceuticals, Plasticisers, POPs, PFCs



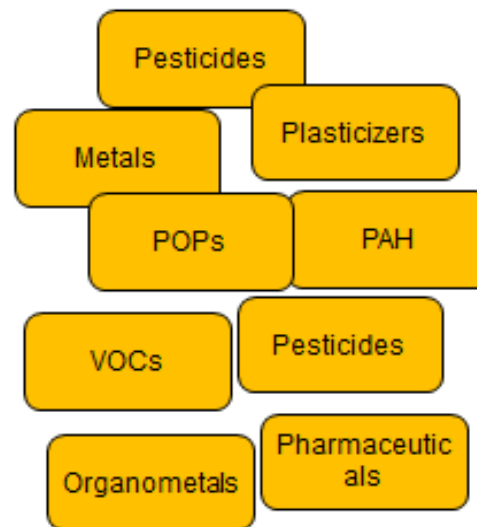
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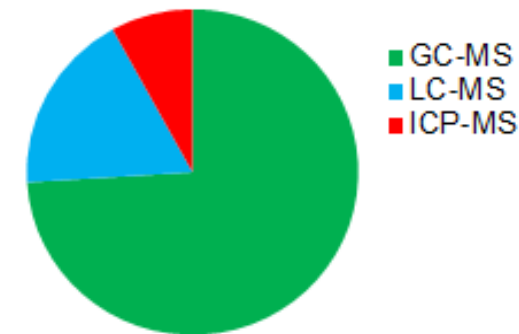
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Priority Hazardous Substances/Technique to be used



Analysis by various techniques



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SCIENTIFIC

Main Problems encountered in Environmental Analysis:

Low Detection Limits: Water Framework Directive 2000/60/EC required LoD for 17-alpha-ethinylestradiol (EE2) is 0.03 ng/L (0.03 ppt).

Complex Matrices: Soil, effluent and biota are just some of the complex matrices that can cause signal suppression and high background signal.

100s of analytes: The demand, especially for pesticide analysis, is for ever increasing numbers of analytes.



With sufficient sensitivity, samples can be diluted more and injections volumes reduced.

Main Problems encountered in Environmental Analysis:

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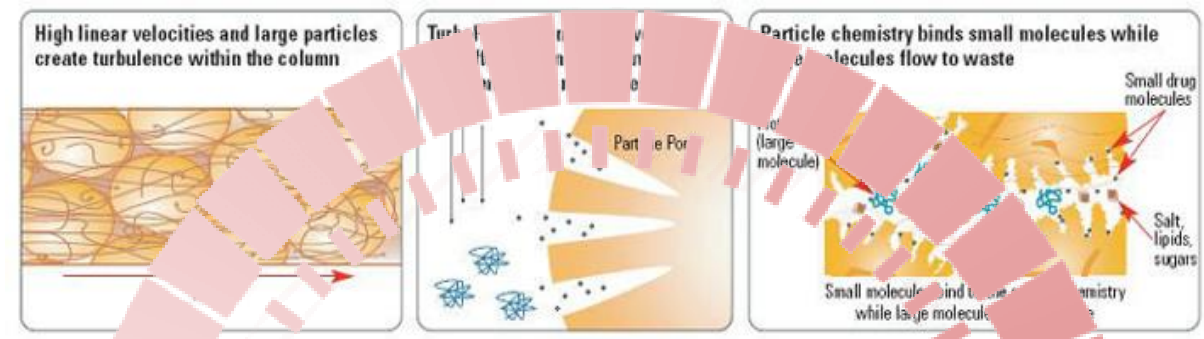
Method Filter Condition Extract Wash Dry

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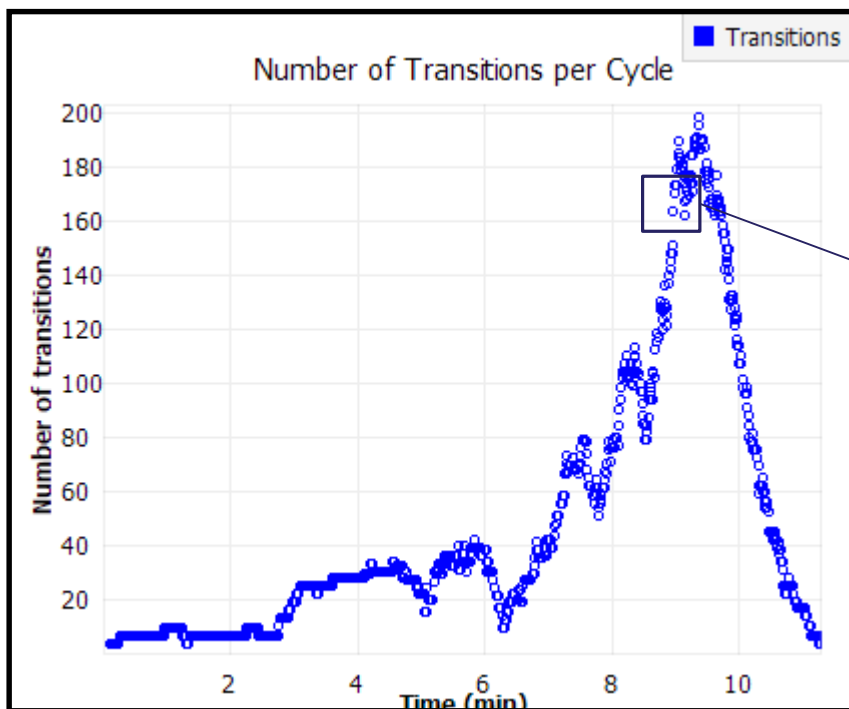
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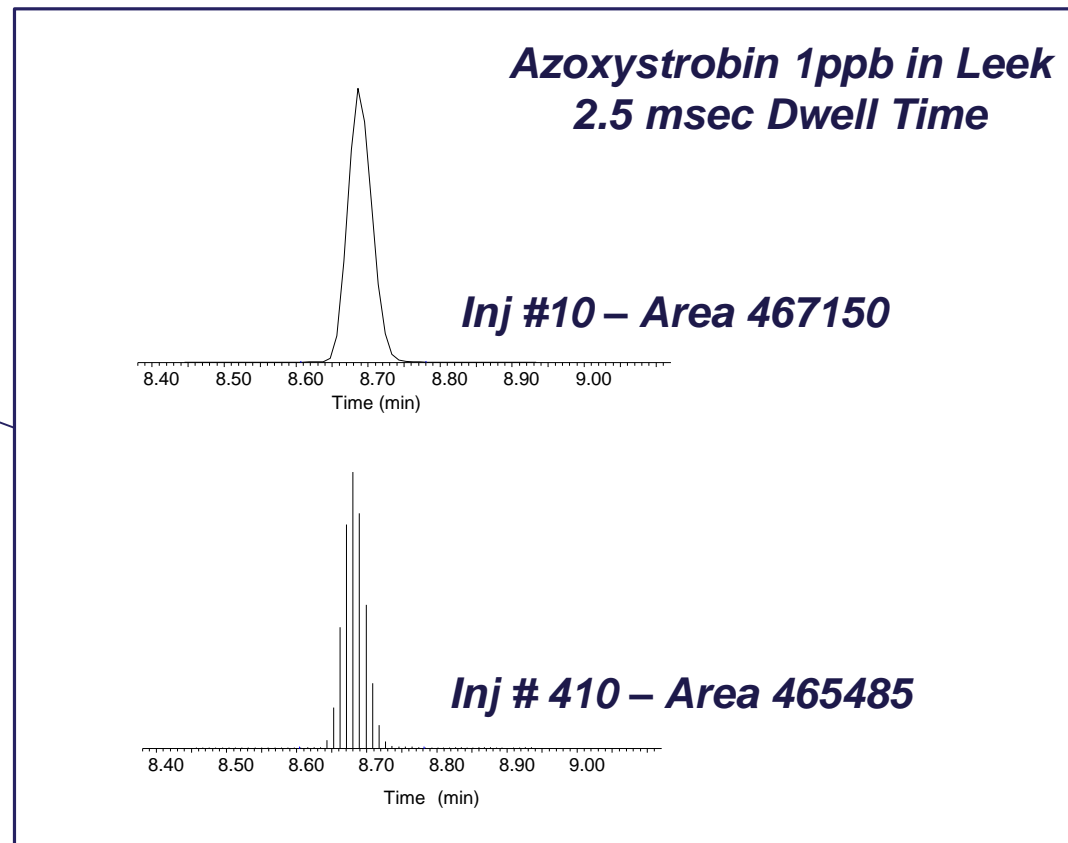
Turbom technology can reduce sample complexity for the most challenging matrices: Milk, honey, effluent, biota.

Main Problems encountered in Environmental Analysis: 100s of Analytes

Excellent Quantitative Performance at Lower Dwell Times!



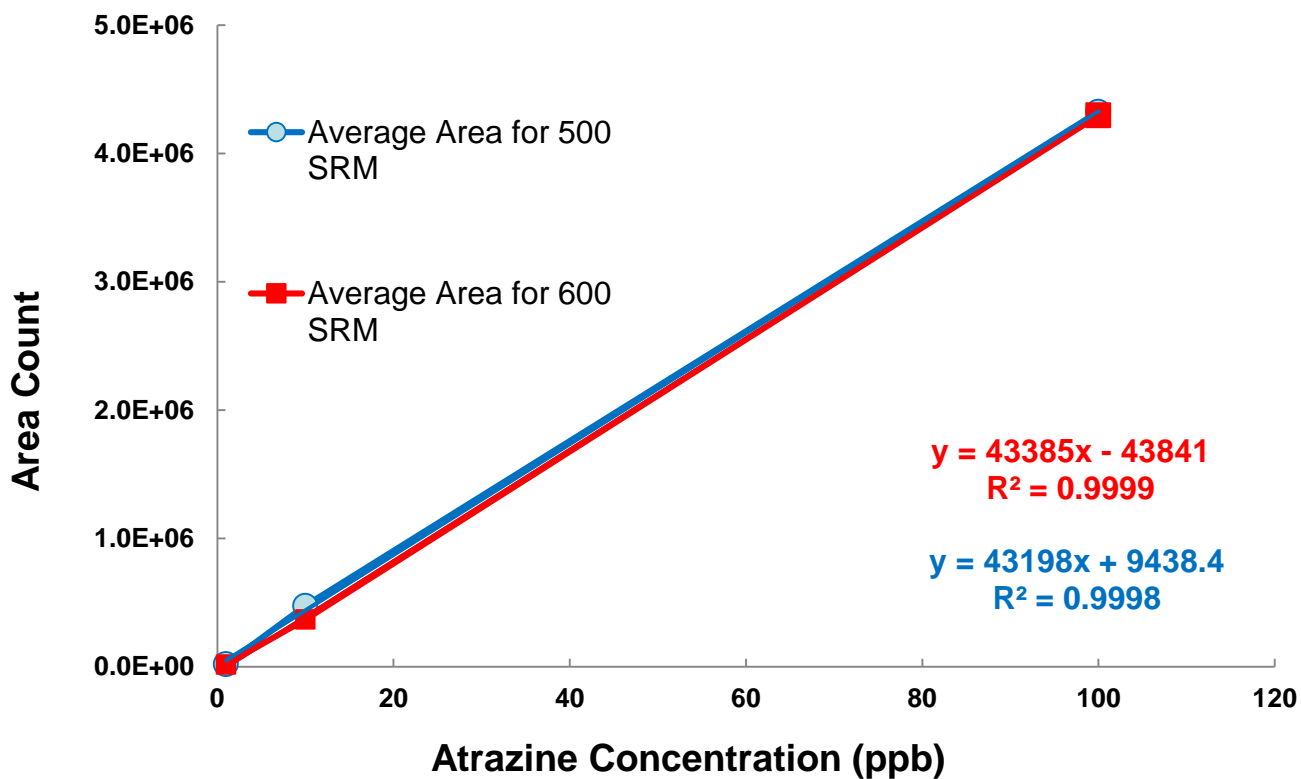
SRM Visualization from Instrument Control Software 3.0 displaying the number of transitions per unit time



~ 160 Transitions Monitored Simultaneously with
Polarity Switching. Excellent Reproducibility (% RSD 2.3) below the MRL

Performance at extreme speeds – 500 SRMs/sec vs 600 SRMs/sec

**Equivalent Quantitative performance between 500 and 600 SRMs/sec!
Good Performance at extremely low dwell times!**



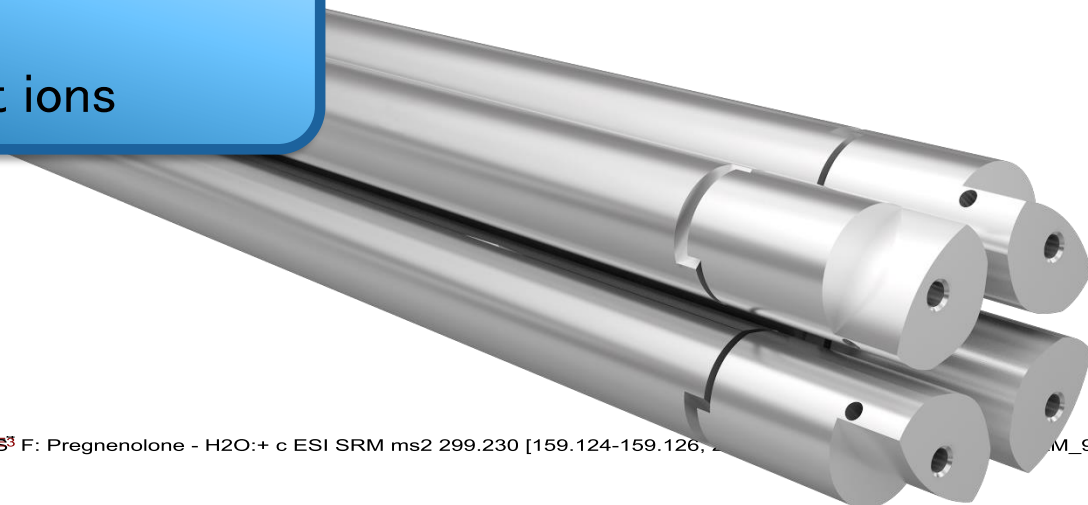
SRMs/Sec	Total Number of Transitions	Dwell Time (mSec)
500	1075	0.769
600	1291	0.437

Atrazine Concentration (ppb)	500 SRM/Second		600 SRM/Second	
	Average Area	%CV	Average Area	%CV
1	21682	9	18090	9
10	475465	4	369612	5
100	4326117	1	4296555	1

Selectivity with High Resolution SRM (H-SRM)

RT: 6.99-12.95, m/z: 158.60-159.16 MS¹ F: Pregnenolone - H₂O:+ c ESI SRM ms2 299.230 [159.124-159.126, 281.213-281.215] SLU_Test_94

Q1 Res = 0.7 FWHM
Pregnenolone
Overlay of both product ions



RT: 7.01-13.02, m/z: 158.60-159.16 MS¹ F: Pregnenolone - H₂O:+ c ESI SRM ms2 299.230 [159.124-159.126, 281.213-281.215] SLU_Test_95

Q1 Res = 0.2 FWHM
Pregnenolone
Overlay of both product ions

*New segmented quadrupoles
with hyperbolic surfaces*

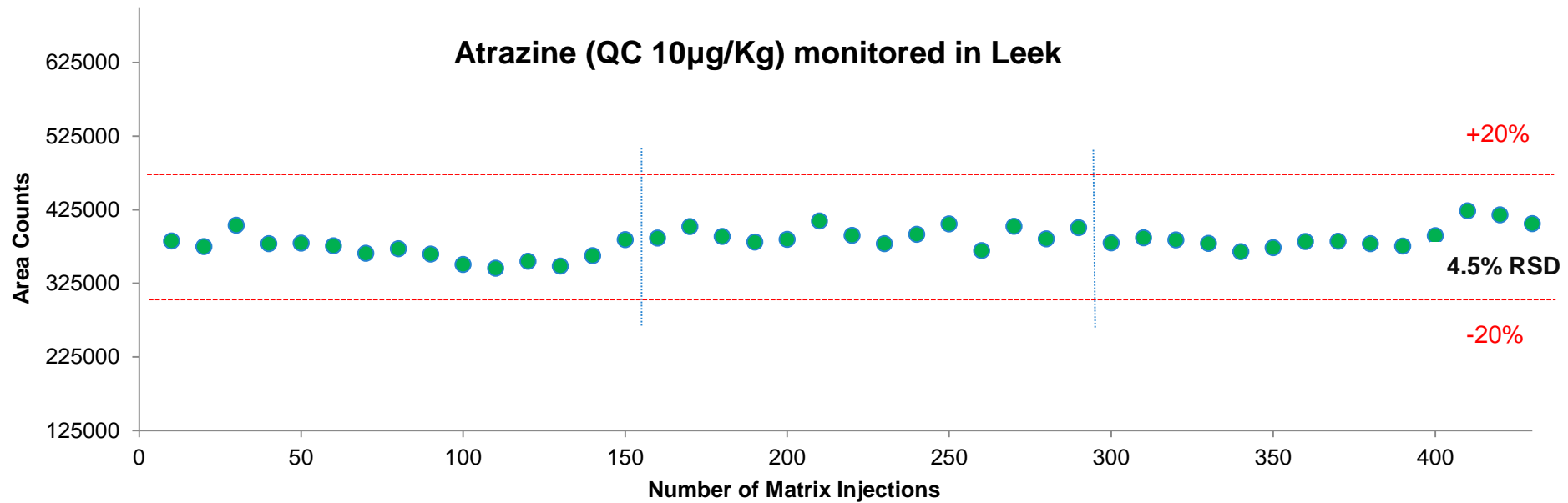
TSQ Altis – 0.2 Da FWHM

TSQ Quantis – 0.4 Da FWHM

*Reduced noise when
analyzing complex matrices –
better S/N – lower LOD/LOQ*

Demonstration of Robustness

Atrazine QC monitored in matrix for more than 400 injections with 4.5% RSD . Red lines represent $\pm 20\%$ response at $10 \mu\text{g}/\text{Kg}$. Blue lines show the time the system was placed in standby mode for 12h to demonstrate consistent performance after standby period



Improved Robustness for TSQ Triple Quadrupole Mass Spectrometers

Robustness

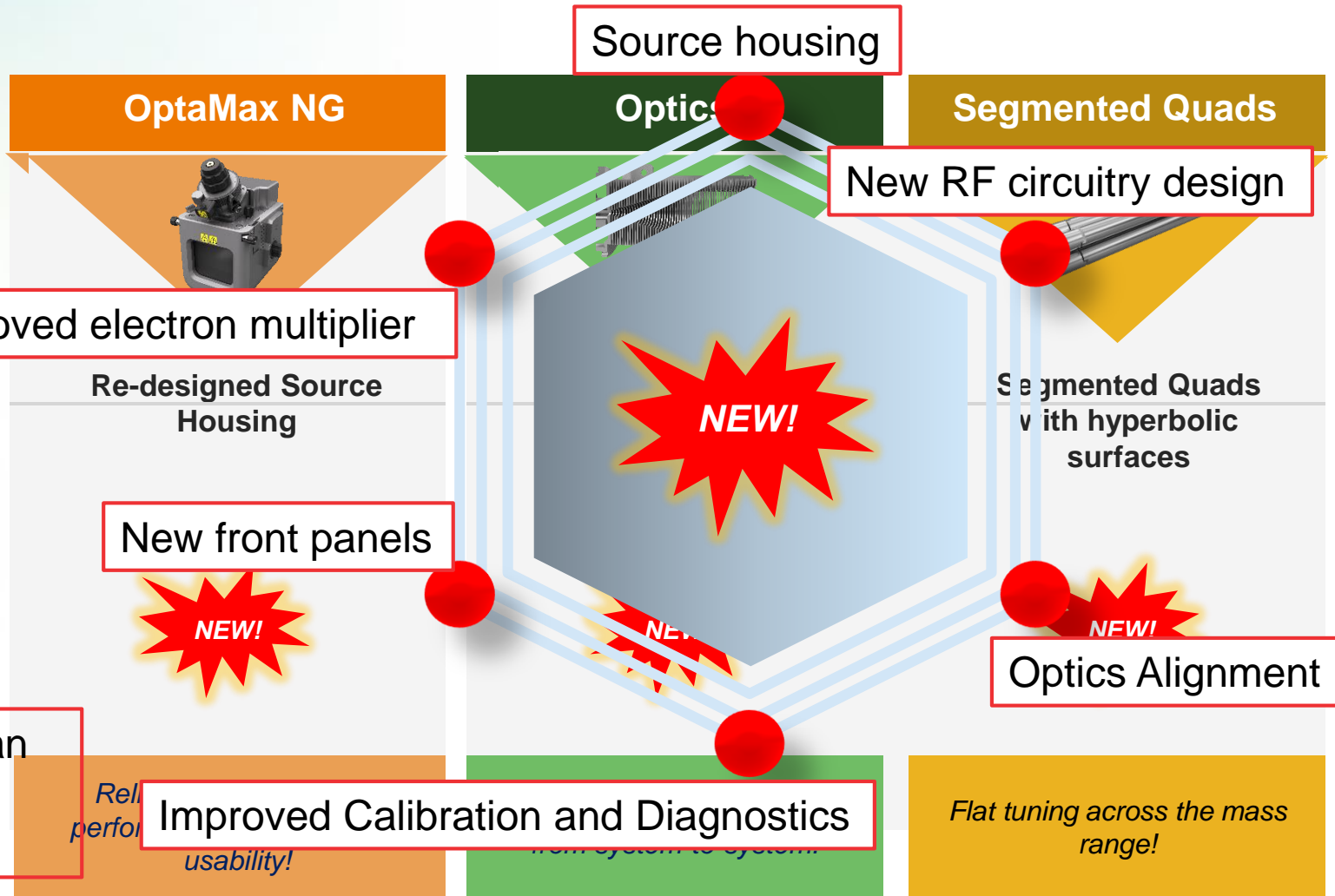
The ability to perform at the expected level (LOD, LOQ, MRL) under adverse conditions (complex samples, limited sample preparation) for the desired period of time without maintenance.

Consistency

The ability to report equivalent results every time independently of the system or the user (day-to-day and system-to-system)

Reliability

Increased time between service calls (mean time between failure- MTBF)
Increased uptime



Critical Resources Worth Looking At

<https://www.thermofisher.com/uk/en/home/industrial/environmental.html>

<https://www.thermofisher.com/uk/en/home/industrial/mass-spectrometry/liquid-chromatography-mass-spectrometry-lc-ms/lc-ms-systems/triple-quadrupole-lc-ms.html>

<https://appslab.thermofisher.com/>

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Testing robustness: Immunosuppres

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pesticides in food matrices
Pesticide Explorer Collection – Standard Quantitation

Authors
Katerina Bousova,¹ Michal Godula,¹

Goal
To present a fully tested LC-MS/MS methodology for rapid and robust

thermoscientific

Reduced injection volume applied to the quantification of cylindrospermopsin and anatoxin-a in drinking water according to EPA Method 545

APPLICATION BRIEF 64972

Authors
Ali Haghani,¹ Andy Eaton,¹
Nelson Wijeratne,² Claudia Martins²

Goal
To demonstrate a sensitive, accurate, and reliable LC-MS/MS methodology in the quantification of anatoxin-a and cylindrospermopsin in drinking water according to EPA Method 545, and to reduce the injection volume while maintaining adequate sensitivity.

¹Eurofins Eaton Analytical,
²

thermoscientific

Pesticides in Food: Targeted Quantitation Solution Guide

Your lab, your challenges—our solutions to help you address them

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Trace analysis of pharmaceuticals and organic contaminants in water

Instrument Type: LCMSMS

We present the reliable and accurate quantitative analysis of contaminants at the pg/mL level in drinking water using the Thermo Scientific EQuan MAX Plus LC-MS system coupled to the Thermo Scientific TSQ Endura triple quadrupole mass spectrometer. Excellent reproducibility was shown for the target compounds in tap water using 1 mL injections at 0.37x maximum effluent concentration.

Identification and Quantitation of Plastic Additives in Medicine Containers by HR LCMS, GCMS and ICPMS

Instrument Type: LCMSMS

Purpose: Identification and Quantitation of Plastics Additives in Medicine Containers by HR LCMS, GCMS and ICPMS. Methods: HR-LCMS, GCMS and ICPMS and data processing software. Results: Comprehensive analysis of extractable for medicine container by multiple techniques, and data analysis software. Confident component detection, unknown structure identification, and quantification were achieved.

Comparing LC and GC Triple Quadrupole MS for the Screening of 500 Pesticides in Matrix

Instrument Type: LCMSMS

Modern pesticide analysis is extremely challenging due to the diversity of compounds required to be reported, especially in the area of food safety control. The pressure to report large numbers of pesticides quickly makes it attractive to use large single injection methods. Triple quad MS has emerged as a primary screening technique due to its high sensitivity and selectivity against matrix. Presented is a comparison of both LC and GC sample introduction techniques coupled to triple q...

High-Resolution Accurate-Mass (HRAM) Phthalate Screening using Direct Analysis in Real Time (DART) Ambient Ionization

Instrument Type: MSMS

Phthalic acid diesters (PAEs), or phthalates, are widely used in industry as a plasticizer in products like toys, flooring, personal care products and food packages. Some PAEs are classified as hazardous, affecting mainly the reproductive system and possibly contributing to cancer. Though regulated, these phthalates might be present and used during production of goods. We demonstrate the possibility of using precursor ion selection and full scan MS2 spectrum, and utilize it as a finge...

Non-Targeted Screening of Lipophilic Marine Biotoxins by Liquid Chromatography-High-Resolution Mass Spectrometry

Instrument Type: LCMS

Marine biotoxins are produced by naturally occurring microalgae, whose populations can increase significantly under certain environmental conditions to form a harmful algal bloom (HAB). Marine biotoxins pose a significant food safety risk when bioaccumulated in shellfish that are ingested by humans. We describe the use of the Thermo Scientific Exactive benchtop LC/MS system powered by Orbitrap technology for screening lipophilic marine biotoxins commonly found in shellfish. The...

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without compromise. The TSQ Altis es segmented quadrupoles with crete-dynode electron multiplier M) for unprecedented sensitivity, analytical flexibility, reproducibility, every analytical laboratory to olications.

C-MS

ne TSQ Quantis Triple Quadrupole y robustness and the sensitivity to ed quadrupoles, an enhanced dual-ector, and high-resolution SRM (0.4 itivity with outstanding robustness eted quantitation workflow

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