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Thermo Scientific TSQ 9000 – Unstoppable Routine Analysis

EPRW 2018

Paul Silcock, GC GC-MS

TSQ 9000 GC-MS/MS

Ultimate **sensitivity** with Advanced Electron Ionization

Incredible **uptime** with inherent robustness and NeverVent™ technology

Routine **ease of use** from method development to daily operation

True **scalability** for growing laboratory requirements

UNSTOPPABLE

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Perfect for today, ready for tomorrow

- Grows with laboratory requirements
- Base to advanced configurations
- Full field upgrade path

Ultra high performance and robustness
TSQ 9000 AEI

High-throughput solution
TSQ 9000 NeverVent EI & CI

High-throughput solution
TSQ 9000 NeverVent EI

Affordable performance
300L/s ExtractaBrite

Most accesible entry from SQ>TQ
240L/s ExtractaBrite

Reaching into the attogram range

ag
10^{-18}

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Inheriting from the ExtractaBrite ion source

- Highly inert material
- Independent dual heater
- Proprietary RF lenses
- Dual filament design

Adding innovative design for superior sensitivity and robustness

- Highly efficient ionization
- Tightly focused ion beam
- Detection into the attogram range

ag
10^{-18}

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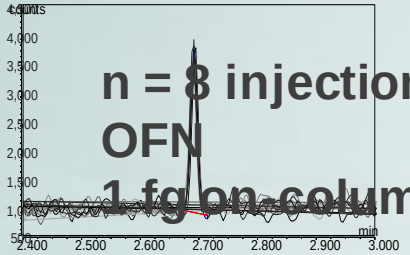
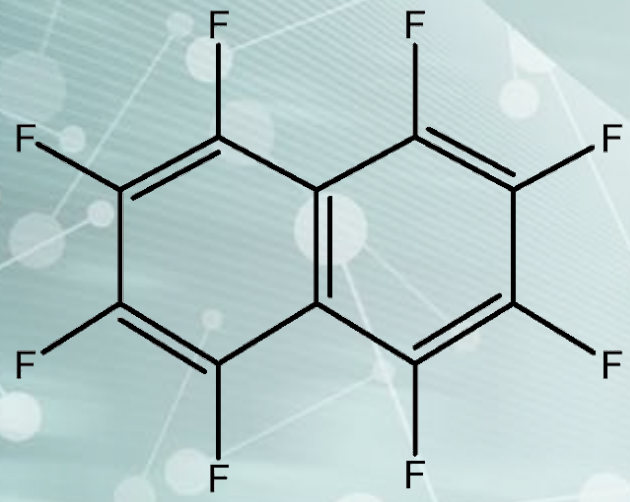
AEI Sensitivity Octafluoronapthalene (OFN)

IDL performance of the TSQ 9000 (AEI) for OFN using repeated injections of 1 fg on-column



n = 8 injections
OFN
1 fg on-column

IDL_{RSD} = 120 ag



*IDL <0.4 fg verified at installation under predefined conditions

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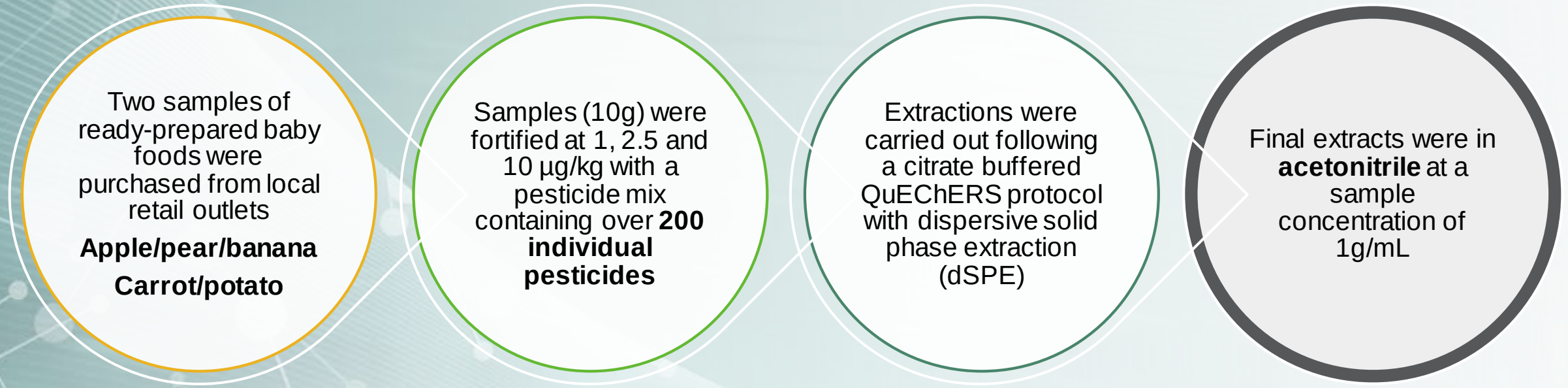
Pesticides in Baby Food : Sample preparation



Software

Thermo Scientific™ Chromeleon™ 7.2 Chromatography Data System (CDS) software was used for instrument control, data acquisition, processing and reporting.

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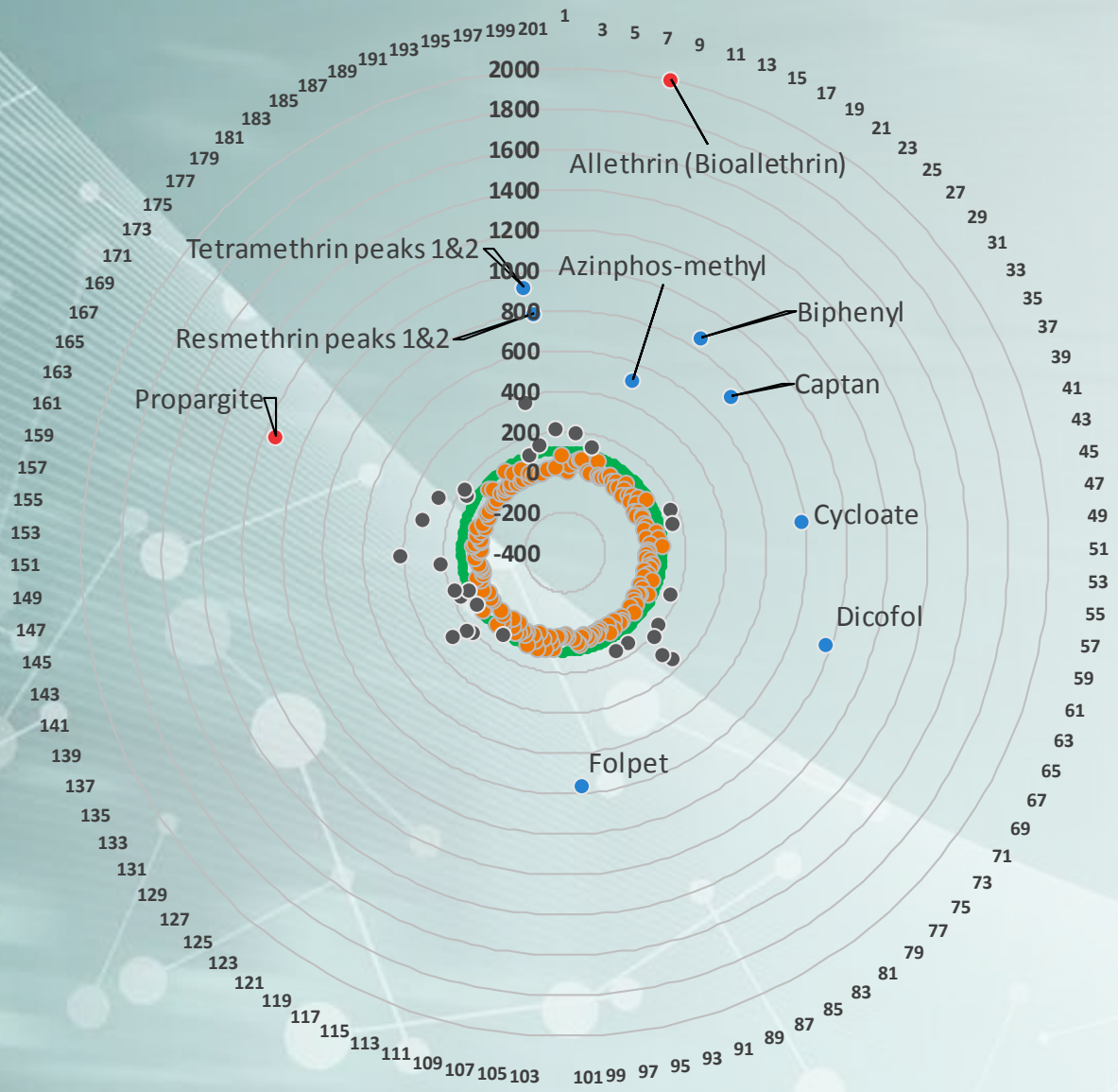
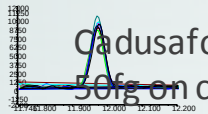
Instrumental detection limit (IDL)

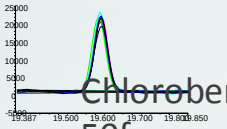


- 100 fg
- IDL (5 - 100 fg)
- IDL (100 - 500 fg)
- IDL (0.5 - 1.0 pg)
- IDL (1.0 - 2.0 pg)



Cadusafos, 50fg on column

10 replicate injections
RSD 4.7%
IDL – 7 fg on-column



Chlorobenzilate, 50fg on column

10 replicate injections
RSD 3.2%
IDL – 5 fg on-column

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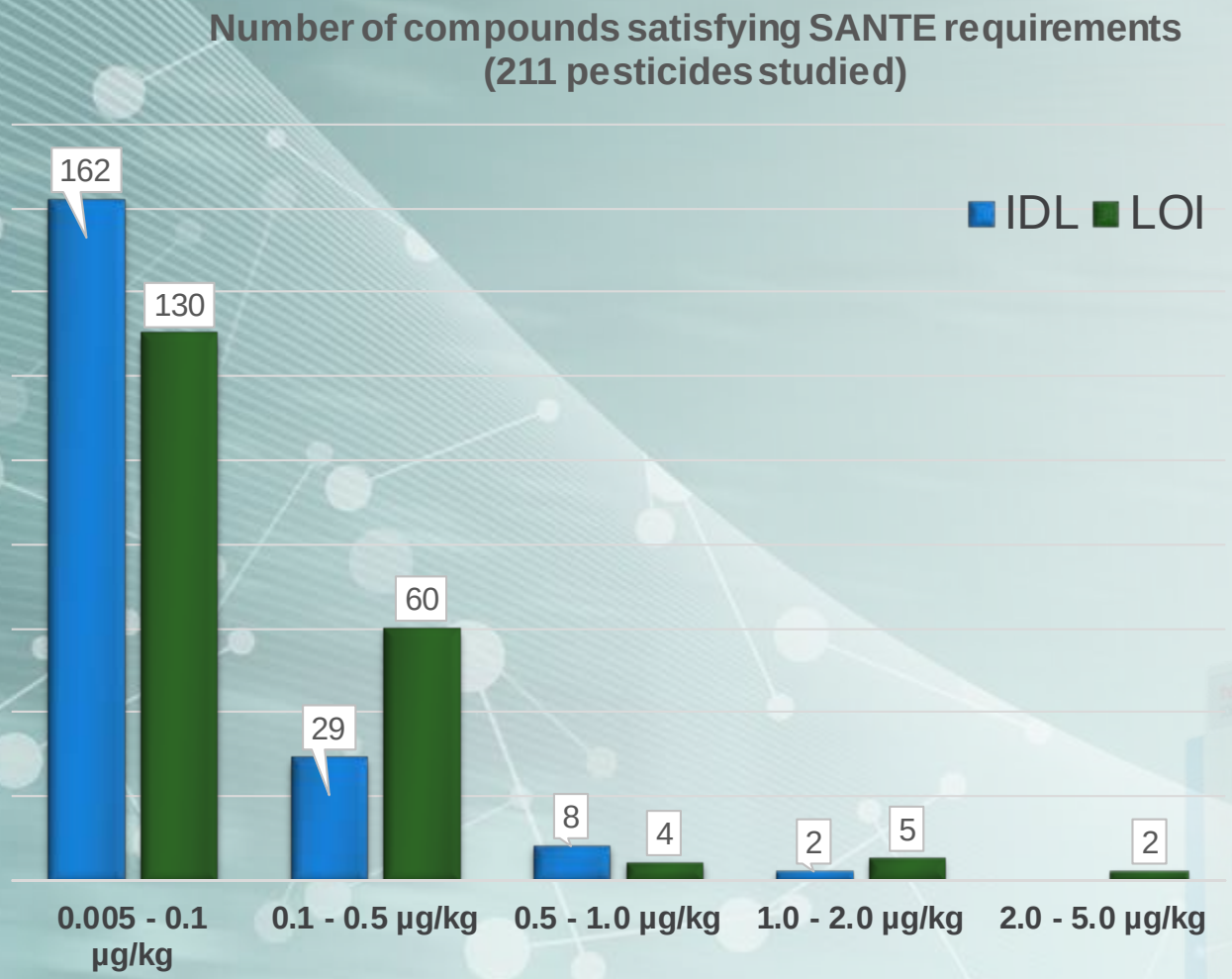
AEI Pesticides in Baby Food - Limit of detection and identification



>60% identified <0.1 µg/kg – 100 x lower than default maximum residue limit (MRL)

>90% identified <0.5 µg/kg – 20 x lower than default maximum residue limit (MRL)

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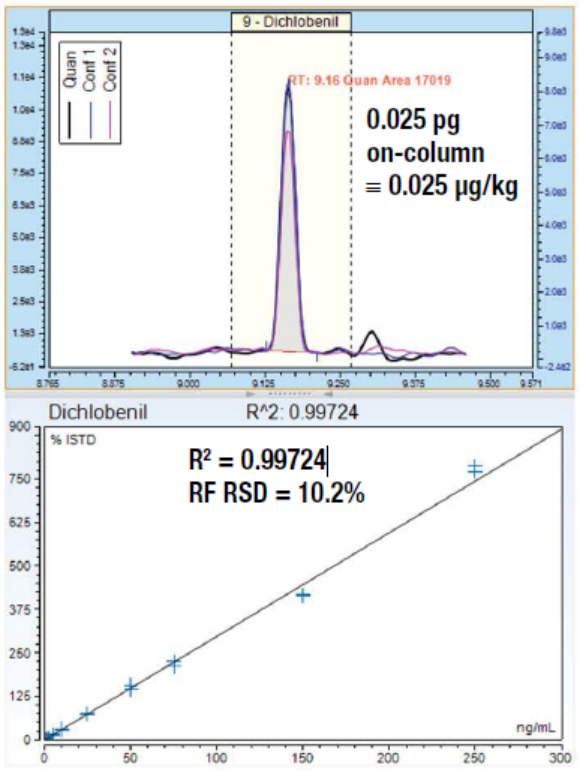
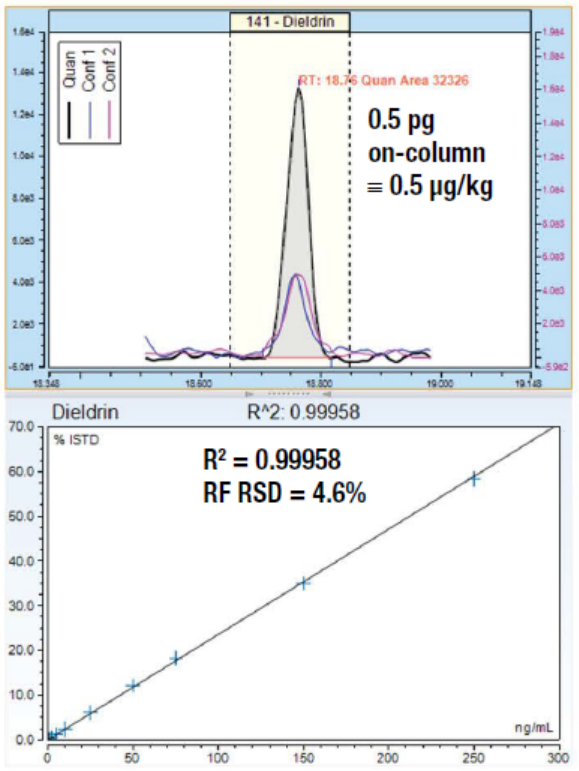
AEI Pesticides in Baby Food

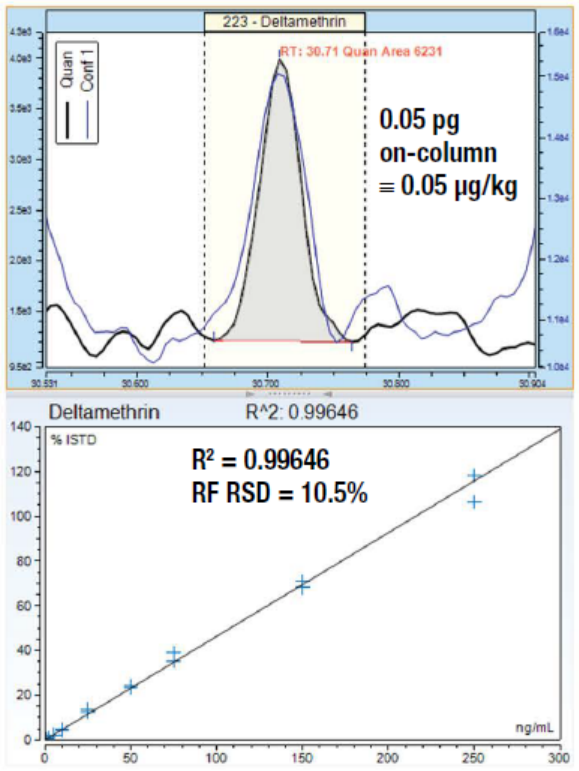
Dichlobenil – MRL 10 µg/kg



Dieldrin– MRL 3 µg/kg



Deltamethrin– MRL 10 µg/kg



Lowest detectable matrix matched standard which meets SANTE identification requirements

Calibration curves
0.025 to 250fg on column
Duplicate injection at 14 levels

Low level detection and identification and quantitative linearity

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Linearity

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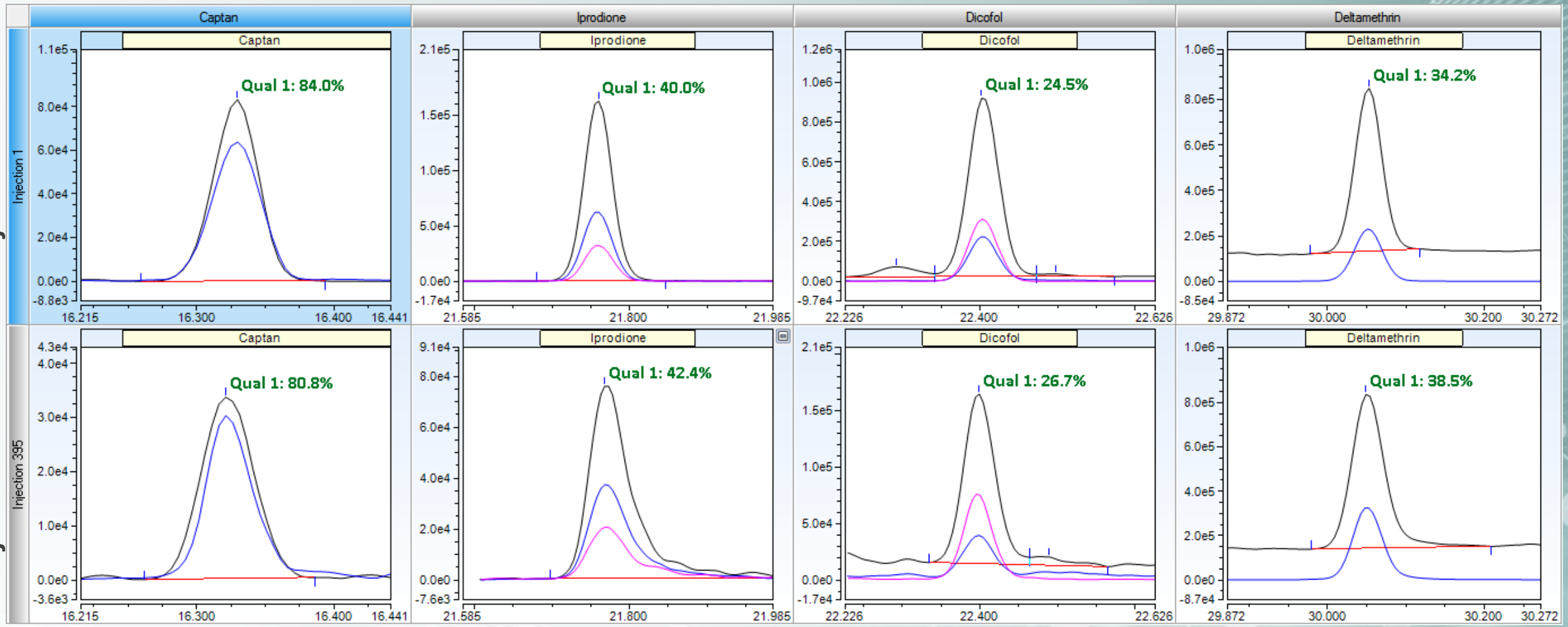
Repeatability of SRM ratio - Challenging pesticides



Sample - 10 µg/kg carrot/potato extract

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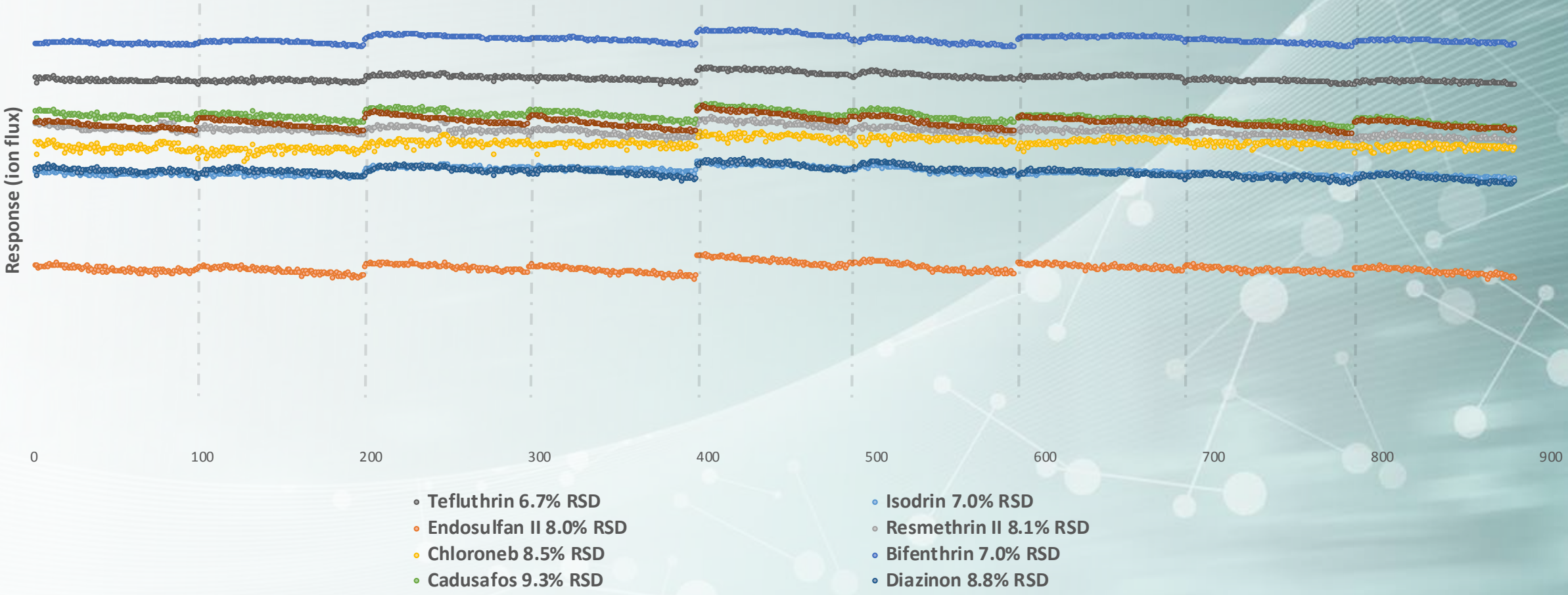
AEI Robustness ~900 Acetonitrile QuEChERS Injections

150 pesticides monitored at 10 ppb in **carrot and potato baby food**

Liner change and SmartTune every ~100 injections

No AEI source cleaning →

<20% RSD for >90% of pesticides monitored



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The Impact of TSQ 9000 AEI for Routine Analysis

Ultra robust

Remain in result production for longer

Ultra high sensitivity

- Take less sample
- Reduce / remove preconcentration
- Dilute extracts
- Inject less / split injection

Measure more comfortably current compounds

Address toughest detection limit challenges

Reduced

- Source cleaning

Reduced

- Sample prep time & cost
- Matrix pressure on system
- GC inlet & column maintenance
- Source cleaning

Reduced

- Manual peak reintegration
- Reanalysis for quality issues

Increased

- Uptime
- Result production
- On time delivery
- Quality
- Margins
- Analytical scope
- Confidence

Authors
Richard Law, Aaron Lamb, Paul Silcock, and Cristian Cojocariu

Thermo Fisher Scientific, Runcorn, UK

Keywords
TSQ 9000, advanced electron ionization, AEI, baby food, sensitivity, robustness, pesticide residue, QuEChERS, triple quadrupole mass spectrometry, GC-MS/MS, Programmable Temperature Vaporization, food safety

Goal
The aim of the study was to assess the quantitative performance of the Thermo Scientific™ TSQ™ 9000 triple quadrupole GC-MS/MS system fitted with the Advanced Electron Ionization (AEI) source for the analysis of pesticide residues at ultra low levels in baby food.

Introduction
The detection and subsequent quantification of pesticides, contaminants, and other chemical residues are of paramount importance, especially when the food stuff is intended to be consumed by infants or young children. The maximum residue level (MRL) for the majority of pesticide-commodity combinations is set at the default level of 10 µg/kg.[1–3] However, the European Union (EU) has established LOD MRLs between 3–8 µg/kg for specific pesticides prohibited in baby foods.[4] These pesticides and their metabolites may cause infants and young children (under worst-case intake conditions) to exceed the acceptable daily intake (ADI) values. The high sensitivity and selectivity of GC-MS/MS enables the detection and identification of residues of prohibited compounds, in compliance with the residue definitions, even when dealing with the diverse composition of multi-ingredient baby foods.

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Routine-grade robustness with the Advanced Electron Ionization source: confirmation of contaminants in food products at trace levels by GC-MS/MS

Authors
Richard Law,[1] Paul Silcock,[1] Tim Anderson,[2] and Cristian Cojocariu[1]

[1]Thermo Fisher Scientific, Runcorn, UK
[2]Thermo Fisher Scientific, Austin TX

Keywords
Advanced electron ionization, AEI, robustness, pesticides, triple quadrupole mass spectrometry, GC-MS/MS, SmartTune

Goal
The aim of this study was to demonstrate the robust and routine performance of the Thermo Scientific™ TSQ™ 9000 triple quadrupole GC-MS/MS system with Advanced Electron Ionization source for the analysis of pesticide residues in food matrix.

Introduction
In today's modern, high-throughput analytical laboratory, instrument downtime can have a significant impact on laboratory productivity. Analysts working in such fast-paced environments are required to investigate large numbers of samples and to deliver accurate and valid results consistently. Having to disrupt this process causes sample turn-around times to increase and, as a result, the cost per sample to surge.

The advent of gas (and liquid) chromatography with triple quadrupole mass spectrometry (GC-MS/MS and LC-MS/MS) increased selectivity and drove detection limits down, reducing the requirement for sample clean-up and leading to quicker, cheaper methods (ex. QuEChERS[1]). However, these sample preparation methods often allow for more of the matrix to make its way into the chromatographic system and the ionization source, affecting the system robustness and increasing the maintenance intervals. Without a highly sensitive and robust ion source, detector responses can quickly drop off, leading to quality control (QC) failures, higher detection limits, and ultimately a failure to deliver acceptable and compliant results. Ensuring that the analytical systems used for these workflows are rugged enough to deal with the challenges faced is of the utmost importance to the user.

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ISQ 7000 GC-MS and TSQ 9000 GC-MS/MS

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