Introducing the P&EP 3.0

GC/MS/MS Pesticides and Environmental Pollutants Analyzer

Confirming Pesticide Residues with Confidence

May 2014

How Many Pesticides Are There?

> 1600 parent compounds

+ metabolites, degradation products and impurities

The Pesticide Manual, 16th Edition, 2012

Pesticide Multi-Residue Analysis
Motivation

- **Food safety and regulations to protect public**
- **Need for analysis of a large number of analytes**
- **Unknown “history” of the analyzed sample (field treatment, post-harvest application, contamination)**
- **Economic aspects (costs, time, and labor)**

Pesticide Residue Analysis

Drivers – Governance of Pesticide Use

Maximum Residue Limits – Amount On or In Food

Tolerance – Level that Triggers Enforcement Action

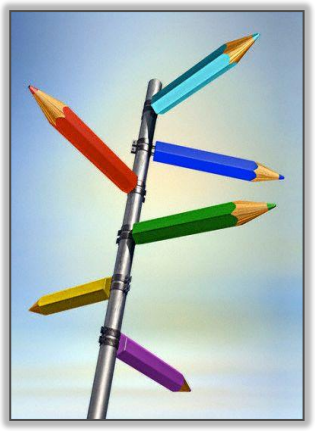
Safety – Toxicity of pesticide and breakdown product

Use – Reasonable Certainty of "No Harm"

Pesticides Residue Analysis

The Analytical Iceberg

Pesticide Multi-Residue Analysis



Classical approach:

Multiple methods and techniques to cover different analytes/classes of interest

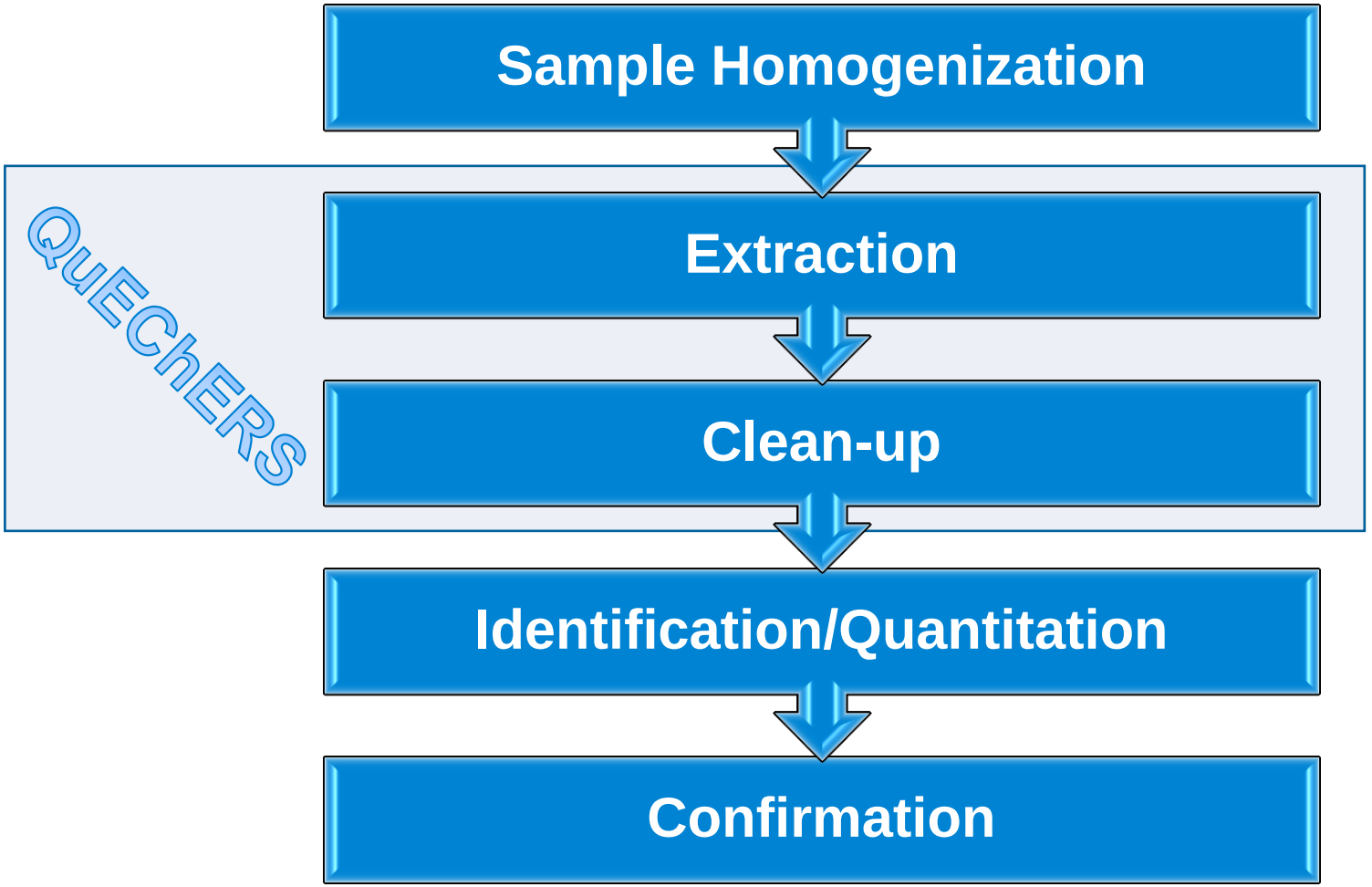
e.g.: GC-FPD, NPD, ECD, ELCD
LC-UV or LC-FLD

Modern approach:

Multi-analyte methods with simultaneous quantification and identification using

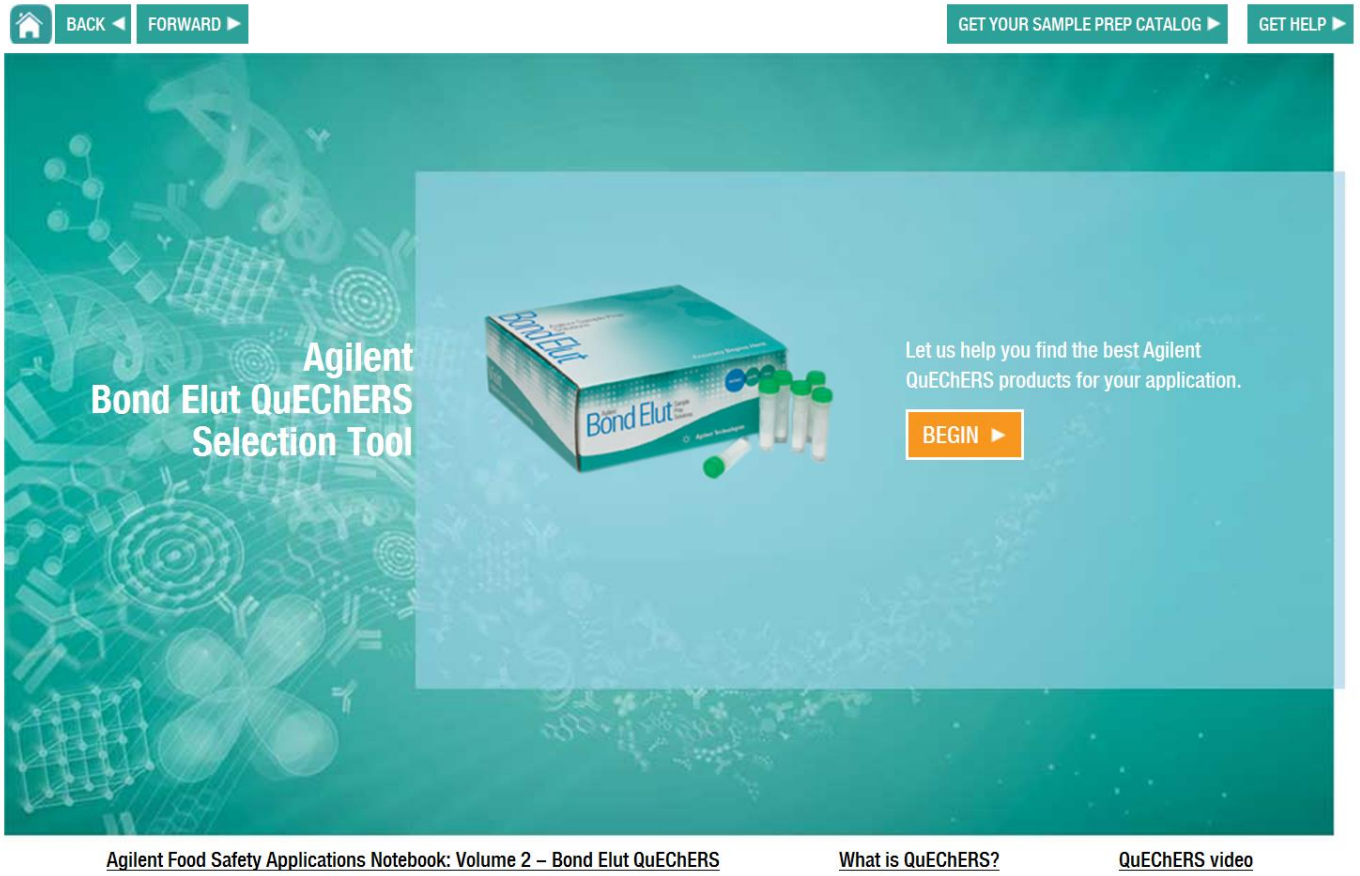
GC-MS and **LC-MS**, especially with **MS/MS** capabilities for increased selectivity

Pesticide Multi-Residue Analysis



QuEChERS = Quick, Easy, Cheap, Effective, Rugged, and Safe

The Bond Elut QuEChERS Selection Guide



www.agilent.com/chem/selectQuEChERS

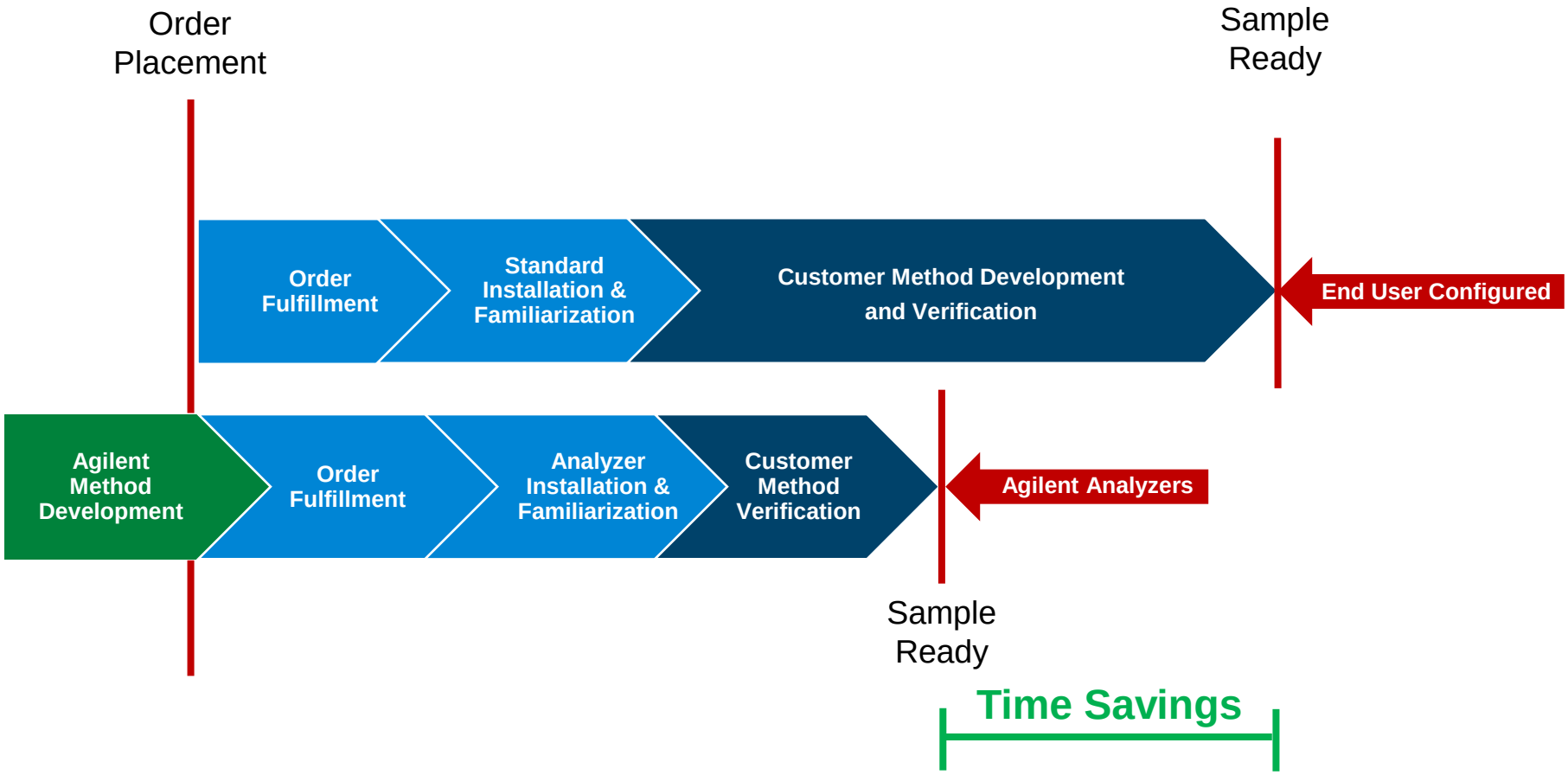
The Agilent Pesticide Analysis Reference Guide
Available from Your Local Agilent Representative

P&EP 3.0
GC/MS/MS Pesticides Analyzer

Get Customers on the Analytical ***FAST TRACK***

Customer Concerns

Confident Identification of Pesicide Residues



…Faster Application Startup with a Guaranteed Method

The Pesticide Analyst Needs

Agilent Analyzer Solutions

Customer's Responsibility

Agilent's Analyzers Provide

Customer's Responsibility

Feature Elements for P&EP 3.0 Analyzer

GC/MS/MS Pesticides and Environmental Pollutants Analyzer

- **MRM database** with **~1100** compounds and **~8500** optimized transitions including 710+ pesticides and breakdown products
- **GUI** that facilitates building MRM acquisition and quantitation methods based on *customer's compound list*
- **Retention Time Locked** separation for reliable peak identification and quantitation for CF and CP BF methods
- **Multimode inlet** for large volume injection helps optimize detection limit performance
- **Opt 114 UI S/SL** for when there is no requirement for optimal LOD performance
- **Capillary Flow Technology Backflush** for faster cycle time and reduced system maintenance

Key

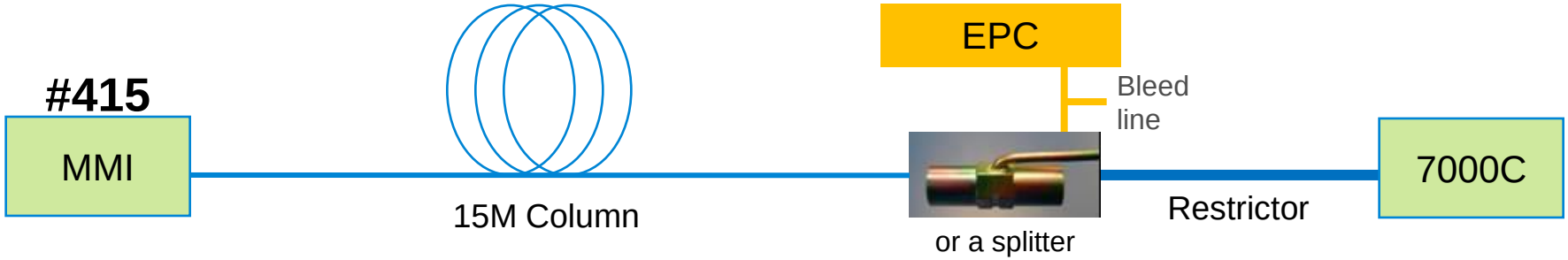
NEW

NEW

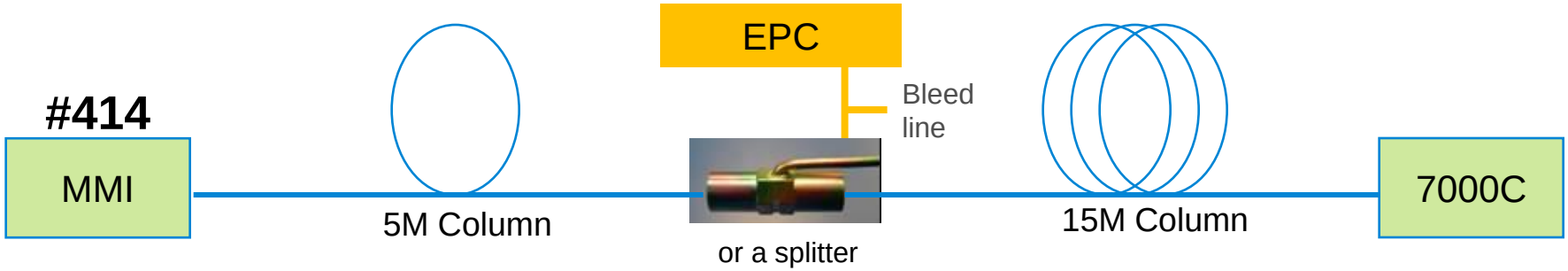
Pesticide & Environmental Pollutant Analyzer 3.0

P&EP 3.0 New Method Configurations – **Constant Pressure** and **Constant Flow** Modes

– post-column backflush components

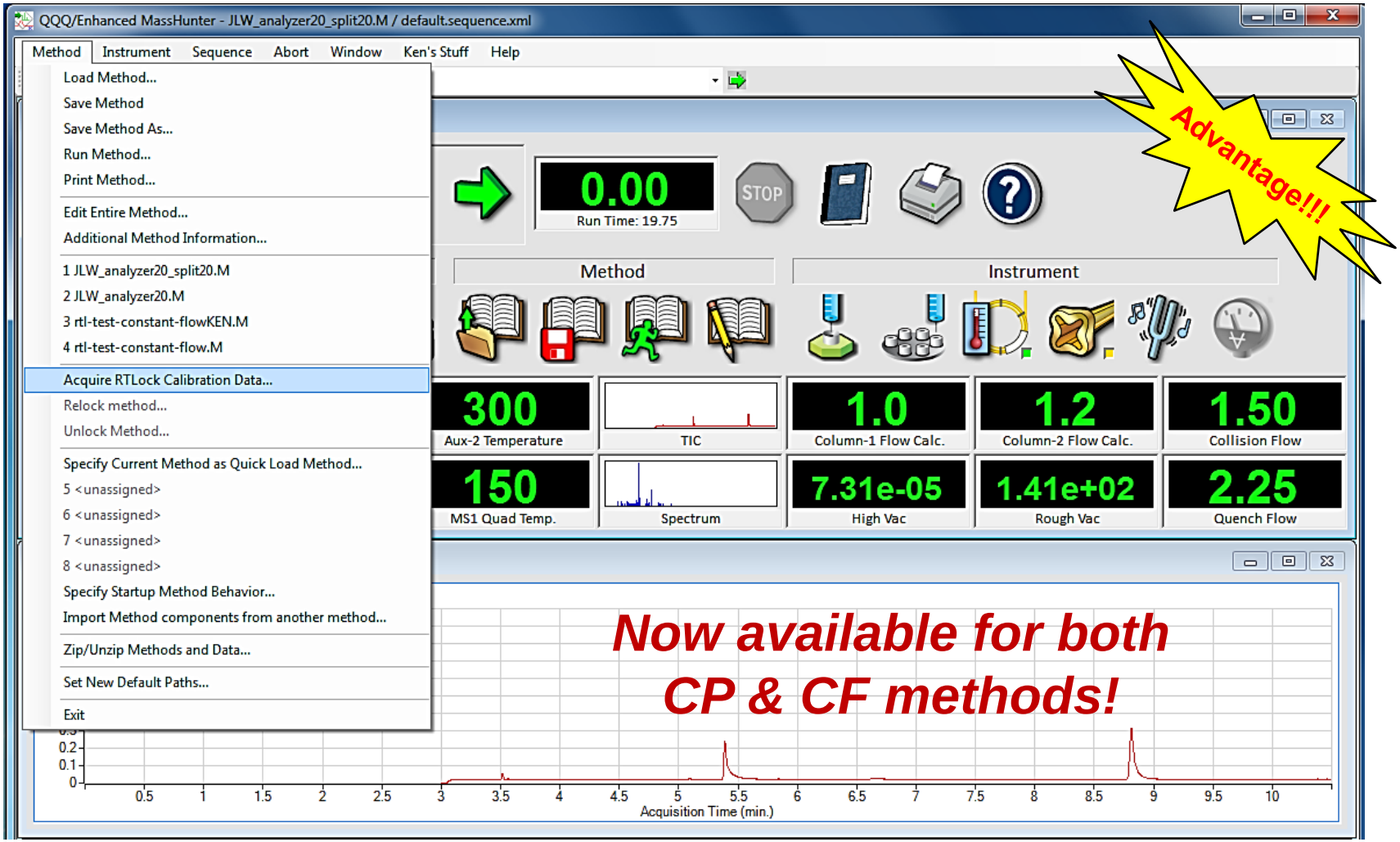


Flexibility to add GC detectors and easily scaled for shorter runtime



Provides ultimate performance and shortest cycle time

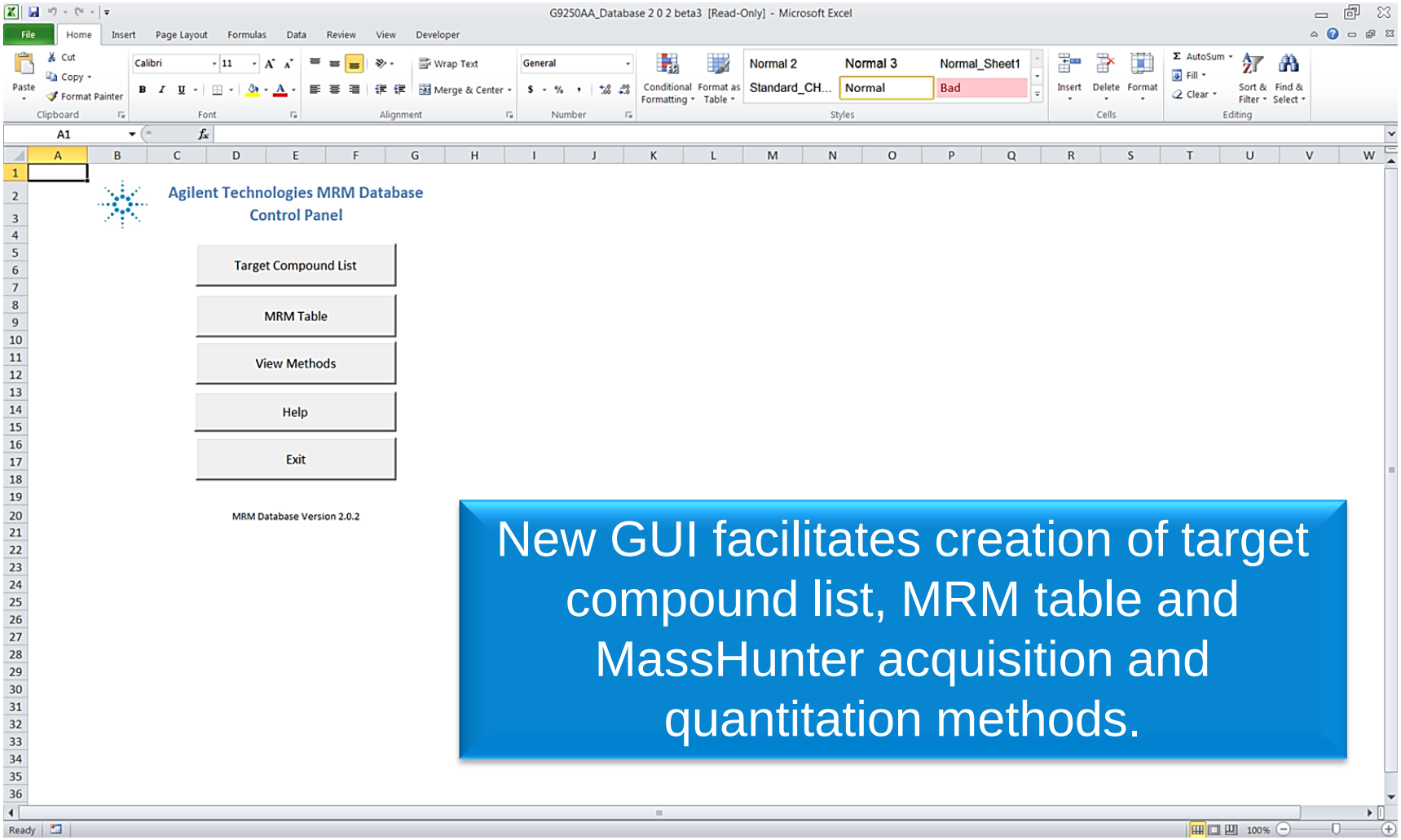
Acquire Retention Time Locking (RTL) Calibration Data



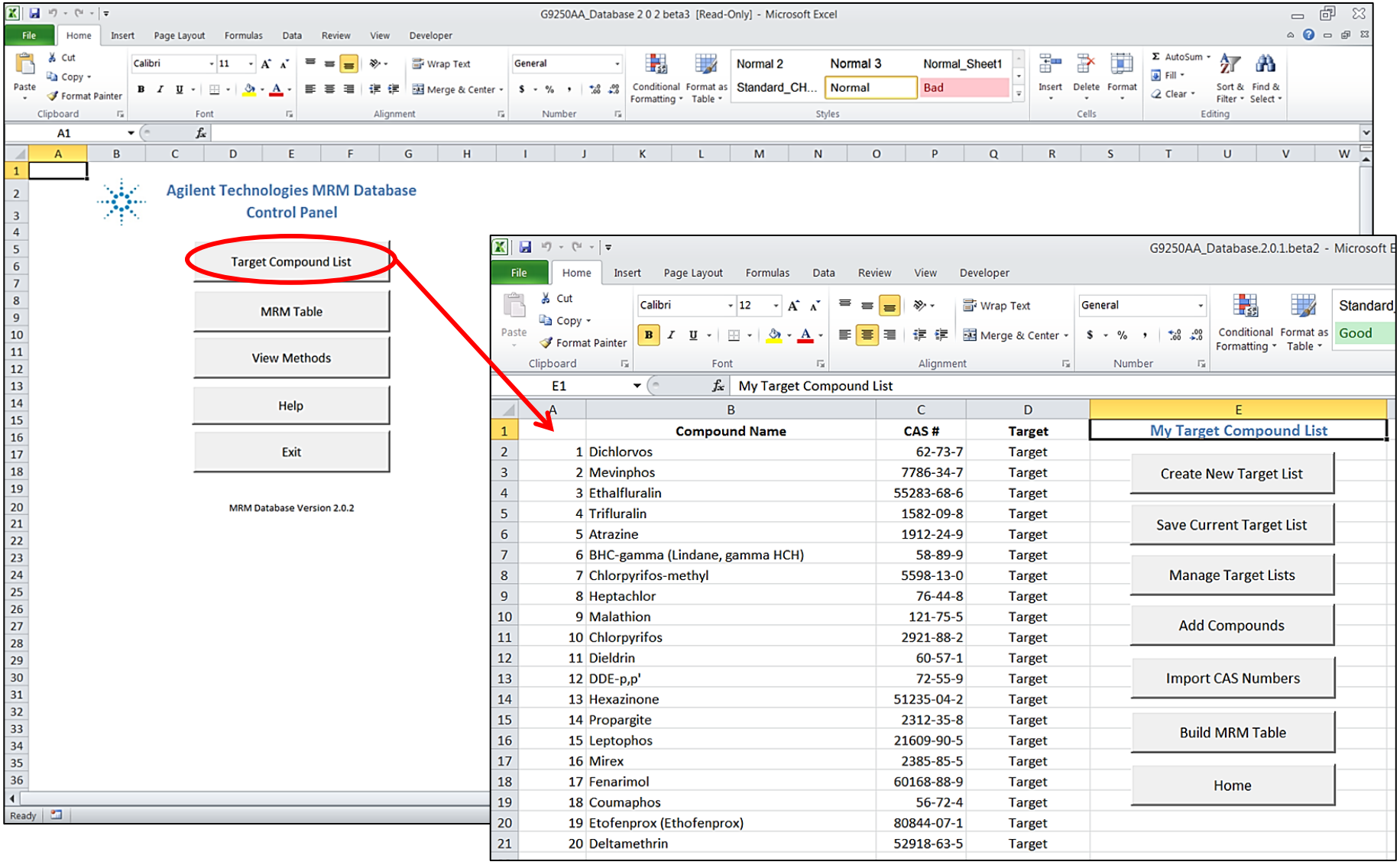
Note: In this example, the acquisition is in full-scan mode.

Home Screen of the MRM Database

Sure it's an Excel file, but…



View of “Target Compound List”

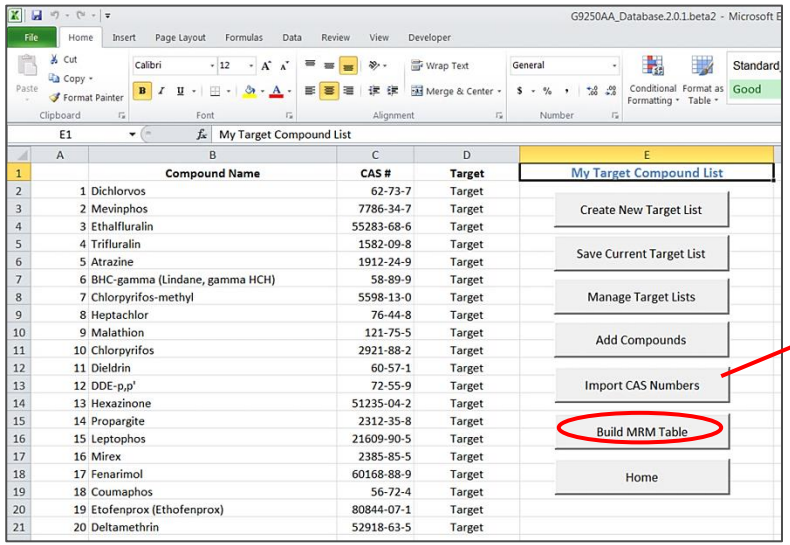


	Compound Name	CAS #	Target
1	Dichlorvos	62-73-7	Target
2	Mevinphos	7786-34-7	Target
3	Ethalfluralin	55283-68-6	Target
4	Trifluralin	1582-09-8	Target
5	Atrazine	1912-24-9	Target
6	BHC-gamma (Lindane, gamma HCH)	58-89-9	Target
7	Chlorpyrifos-methyl	5598-13-0	Target
8	Heptachlor	76-44-8	Target
9	Malathion	121-75-5	Target
10	Chlorpyrifos	2921-88-2	Target
11	Dieldrin	60-57-1	Target
12	DDE-p,p'	72-55-9	Target
13	Hexazinone	51235-04-2	Target
14	Propargite	2312-35-8	Target
15	Leptophos	21609-90-5	Target
16	Mirex	2385-85-5	Target
17	Fenarimol	60168-88-9	Target
18	Coumaphos	56-72-4	Target
19	Etofenprox (Ethofenprox)	80844-07-1	Target
20	Deltamethrin	52918-63-5	Target

Build MRM Table

Step 1 – Select Method of Choice

Step 2 – Select Quant & Qualifier ions



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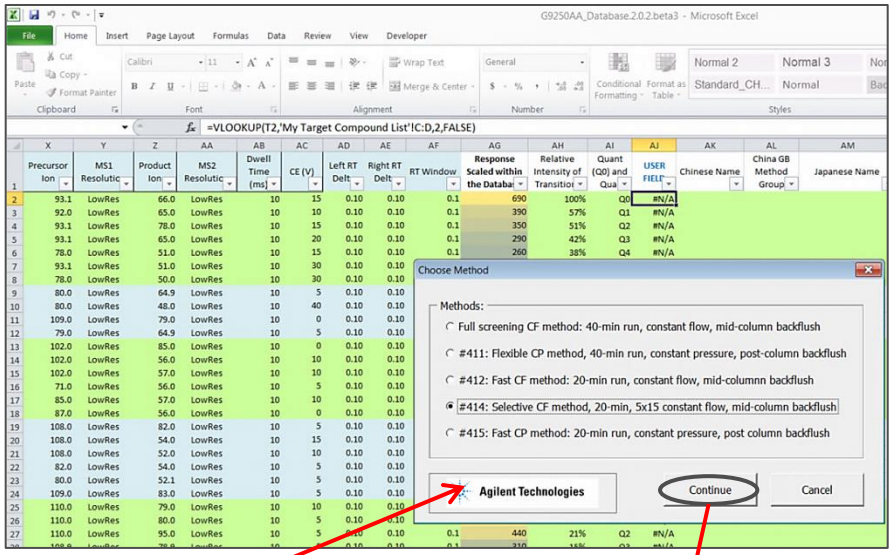
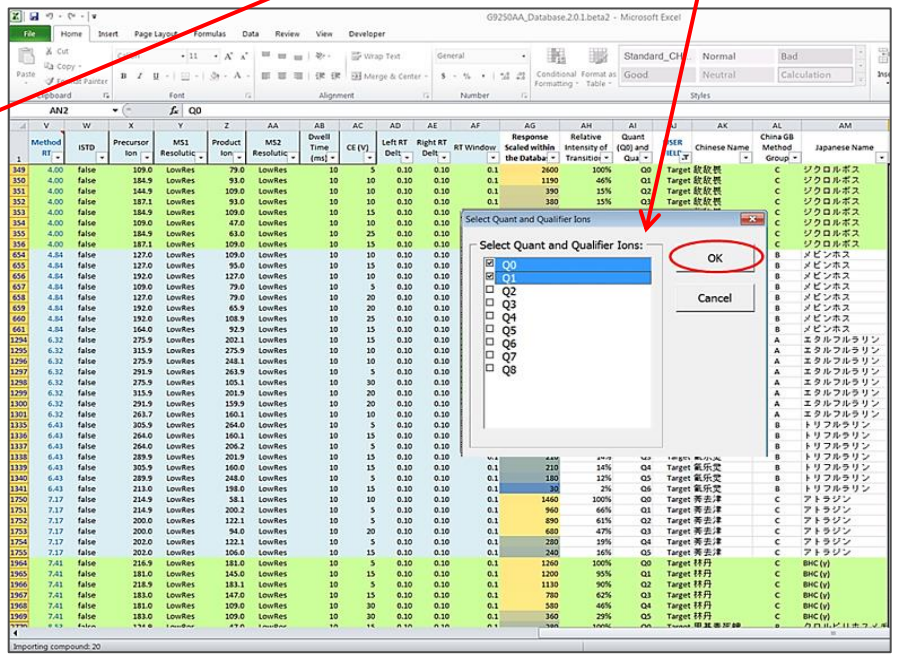
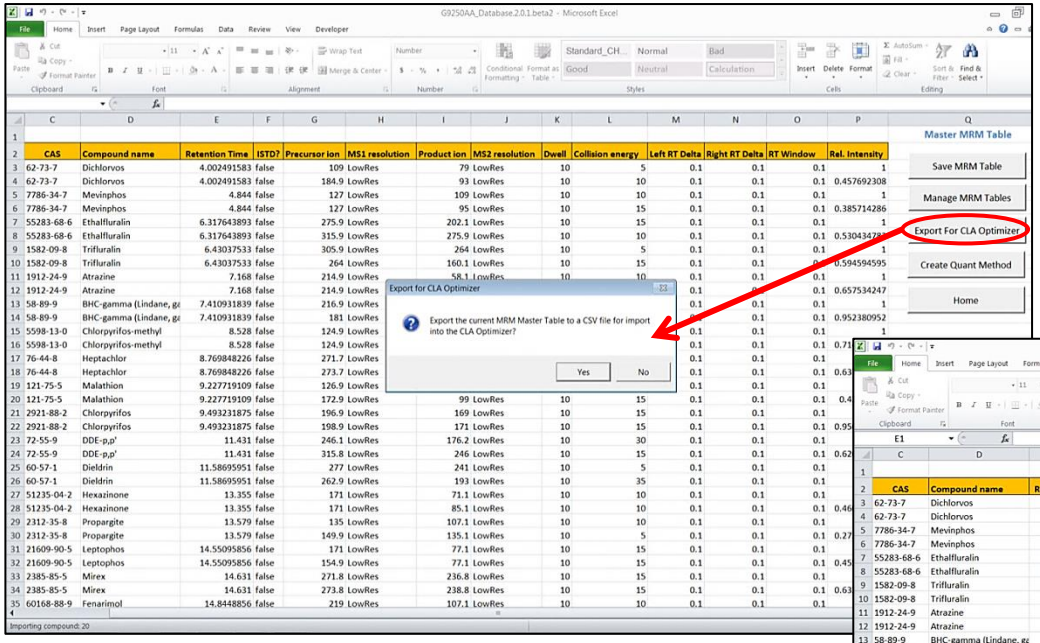




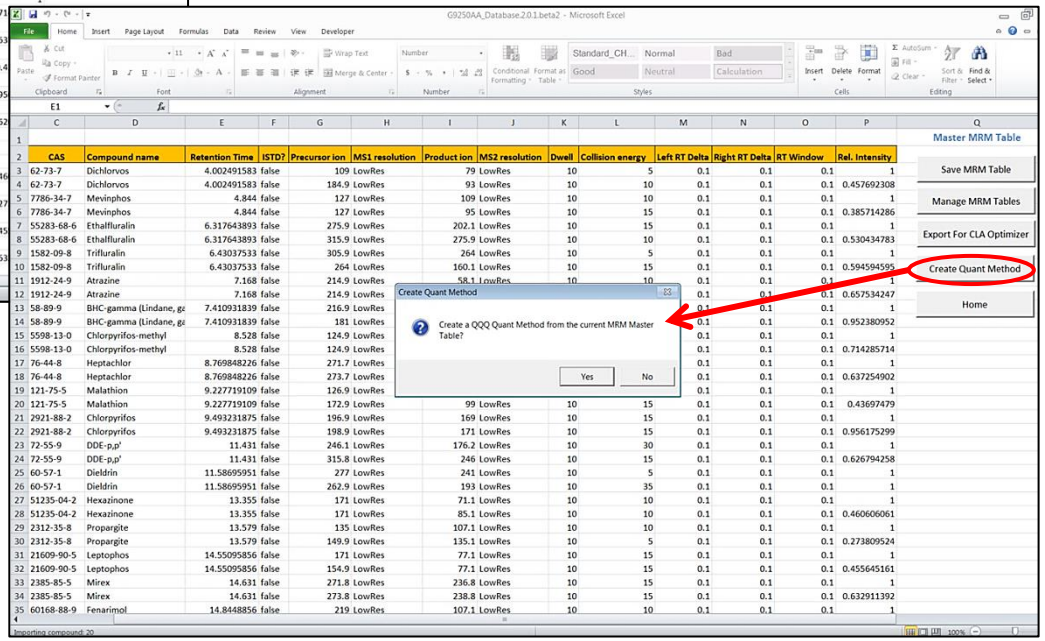
Develop MassHunter Methods

Easy interface to MassHunter Method Development Tools



MRM Acquisition Method

via MH Compound List Assistant (**CLA**)



MH Quantitation Method

via the MRM database

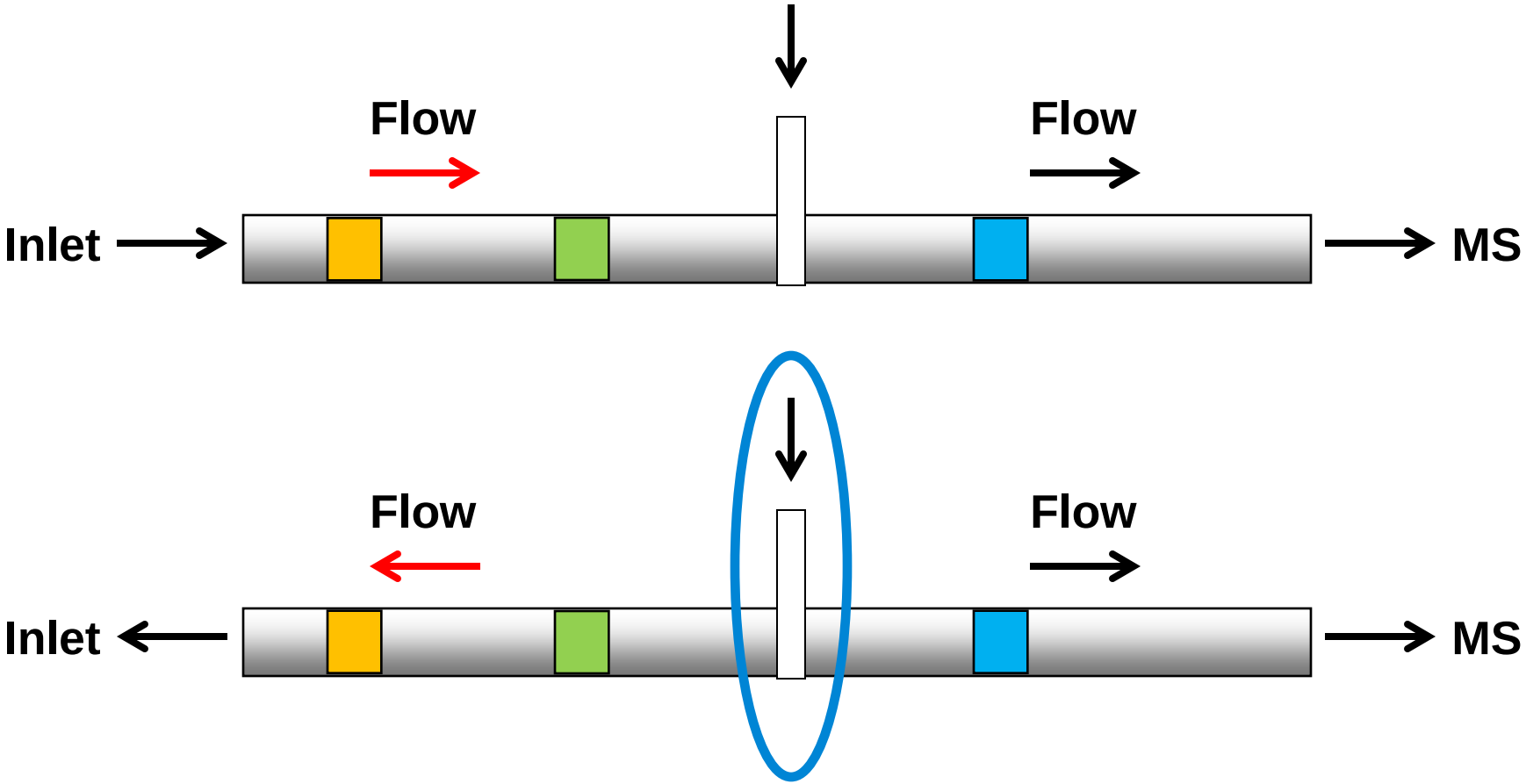
P&EP 3.0
GC/MS/MS Pesticides Analyzer

Value Overview and Summary

The Measure of Confidence

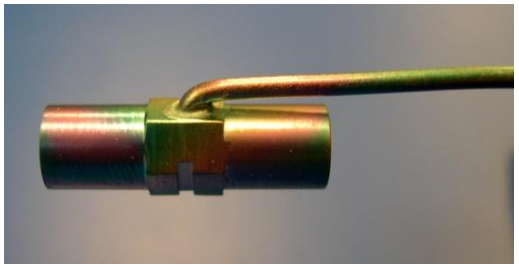
Column Backflush

Eliminates less volatile matrix components from the GC column by reversing the column flow at a pressure junction point:

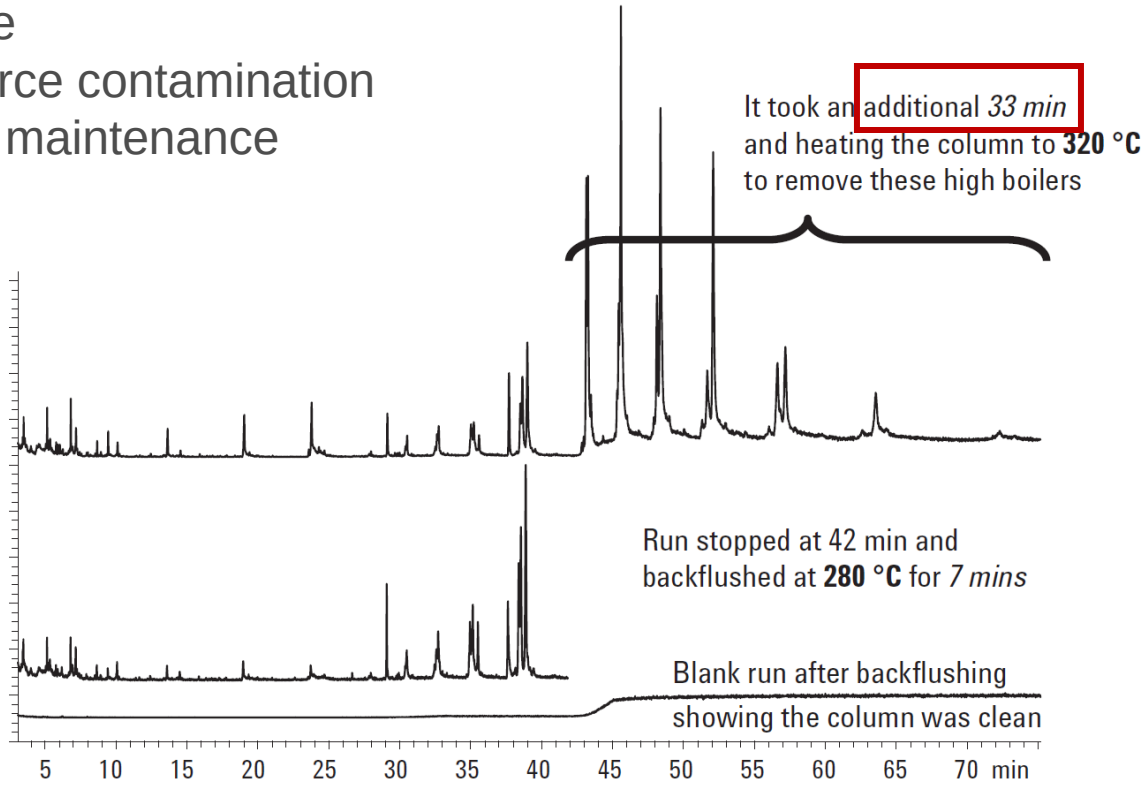


Column Backflush - Benefits

- Elimination of long “baked out” at a high temperature to remove less volatile, late eluting matrix components
- Reduced analysis time
- Increased column life time
- Prevention of the MS source contamination
- Less frequent MS source maintenance

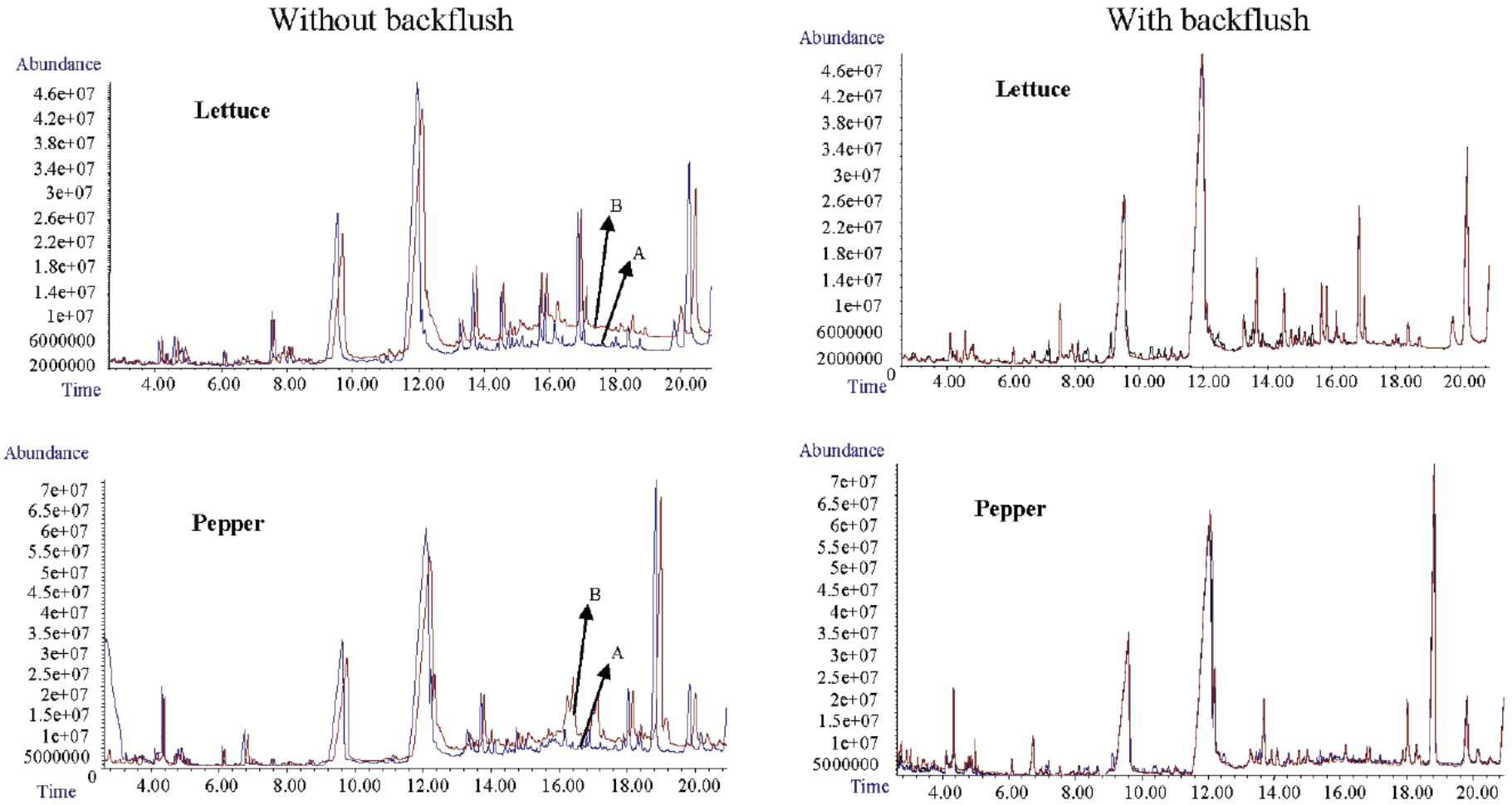


Purged Ultimate Union



C.-K. Meng, Agilent Application Brief 5989-6018EN

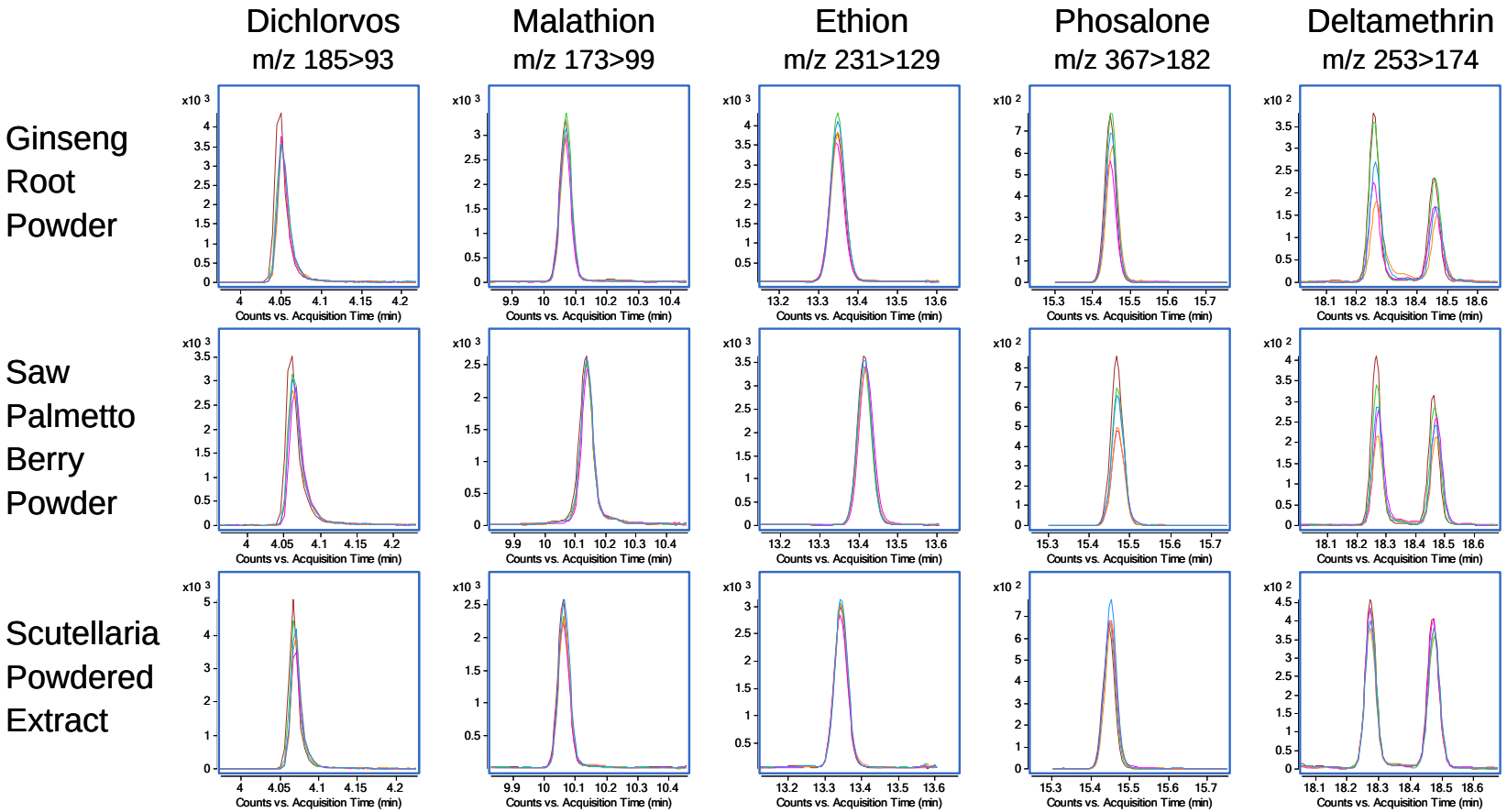
Column Backflush - Benefits



M. Mezcua, M.A. Martinez-Uroz, P.L. Wylie, A.R. Fernandez-Alba, *J. AOAC Int*. **92** (2009) 1790-1806.

Column Backflushing - Benefits

Overlays of GC-MS/MS chromatograms for selected analytes (at 50 ng/g) obtained within a 2.5-day sequence of 125 dietary supplement sample injections

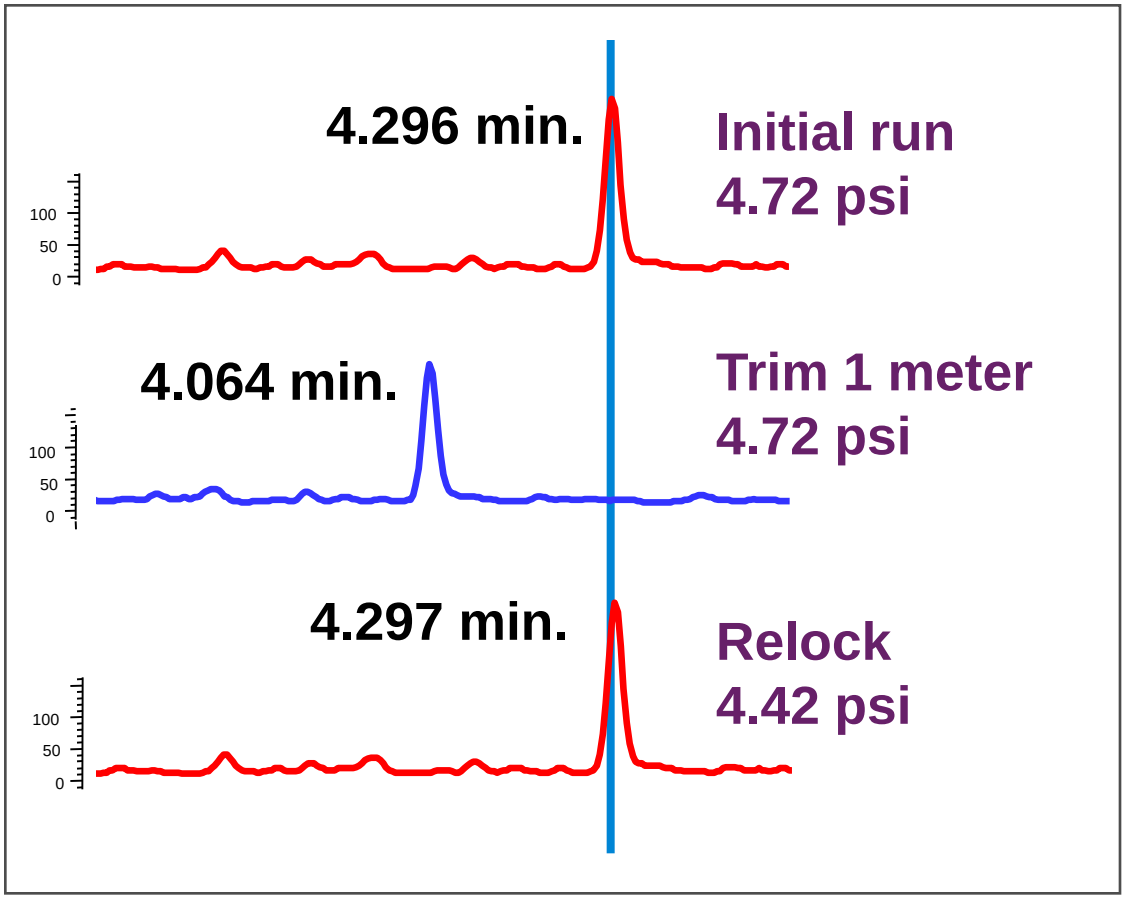


K. Mastovska and P.L. Wylie,
J. Chromatogr. A **1265** (2012) 155-164

Retention Time Locking (RTL)

Improve Confidence with Retention Time Locking

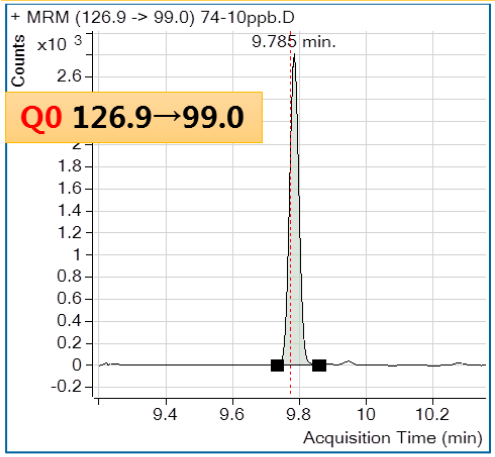
- **MRM Spectrum Unchanged**
- **Troubleshooting**
- **Repeatability**
  - Run-to-run
  - Operator-to-operator
  - Instrument-to-instrument

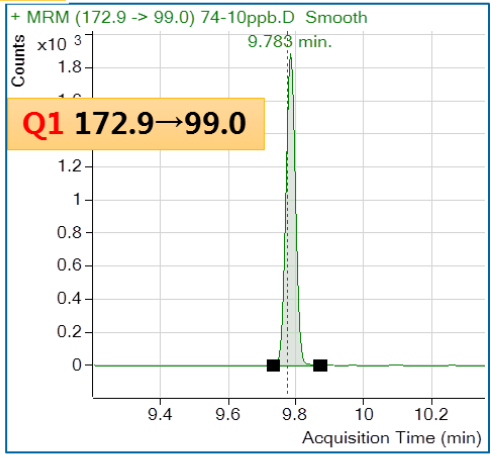


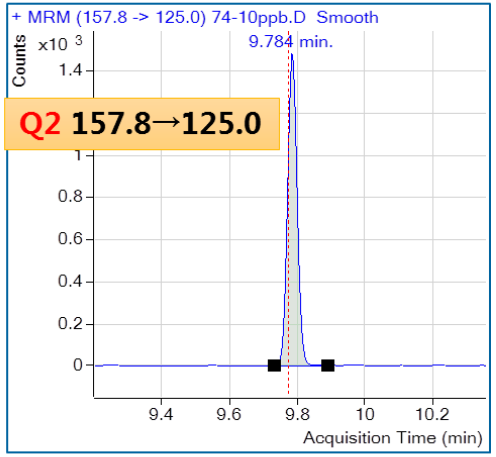
Importance of MRM Transitions

Malathion Identification

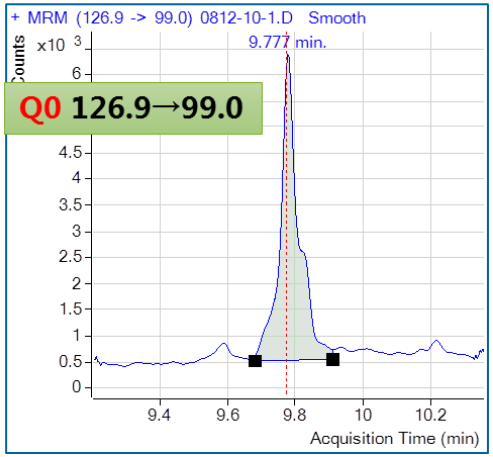
Malathion 10ppb standard MRM

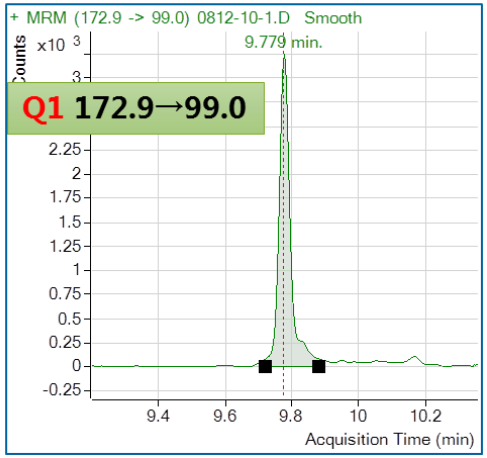


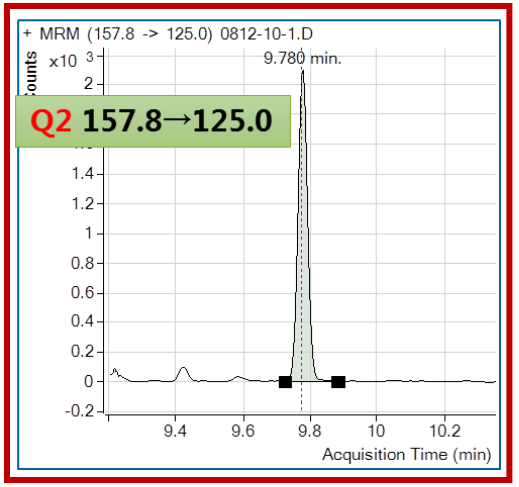




Malathion10ppb MRM spiked in sample



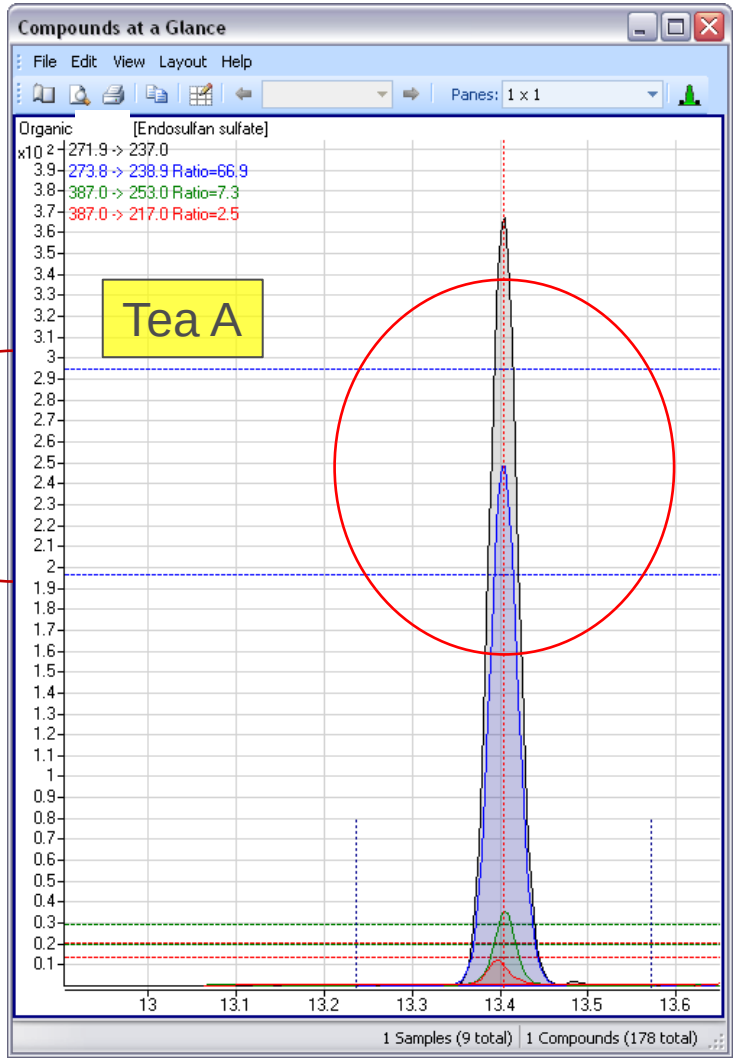




Why are MRM Transitions Important?

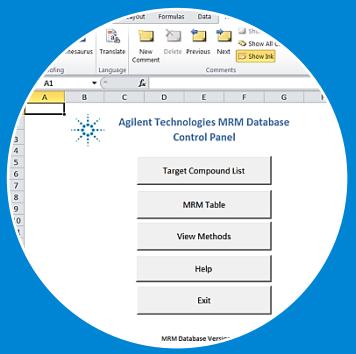
Endosulfan Sulfate (?) in Tea Extract – Two (2) Transitions

- Rerun of data
- Ion Ratio within 80-120% confidence band
- CONFIRMED!!



- Demonstrates the value of multiple optimized transitions in the MRM Database.
- Not just to avoid matrix interferences but also for additional confirmation!

GC/MS/MS Pesticide Analyzer
Value Overview

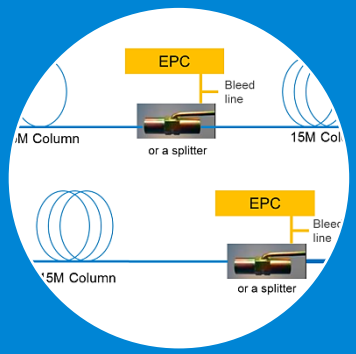


Powerful MRM Database

- The most Comprehensive and Flexible MRM database!
- New User Interface that streamlines the creation of custom MRM acquisition and quant methods.

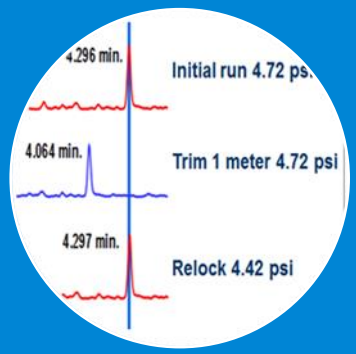
MultiMode Inlet (MMI)

- Large volume injection helps optimize LOD performance
- Opt 114 UI S/SL for customers that do not require for optimal LOD performance



Includes New Analytical Methods

- Expands analysis options:
  - Constant Pressure methods: #411 & #415
  - Constant Flow methods: #412 & #414



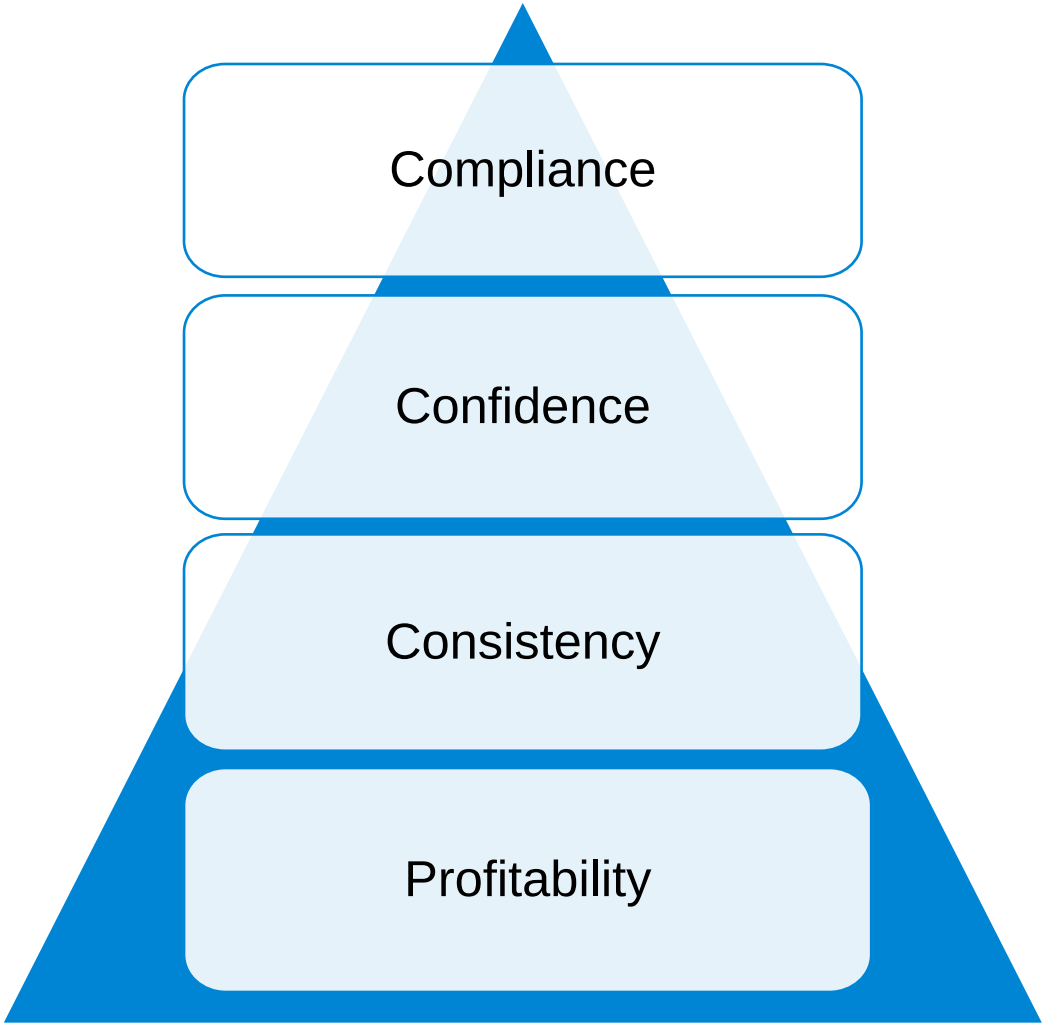
Auto RTL for CFT BF Methods

- Auto RTL for CF and CP BF method
  - Facilitates relocking methods

Accurately confirm target pesticides while reducing the time required from start-up to results

Agilent GC/MS/MS Pesticide Analyzer

Confident Identification of Pesticide Residues



Questions…

Thank you for your attention

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