Expanding Lab Capability using Agilent’s GC/QQQ Analyzer with a New Versatile 1000-compound Pesticide MRM Database

-- “Ready to Go” Analyzer based on the most comprehensive MRM database

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What is a Pesticide GC/MS/MS Analyzer?

A pre-configured and chemically tested GC/TQ system loaded with methods and a 1000-compound Pesticide MRM database for quick installation and start-up.

**Backflush:** reversing the column flow

- Hot split/splitless
- Cold splitless
- Solvent vent (LVI)
Pesticide Analyzer System Configuration

**SP1 7890-0501 Setup**

- **Inlet**
- 30 m
- **EPC**
- 1000-compound MRM Database
- **MS**
- **Constant Pressure Post-column Backflush**

Flexible to add GC detectors and easily scaled for shorter runtime

**SP1 7890-0502 Setup**

- **Inlet**
- 15 m
- **EPC**
- **Purged Ultimate Union**
- **15 m**
- **MS**
- **Constant Flow Mid-column Backflush**
- 1000-compound MRM Database

Provides ultimate performance and shortest cycle time
Why Do We Need Backflush?

• With the selectivity of MS/MS, users cannot see “dirty matrix”

• MS/MS users want the LOWEST detection limits – inject more with large volume injection

• Many late eluting peaks are not “chromatographically ideal” and leave a residue throughout the column

• Heavy matrix contaminates the source faster --- performance is LOST!

Backflush ensures the highest data quality with GC/MS/MS!
The trade-off is 10-20% decrease in sensitivity.
10% Fish Oil In Acetone: Retention Time Shifts Eliminated With Backflushing

10 Runs without Backflushing: Retention times shift ~4-5 sec during 10 runs

10 Runs with Backflushing: RT shift eliminated
Milk Extract - Using Bakeout To Remove High Boilers

Cleaning out high boilers is a real problem.

Run time > 75 min to clean out the column.

Oven ramps to 320°C to bake off late eluters.

RT range of analytes.
Backflush

During GC Run

Split Vent Trap
Inlet
Aux EPC
4 psi
MSD

25 psi

Column

Purged Ultimate Union

After GC Run

Split Vent Trap
Inlet
Aux EPC
60 psi
MSD

2 psi

Column

Purged Ultimate Union
Heavy Compounds May Be Left in Head of Column After Each Injection

These heavy materials build up and travel further into the column with each injection.

This buildup of heavy materials causes retention time shifts, peak distortion, higher bleed, and loss of sensitivity.
Backflushing After Each Injection

Backflushing removes heavy materials after each injection.
Milk Extract

Once correct backflushing time is chosen, it will work for ALL high boilers thereafter, because heaviest elute first.

It took additional **33 mins** and column to **320°C** to remove these high boilers.

Run stopped at 42 min and backflushed at **280°C** for **7 mins**

Blank run after backflushing

Column is clean.
Backflush: Many Advantages for GC/MS(/MS) Analysis of Complex Samples (‘Dirty Matrices’)

- Provides more consistent GC retention times
- Provides better, more consistent MS spectra through sequence
  - Reduces chemical noise that due to small carryover of matrix
  - Higher quality quantitation without increase in interfering ions
- Reduces contamination for the source
- Reduces analysis time
- Increases lifetime of analytical column
Benefits of Agilent GC/MS/MS Pesticide Analyzer

- **Retention Time Locking**: No need to update the time segment RTs after a column maintenance.

- **Multimode inlet (MMI)**: Injector adds flexibility by including standard, cold split/splitless, solvent vent (LVI) capabilities.

- **Capillary Flow Technology (CFT) and backflush**: Shorter analysis time, more consistent retention times and spectra, longer column life, and less frequent source cleaning -- **improve uptime**.

- **MS/MS MRM Database**: Optimized and flexible MRM database of hundreds of compounds.

- **Pre-config. and factory setup analyzer**: Factory setup and checked out on pesticide mixture - ready to generate results on Day One.
But…

How does the Analyzer work with the list of target pesticides in my lab?
Agilent’s New Comprehensive MRM database with Extensive Flexibility

- **Contains 7000 optimized MRMs for 1000 pesticides**
  - over 3000 injections on $70,000 worth of **chemical standards**

- **Extensive flexibility allows method optimization**
  - average of 7 MRM transitions with relative intensity for each compound
    - provides alternatives to avoid matrix interference
  - compound classification, CAS number etc. in excel format
    - allows **easy searching and sorting** for method customization
  - three chromatographic methods (constant flow or pressure) with Retention Time and Retention Index
    - allows maximum freedom to follow **customer’s workflow**
  - absolute intensity for each MRM transition
    - allows **semi-quantitation** without standards
The Flexibility: 7 transitions; classifications; 3 RTs and RIs

Database has RTs (and RIs) to be used with three GC methods (CP, CF, and CF-screening).

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Average and exact Molecular Weight

Each pesticide is classified in two categories
The Flexibility: Excel format, relative and absolute Transition intensity

MassHunter Format

The absolute and relative intensities of transitions

(Color Scales): Red denotes strong intensity and blue denotes weak intensity among ALL transitions.

One Quant and several Qualification ions for each compound

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Click on the sorting button to show/hide Quant and Qualifier Ions
Use the sorting function to quickly select a Quant (Q0) and top three Qualifier ions (to build a method)!

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<td>202.0</td>
<td>Wide</td>
<td>20</td>
<td>10</td>
<td>360</td>
<td>12%</td>
<td>Q3</td>
<td>エトキシシリン</td>
<td></td>
</tr>
<tr>
<td>28</td>
<td>Dicloran (Dichloran)</td>
<td>FALSE</td>
<td>206.0</td>
<td>Wide</td>
<td>176.0</td>
<td>Wide</td>
<td>20</td>
<td>15</td>
<td>2480</td>
<td>100%</td>
<td>Q0</td>
<td>二クロラン</td>
<td></td>
</tr>
<tr>
<td>29</td>
<td>Dicloran (Dichloran)</td>
<td>FALSE</td>
<td>207.9</td>
<td>Wide</td>
<td>178.0</td>
<td>Wide</td>
<td>20</td>
<td>15</td>
<td>1560</td>
<td>83%</td>
<td>Q1</td>
<td>二クロラン</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>Dicloran (Dichloran)</td>
<td>FALSE</td>
<td>214.0</td>
<td>Wide</td>
<td>73.1</td>
<td>Wide</td>
<td>20</td>
<td>15</td>
<td>1410</td>
<td>47%</td>
<td>Q2</td>
<td>二クロラン</td>
<td></td>
</tr>
<tr>
<td>31</td>
<td>Dicloran (Dichloran)</td>
<td>FALSE</td>
<td>216.1</td>
<td>Wide</td>
<td>148.0</td>
<td>Wide</td>
<td>20</td>
<td>15</td>
<td>1100</td>
<td>44%</td>
<td>Q3</td>
<td>二クロラン</td>
<td></td>
</tr>
</tbody>
</table>
Click on the sorting button to select/show the compounds to be added into the acquisition method.

It is easy to add a column to associate each compound with a lab method or study to allow a quick sort to build an acq. method.
Why Do We Need More than 2 MRM Transitions?

Signal-to-Noise Ratio Comparison for MRM Transitions in Spinach and Orange

MRM transitions

- 215 → 58
- 200 → 94
- 173 → 138
- 215 → 200
- 200 → 122

Dash Lines are Absolute Responses (area)
Solid Lines are Signal/Noise

- 50 ppb Spinach, resp.
- 50 ppb Orange, resp.
- 50 ppb Spinach, S/N
- 50 ppb Orange, S/N

S/N
Atrazine
Responses (area)
MRM Transitions are not Universal, Should Choose them According to Matrices
Summary: Pesticide GC/MS/MS Analyzer

The Pesticide GC/MS/MS Analyzer is tested as a unit in the factory to ensure a quick and successful installation.

New flexible and comprehensive Pesticide MRM Database expands the target compound list to 1000 to meet users’ need.

The MRM Database:

- allows users to build acquisition methods without acquiring expensive or hard-to-get pesticide standards (saves time and money);
- applies to either constant flow or constant pressure method (adapts to user’s preference or analytical method);
- has multiple MRM transitions (average 7) for each compound (helps to provide alternatives to work around matrix interference);
- shows relative intensity of each MRM transition (facilitates transition selection and acquisition method creation).