Finding Non-targeted (Unknown) Pesticides Using GC/MS and LC/Q-TOF

Chin-Kai Meng, Ph.D.
Applications Chemist
Wilmington, Delaware

chin_meng@agilent.com
302-633-8388
Outline - Workflow for Non-targeted Pesticides Analysis

• Business Issues and Challenges
  • Sample Prep (QuEChERS) – Lehotay, Anastassiades and Mastovska
  • GC/MSD
  • (GC or LC)-QQQ
  • LC/Q-TOF
Business Issues and Challenges

- Global trade increases the number of pesticides to monitor (> several hundreds)
- Regulation driving lower detection limits
- Speed: doing more analyses in a day
- Need for fast startup
GC-MSD Workflow

GC/MS (PTV) SIM/Scan
– for known and unknown

Deconvolution (+backflush)

Screen
Confirm
Quantify

Final Report
TICs of Surface Water Extracts

How many pesticides (drugs, allergens etc.) are in these samples and how long does it take you to confirm?
17 Surface Water TICs (Scan): Pesticide Analysis Using DRS with Pesticide Database (927 entries)

<table>
<thead>
<tr>
<th></th>
<th>CDFA*</th>
<th>Agilent DRS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Targets Found (not counting ISTD)</td>
<td>37</td>
<td>Same 37 +99 more</td>
</tr>
<tr>
<td>False Positives</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Processing Time</td>
<td>~8 hrs</td>
<td>32 min</td>
</tr>
</tbody>
</table>

DRS: Deconvolution Reporting Software

*CDFA is the California Department of Food and Agriculture

Saving 7.5 hours
What is Deconvolution?

“...in the broad sense of extracting one signal from a complex mixture...” (From AMDIS)

There are four deconvoluted components under the white TIC.
AMDIS

Automatic Mass spectral Deconvolution and Identification System

• Developed by the National Institute of Standards and Technology (NIST)

• Developed to detect chemicals in violation of Chemical Weapons Convention (must minimize false positives and false negatives in reporting)

• Used to identify target compounds in complex matrices
How Does Deconvolution Work?

50 75 160 170 185 280 310
Eliminate Ions Don’t Fit the Criteria

Ion grouping criteria:
1. Same RetTime at apex
2. Same peak width

Extracted Ion Chromatograms (EIC)
Spectrum is Deconvoluted/Cleaned

Related ions are grouped together as a component.
More than 370 peaks found.

TIC of Spinach Extract

Deconvolution

Library Search
The power of deconvolution is appreciated while comparing the top two spectra (raw scan and the compound spectrum hidden in the raw scan).
Scan at 10.776 min

Deconvoluted/extracted spectrum

A component in the scan above.

Library spectrum

Fenbuconazole

Peach
The NIST library was searched for the components that were found in the AMDIS target library.

<table>
<thead>
<tr>
<th>R.T.</th>
<th>Cas #</th>
<th>Compound Name</th>
<th>ChemStation Amount (ng)</th>
<th>Agilent Match</th>
<th>R.T. Diff sec.</th>
<th>Reverse Match</th>
<th>NIST Hit Num.</th>
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</thead>
<tbody>
<tr>
<td>1.823</td>
<td>91203</td>
<td>Naphthalene</td>
<td>0.05</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.2748</td>
<td>97530</td>
<td>Eugenol</td>
<td>78</td>
<td>2.5</td>
<td>76</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>3.3036</td>
<td>86737</td>
<td>Fluorene</td>
<td>76</td>
<td>0.5</td>
<td>89</td>
<td>5</td>
<td></td>
</tr>
<tr>
<td>3.3242</td>
<td>84662</td>
<td>Diethyl phthalate</td>
<td>89</td>
<td>1.4</td>
<td>89</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3.5084</td>
<td>877098</td>
<td>2,4,5,6-Tetrachloro-m-xylene</td>
<td>0.36</td>
<td>98</td>
<td>3.1</td>
<td>87</td>
<td>2</td>
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<tr>
<td>3.6423</td>
<td>126738</td>
<td>Tributyl phosphate</td>
<td>1.3</td>
<td>90</td>
<td>0.9</td>
<td>87</td>
<td>2</td>
</tr>
<tr>
<td>5.3160</td>
<td>84695</td>
<td>Diisobutyl phthalate</td>
<td>2</td>
<td>99</td>
<td>3.1</td>
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<td>63252</td>
<td>Carbaryl</td>
<td>81</td>
<td>1.8</td>
<td>84</td>
<td>7</td>
<td></td>
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<tr>
<td>6.1423</td>
<td>84742</td>
<td>Di-n-butylphthalate</td>
<td>87</td>
<td>0.6</td>
<td>92</td>
<td>2</td>
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<tr>
<td>7.0835</td>
<td>133062</td>
<td>Captan</td>
<td>83</td>
<td>1.5</td>
<td>75</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>7.5430</td>
<td>959988</td>
<td>Endosulfan (alpha isomer)</td>
<td>91</td>
<td>-0.3</td>
<td>80</td>
<td>3</td>
<td></td>
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<tr>
<td>8.0082</td>
<td>80057</td>
<td>Bisphenol A</td>
<td>80</td>
<td>11.8</td>
<td>76</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>9.0198</td>
<td>85687</td>
<td>Butyl benzyl phthalate</td>
<td>80</td>
<td>3.5</td>
<td>76</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>9.0713</td>
<td>60207901</td>
<td>Propiconazole-l</td>
<td>76</td>
<td>16.8</td>
<td>72</td>
<td>2</td>
<td></td>
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<tr>
<td>9.5285</td>
<td>732116</td>
<td>Phosmet</td>
<td>96</td>
<td>5.4</td>
<td>85</td>
<td>2</td>
<td></td>
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<tr>
<td>10.7788</td>
<td>119611006</td>
<td>Fenbuconazole</td>
<td>76</td>
<td>6.9</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.7788</td>
<td>00000</td>
<td>Piperazine-2,5-dione, 3-hydroxy-6-isopropyl-3-trifluoromethyl-</td>
<td>59</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### MSD Deconvolution Report

**Sample Name:** peach  
**Data File:** C:\msdchem1\DATA\FDA\08_03_07 FDA_S_CL\peach_SIM.D  
**Date/Time:** 05:20 PM Monday, Oct 1 2007

The NIST library was not searched for the components that were found in the AMDIS target library.

<table>
<thead>
<tr>
<th>R.T.</th>
<th>Cas #</th>
<th>Compound Name</th>
<th>Agilent ChemStation Amount (ng)</th>
<th>Agilent Match</th>
<th>AMDIS R.T. Diff sec.</th>
<th>Reverse Match</th>
<th>Hit Num.</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.6148</td>
<td>63252</td>
<td>Carbaryl</td>
<td>0.09</td>
<td>100</td>
<td>2.2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7.0856</td>
<td>133062</td>
<td>Captan</td>
<td>0.2</td>
<td>99</td>
<td>1.9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.0028</td>
<td>60207901</td>
<td>Propiconazole-I</td>
<td>0.03</td>
<td>100</td>
<td>4.4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9.0727</td>
<td>999048032</td>
<td>Propiconazole-II</td>
<td>0.07</td>
<td>100</td>
<td>4.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10.7813</td>
<td>119611006</td>
<td>Fenbuconazole</td>
<td>0.65</td>
<td>100</td>
<td>7.4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Done**
Can We Quant on Deconvoluted Ions?

• Yes!
• MSD ChemStation (G1701AA) E.02
• Deconvolution Reporting Software, DRS (G1716AA) A.04
• Pesticide RTL Library (G1672AA) – 927 entries
QEdit, p,p’-DDT selected

5 ion overlay

3 spectra

“x” and “A” indicators

MSD & AMDIS areas & amounts

MSD ion

AMDIS ion

MSD & AMDIS

QEdit, p,p’-DDT selected

5 ion overlay

3 spectra

“x” and “A” indicators

MSD & AMDIS areas & amounts

MSD ion

AMDIS ion

MSD & AMDIS
Graphics Report

MSD and AMDIS 5-ion overlay

Raw, deconvoluted and library spectra

MSD and AMDIS areas and amounts
Summary Quant Report optionally includes both MSD ChemStation and AMDIS amounts

<table>
<thead>
<tr>
<th>Compound</th>
<th>R.T.</th>
<th>Q1m</th>
<th>Response</th>
<th>Conc Units</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Internal Standards</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1) Phenanthrene-d10</td>
<td>13.718</td>
<td>188</td>
<td>4953294</td>
<td>10.00 ppm</td>
</tr>
<tr>
<td><strong>Target Compounds</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18) Di-n-butylphthalate</td>
<td>18.445</td>
<td>149</td>
<td>989364m</td>
<td>7.18 ppm</td>
</tr>
<tr>
<td>22) Bisphenol A</td>
<td>23.974</td>
<td>213</td>
<td>2119577m</td>
<td>15.39 ppm</td>
</tr>
<tr>
<td>24) p,p'-DDE</td>
<td>24.060</td>
<td>246</td>
<td>79791m</td>
<td>0.58 ppm</td>
</tr>
<tr>
<td>25) p,p'-DDD</td>
<td>25.705</td>
<td>235</td>
<td>21489m</td>
<td>0.16 ppm</td>
</tr>
<tr>
<td>26) p,p'-DDT</td>
<td>26.998</td>
<td>235</td>
<td>17838m</td>
<td>0.13 ppm</td>
</tr>
<tr>
<td>27) Butyl benzyl phthalate</td>
<td>27.009</td>
<td>149</td>
<td>35766m</td>
<td>0.26 ppm</td>
</tr>
<tr>
<td>30) Piperonyl butoxide</td>
<td>27.928</td>
<td>176</td>
<td>5208006m</td>
<td>37.80 ppm</td>
</tr>
<tr>
<td>31) Bis(2-ethylhexyl)phtha...</td>
<td>29.669</td>
<td>149</td>
<td>429941m</td>
<td>3.12 ppm</td>
</tr>
<tr>
<td>34) Permethrin II</td>
<td>31.614</td>
<td>183</td>
<td>29430854m</td>
<td>213.63 ppm</td>
</tr>
</tbody>
</table>

**AMDIS Imported Quantitation Results**

<table>
<thead>
<tr>
<th>Compound</th>
<th>R.T.</th>
<th>Q1m</th>
<th>Response</th>
<th>Conc Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>18) Di-n-butylphthalate</td>
<td>18.443</td>
<td>149</td>
<td>861673</td>
<td>6.25 ppm</td>
</tr>
<tr>
<td>22) Bisphenol A</td>
<td>23.975</td>
<td>213</td>
<td>1754970</td>
<td>12.74 ppm</td>
</tr>
<tr>
<td>24) p,p'-DDE</td>
<td>24.065</td>
<td>246</td>
<td>25906</td>
<td>0.19 ppm</td>
</tr>
<tr>
<td>25) p,p'-DDD</td>
<td>25.715</td>
<td>235</td>
<td>17508</td>
<td>0.13 ppm</td>
</tr>
<tr>
<td>26) p,p'-DDT</td>
<td>26.993</td>
<td>235</td>
<td>12496</td>
<td>0.09 ppm</td>
</tr>
<tr>
<td>27) Butyl benzyl phthalate</td>
<td>27.010</td>
<td>149</td>
<td>21499</td>
<td>0.16 ppm</td>
</tr>
<tr>
<td>30) Piperonyl butoxide</td>
<td>27.927</td>
<td>176</td>
<td>4563220</td>
<td>33.12 ppm</td>
</tr>
<tr>
<td>31) Bis(2-ethylhexyl)phtha...</td>
<td>29.665</td>
<td>149</td>
<td>377561</td>
<td>2.74 ppm</td>
</tr>
<tr>
<td>34) Permethrin II</td>
<td>31.613</td>
<td>183</td>
<td>27779700</td>
<td>201.65 ppm</td>
</tr>
</tbody>
</table>
**DRS A.04 Report after importing AMDIS results**

QEdit reviewed with manual integrations

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**MSD Deconvolution Report**

- **Sample Name:** + 400 ppb ISTDs, 25 µL PTV
- **Data File:** C:\msdchem\DATA\Trifecta\SPINACH.D
- **Date/Time:** 07:41 AM Thursday, Apr 10 2008

The NIST library was searched for the components that were found in the AMDIS target library.

<table>
<thead>
<tr>
<th>R.T.</th>
<th>Cas #</th>
<th>Compound Name</th>
<th>Amount (ppm)</th>
<th>AMDIS</th>
<th>Match</th>
<th>R.T. Diff sec.</th>
<th>Reverse Match</th>
<th>Hit Num.</th>
</tr>
</thead>
<tbody>
<tr>
<td>18.4431</td>
<td>84742</td>
<td>Di-n-butylphthalate</td>
<td>7.18</td>
<td>6.25</td>
<td>95</td>
<td>1.7</td>
<td>92</td>
<td>1</td>
</tr>
<tr>
<td>23.974</td>
<td>80057</td>
<td>Bisphenol A</td>
<td>15.39</td>
<td>12.74</td>
<td>97</td>
<td>8.7</td>
<td>91</td>
<td>1</td>
</tr>
<tr>
<td>24.060</td>
<td>72559</td>
<td>p,p'-DDE</td>
<td>0.58</td>
<td>0.19</td>
<td>66</td>
<td>2.6</td>
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<td>2</td>
</tr>
<tr>
<td>25.705</td>
<td>72548</td>
<td>p,p'-DDD</td>
<td>0.16</td>
<td>0.13</td>
<td>52</td>
<td>1.8</td>
<td>65</td>
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</tr>
<tr>
<td>26.9932</td>
<td>50293</td>
<td>p,p'-DDT</td>
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<td>0.09</td>
<td>53</td>
<td>0.7</td>
<td>43</td>
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<tr>
<td>27.009</td>
<td>85687</td>
<td>Butyl benzyl phthalate</td>
<td>0.26</td>
<td>0.16</td>
<td>54</td>
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<td>57</td>
<td>25</td>
</tr>
<tr>
<td>27.9265</td>
<td>51036</td>
<td>Piperonyl butoxide</td>
<td>37.8</td>
<td>33.12</td>
<td>96</td>
<td>1.6</td>
<td>94</td>
<td>1</td>
</tr>
<tr>
<td>29.6648</td>
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<td>Bis(2-ethylhexyl)phthalate</td>
<td>3.12</td>
<td>2.74</td>
<td>94</td>
<td>1.0</td>
<td>86</td>
<td>3</td>
</tr>
<tr>
<td>31.6131</td>
<td>52645531</td>
<td>Permethrin II</td>
<td>213.63</td>
<td>201.65</td>
<td>90</td>
<td>3.8</td>
<td>91</td>
<td>3</td>
</tr>
<tr>
<td>13.718</td>
<td></td>
<td>Phenanthrene-d10</td>
<td>10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
GC/MSD Workflow Summary

- GC/MS in full scan mode combined with deconvolution reporting software (DRS) enables unknown pesticide analysis at 10 µg/kg (ppb) in various food commodities from one injection.
- Significant time saved on data analysis (screen and quant on 927 pesticides), from hours to minutes.

Application Note 5989-7670EN: Replacing Multiple 50-Minute GC and GC-MS/SIM Analyses with One 15-Minute Full-Scan GC-MS Analysis for Non-targeted Pesticides Screening and >10x Productivity Gain.
LC/MS Workflow

LC/Q-TOF or TOF
Full Spectrum
– for unknown compounds

Exact Mass
Database Search

Molecular
Formula Generation

Another injection for
MS/MS
(QQQ or QTOF)

Screen

Quantify

Confirm
Why Use (Q-)TOF?

QQQ

• Routine target compound screening/quantitation in a single injection
• MRM detection limit meets all regulatory requirements

TOF/Q-TOF

• Always full spectrum
• Un-limited number of routine target and non-target compound screening (using exact mass databases)

Q-TOF

• Full scan accurate MS/MS spectra for added confidence for total unknowns

All systems share SAME software platform, ion source, and collision cell – 100% workflow portability
Agilent Q-TOF Fundamentals

Exact Mass
Mass Accuracy (ppm)

Flight tube
Common with TOF

Collision cell
Common with QQQ

Ion optics
Common with Q & QQQ

Bullet Points:
- Ion optics Common with Q & QQQ
- Flight tube Common with TOF
- Collision cell Common with QQQ

Diagram:
- Octopole 1
- DC Quad
- Collision cell
- Lens 1 and 2
- Quad Mass Filter (Q1)
- Octopole 2
- Ion Pulser
- Detector
- Rough Pump
- Turbo
- Turbo
- Turbo
- Turbo
What does “Exact Mass” mean?

<table>
<thead>
<tr>
<th>Element</th>
<th>Atomic Number</th>
<th>Exact Mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>1</td>
<td>1.007825</td>
</tr>
<tr>
<td>C</td>
<td>6</td>
<td>12.000000</td>
</tr>
<tr>
<td>N</td>
<td>7</td>
<td>14.003074</td>
</tr>
<tr>
<td>O</td>
<td>8</td>
<td>15.994915</td>
</tr>
</tbody>
</table>

- C6H6Cl6 287.8600665 Lindane
- C10H12N2O6S 288.0416000 Carbasulam
- C9H21O2PS3 288.0441285 Terbufos
- C13H21O3PS 288.0949000 Iprobenfos
- C15H17N4Cl 288.1141743 Myclobutanil
- C12H21N2O4P 288.1238937 Diazoxon
- C11H20N4O3PS 288.1256000 Epronaz
- C11H21N4O3P 288.1351000 Pirimethaphos
- C16H20N2O3 288.1473925 Imazamethabenz

Uses accurate mass on TOF/Q-TOF to identify all of them.
Mass Analysis for TOF

\[ v = \frac{d}{t} \]
\[ E = \frac{1}{2} m v^2 = \frac{1}{2} m \left(\frac{d}{t}\right)^2 \]
\[ m = \frac{2E}{d^2} t^2 \]

Energy (E) and Distance (d) are fixed

The measured mass is proportional to the flight time (time-of-flight).

The Key for getting useful TOF results is good mass accuracy.
Calculation of Exact Mass and Error in Measured Mass (MH⁺) of Reserpine

<table>
<thead>
<tr>
<th>Atom</th>
<th>Mass of Atom</th>
<th># of Atoms</th>
<th>Sum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>1.00783</td>
<td>40</td>
<td>40.31300</td>
</tr>
<tr>
<td>Carbon</td>
<td>12.00000</td>
<td>33</td>
<td>396.00000</td>
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<tr>
<td>Nitrogen</td>
<td>14.00307</td>
<td>2</td>
<td>28.00615</td>
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<tr>
<td>Oxygen</td>
<td>15.99492</td>
<td>9</td>
<td>143.95424</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td><strong>608.27338</strong></td>
</tr>
<tr>
<td><strong>Plus H</strong></td>
<td>1.00783</td>
<td>1</td>
<td>1.00783</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td><strong>609.28121</strong></td>
</tr>
<tr>
<td><strong>Minus e-</strong></td>
<td>0.00055</td>
<td>1</td>
<td>0.00055</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td><strong>609.28065</strong></td>
</tr>
</tbody>
</table>

Calculated = exact

\[
\frac{\text{Measured} - \text{Calculated}}{\text{Calculated}} \times 1,000,000 = \text{ppm}
\]

0.9027038 ppm

Error if the electron was not omitted!

Reserpine (C₃₃H₄₀N₂O₉)
How Much Accuracy is Needed?

Reserpine \((C_{33}H_{40}N_2O_9)\) has a protonated ion at 609.28066 (MH\(^+\))

Single quad reports mass to +/- 0.1 = 165 ppm

\((0.1/609.28 \times 10^{e6} = 164.128 \text{ ppm})\)

Number of possible formulas using only C, H, O & N:

<table>
<thead>
<tr>
<th>Accuracy</th>
<th>Mass Difference</th>
<th>Number of Formulas</th>
</tr>
</thead>
<tbody>
<tr>
<td>165 ppm</td>
<td>0.1 amu (609.18 - 609.38)</td>
<td>209</td>
</tr>
<tr>
<td>10 ppm</td>
<td>0.061 amu</td>
<td>13</td>
</tr>
<tr>
<td>5 ppm</td>
<td>0.030 amu (609.25 - 609.31)</td>
<td>7</td>
</tr>
<tr>
<td>3 ppm</td>
<td>0.0018 amu</td>
<td>4</td>
</tr>
<tr>
<td>2 ppm</td>
<td>0.0012 amu (609.2795 - 609.2819)</td>
<td>2</td>
</tr>
</tbody>
</table>

Measured mass accuracy can **narrow the number of hits** in a TOF database search, therefore reduce risk of investing effort on the wrong molecule.
Automatic Internal Referencing (Easy-to-use)

Analytical Sprayer

Reference Sprayer

Dual Spray ESI source and Calibration Delivery System (CDS) → automates the introduction of reference masses

AutoTune
TOF/Q-TOF Unlimited Number of Compound Screening

15 out of 510 compounds had hits from database search.

5556.D (Grape) MS1 Full Spectrum
Run Another Analysis in MS/MS (Targeted) Mode to Confirm Hits Found in MS1 Mode

<table>
<thead>
<tr>
<th>Compound</th>
<th>RT</th>
<th>Precursor Mass (MH)$^+$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spiroxamine</td>
<td>10.884</td>
<td>298.27406</td>
</tr>
<tr>
<td>Terbuconazole</td>
<td>14.139</td>
<td>308.15242</td>
</tr>
<tr>
<td>Tebufenoxide</td>
<td>15.492</td>
<td>353.22236</td>
</tr>
</tbody>
</table>
Next Step: Find compounds by Targeted MS/MS
The compound name Spiroxamine came up in the MS1 mode. Use formula results and MS/MS results to confirm the hit.
Terbuconazole

The compound name Terbuconazole came up in the MS1 mode.

Use formula results and MS/MS results to confirm the hit.

Boxes represent theoretical isotope ratios
Screen Pesticides with LC-TOF/Q-TOF

• Accurate Mass provides added compound selectivity
• Higher resolution provides added interference selectivity
• Always full spectral data
• Unlimited number of compounds can be screened (search exact mass compound database for identification)
• Sensitivity is the same regardless of number of compounds screened*
• MS/MS (Q-TOF) assists compound confirmation

*Triple quadrupole (QQQ) mass spectrometer can be more sensitive up to a limited number of compounds. That limit has not been definitively determined.
Pesticide Workflow: Screen S, Confirm C and Quantify Q

Representative Sample

QuEChERS

Extraction

Clean-up

GC/MS (PTV) SIM/Scan – for known and unknown (+backflush)

Deconvolution Final Report

GC/QQQ MRM – for known targets

LC/QQQ MRM – for known targets

LC/QTOF or TOF Full Spectrum – for unknown compounds

Exact Mass Database Search

Molecular Formula Generation

Another injection for MS/MS (QQQ or QTOF)
Summary

- GC/MS and Deconvolution to Screen, Confirm and Quantify
- QQQ for **Targeted** analysis in complex matrix
  - Sensitivity unsurpassed
  - Complex matrix with less clean-up
- TOF/Q-TOF for **Targeted and Unknown** Screening
  - Sensitive full scan analysis
  - Searching exact mass database leads to identification
  - Quantitative
  - Accurate mass MS/MS for identification of fragments and structure elucidation
Wrap-up E-Seminar Questions

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