



## Screening method QTOF

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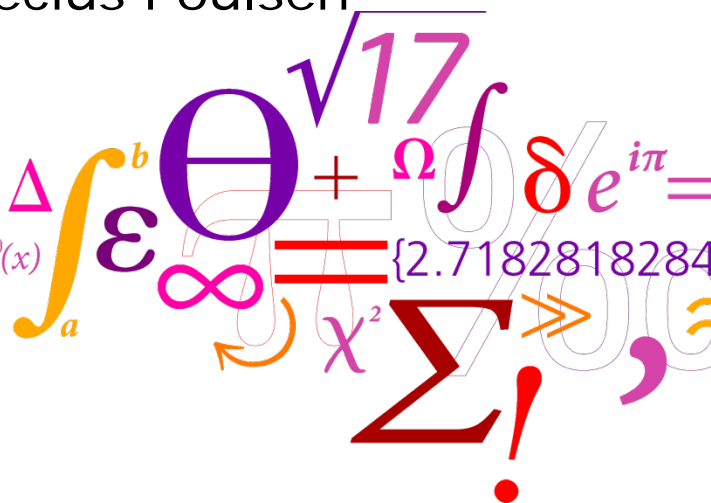
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# Screening method QTOF

Anne Kruse Lykkeberg and Mette Erecius Poulsen  
Copenhagen, 4<sup>th</sup> September 2014

$$f(x+\Delta x) = \sum_{i=0}^{\infty} \frac{(\Delta x)^i}{i!} f^{(i)}(x)$$


# Disposition

LC-QTOF screening - MassHunter Qualitative

LC-QTOF - Validation

GC-QTOF screening - MassHunter Quantitative

GC-QTOF - Validation

# Disposition

LC-QTOF screening - MassHunter Qualitative

LC-QTOF - Validation

GC-QTOF screening - MassHunter Quantitative

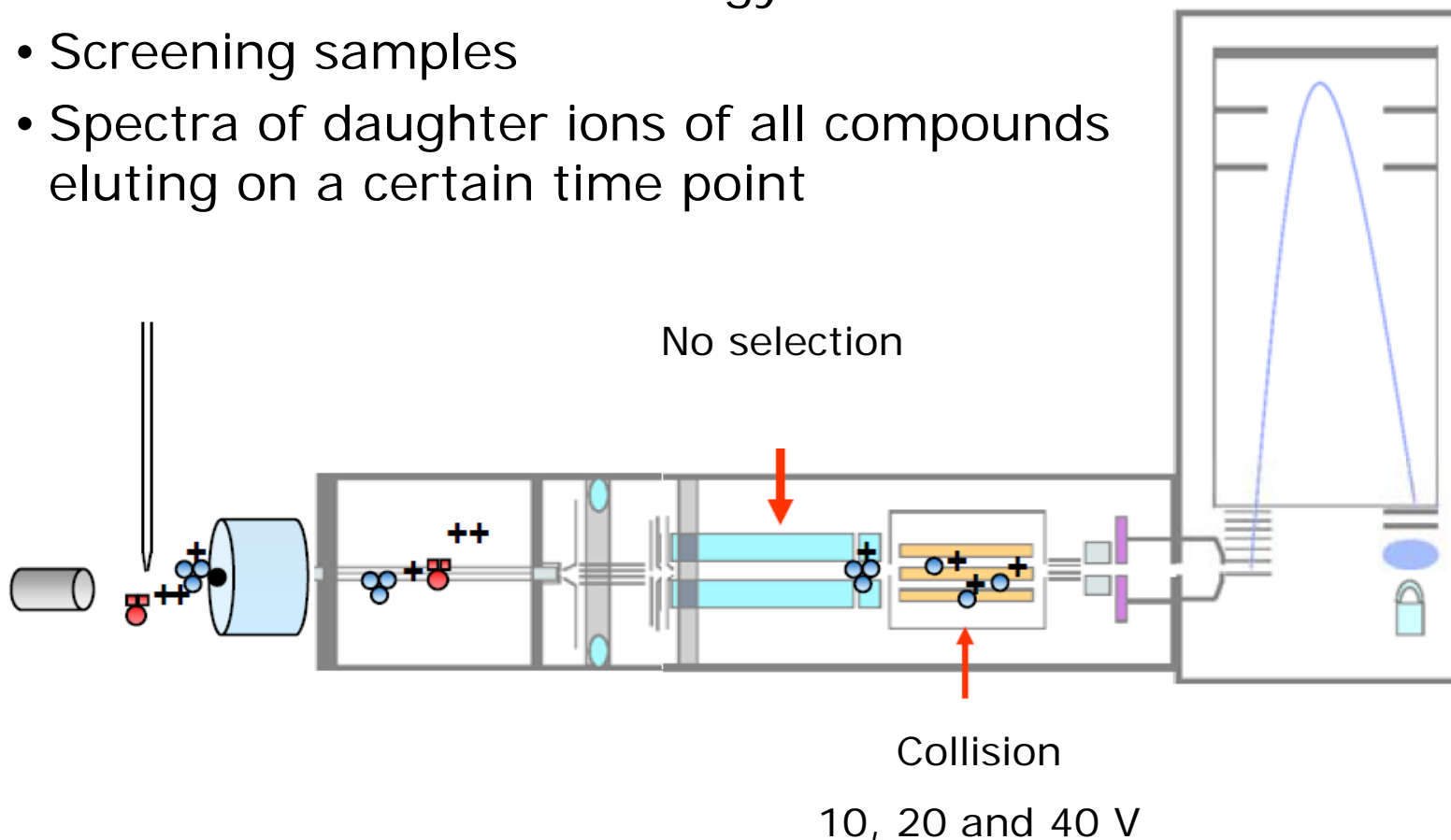
GC-QTOF - Validation

# LC-QTOF instruments

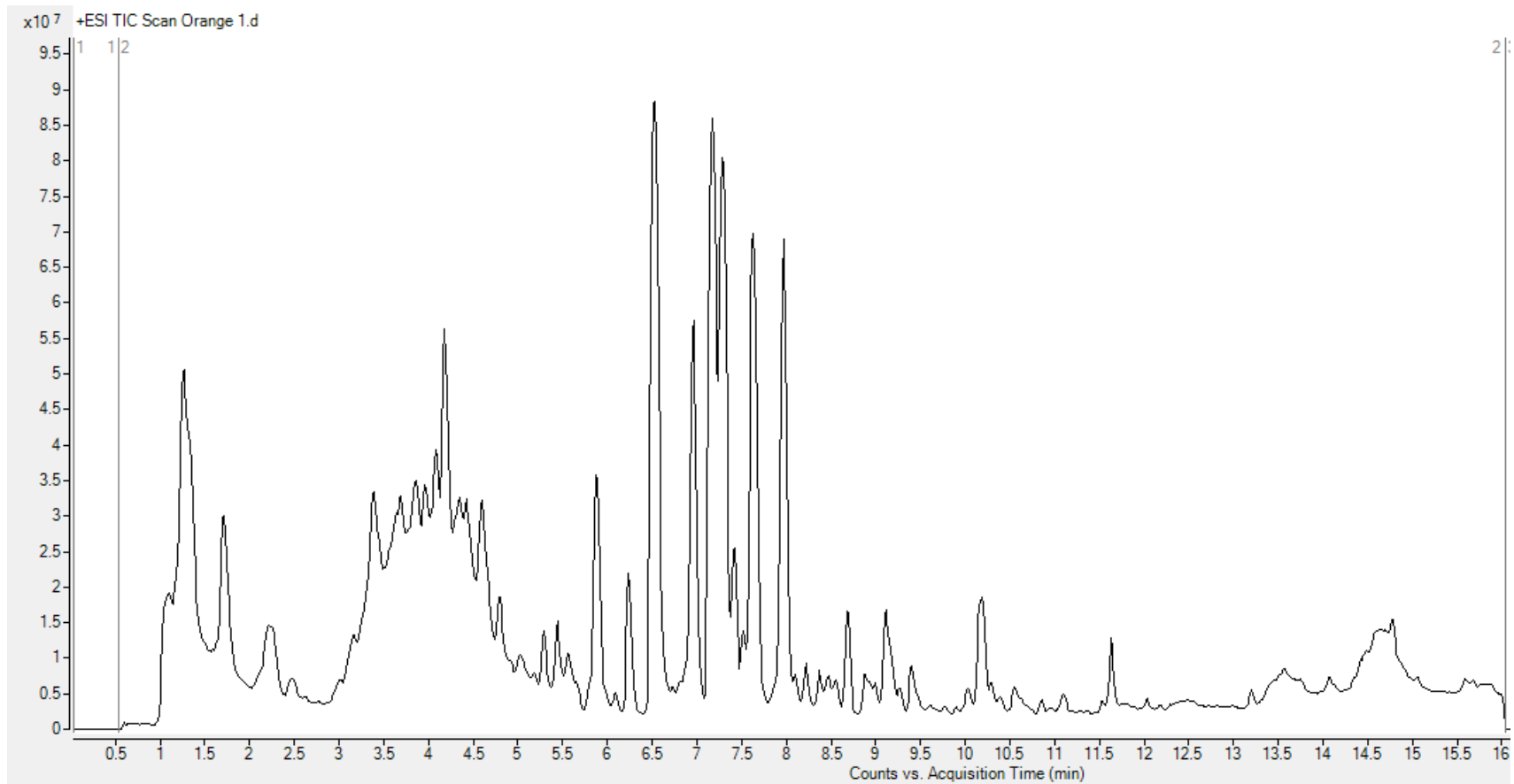


# QTOF-analysis – All ion MS

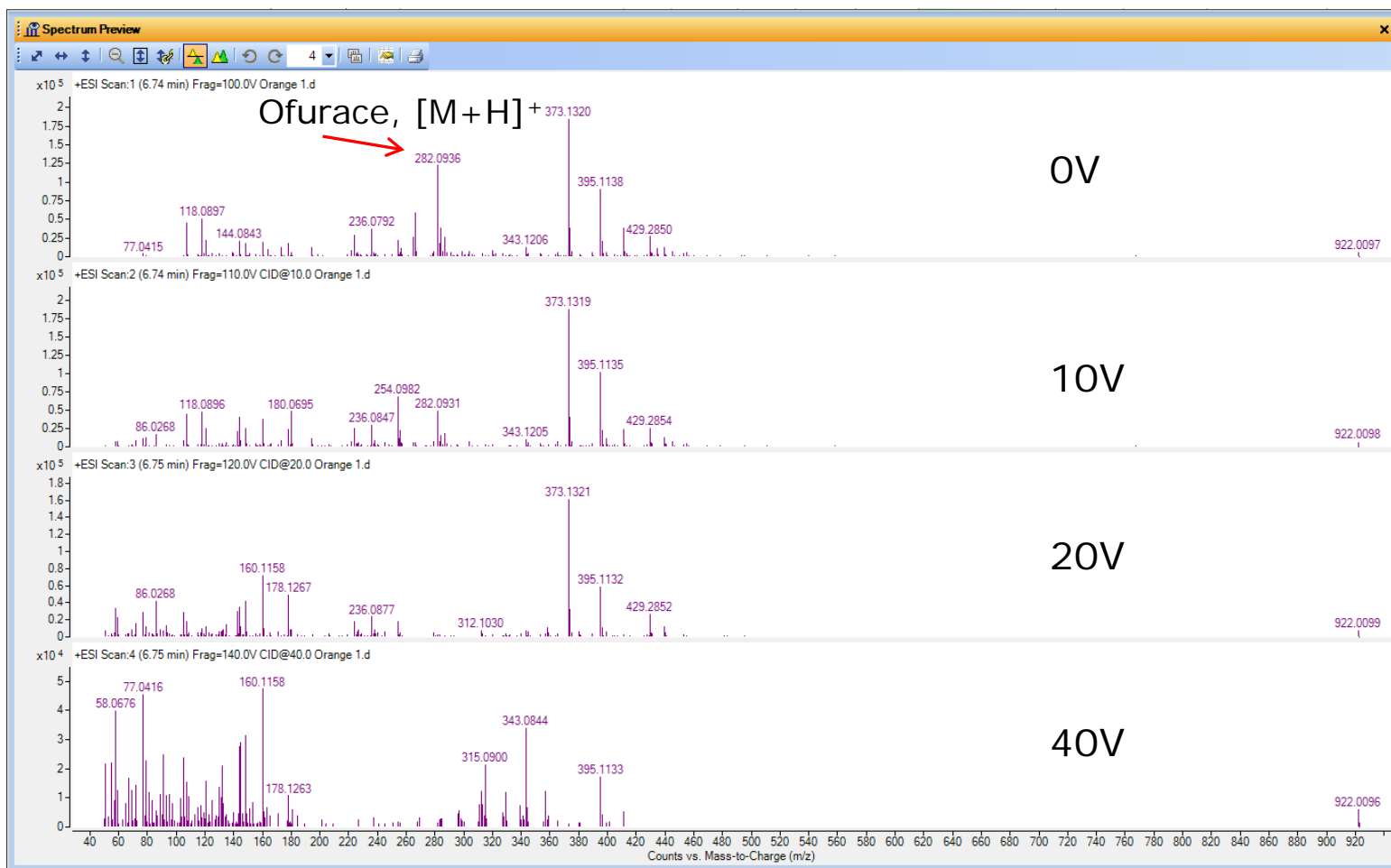
- MS scan with collision energy
- Screening samples
- Spectra of daughter ions of all compounds eluting on a certain time point



# Chromatogram - TIC



# Spectra – MSscan incl. collision





# PCDL - library

MassHunter PCDL Manager for Pesticides - G:\Agilent TOF\PCDL\Pesticides pos 20130821.cdb

File Edit View PCDL Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds Spectral Search Browse Spectra Edit Spectra

Mass:  [M+H]<sup>+</sup>  Neutral  [M-H]<sup>-</sup> Formula:

Molecule:  Structure MOL Text

Compound Name	Formula	Mass	Anion	Cation	RT (min)	CAS	ChemSpider	IUPAC Name	Num Spectra
Acetazolamide	C4H6N4...	221.98813	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">59-66-5</a>	<a href="#">1909</a>	N-(5-Sulfamoyl-1,3,4-thiadiazol-2-yl)acetamide	3
Acetochlor	C14ClNO...	269.11826	<input type="checkbox"/>	<input type="checkbox"/>	9.390	<a href="#">34256-82-1</a>	<a href="#">1911</a>	2-Chloro-N-(ethoxymethyl)-N-(2-ethyl-6-methylphe...	3
Acetyl-Seneciophylline	C20H25N...	375.16819	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">90341-45-0</a>	<a href="#">4945366</a>	11,16-Dioxo-13,19-didehydrosenecionan-12-yl ac...	0
Acibenzolar-S-methyl (CGA 245704)	C8N2OS2...	209.99215	<input type="checkbox"/>	<input type="checkbox"/>	8.490	<a href="#">135158-5...</a>	<a href="#">77928</a>	S-Methyl 1,2,3-benzothiadiazole-7-carbothioate	0
Acifluorfen	C14ClF3N...	360.99648	<input type="checkbox"/>	<input type="checkbox"/>	8.758	<a href="#">50594-66-6</a>	<a href="#">40113</a>	5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenz...	3
Acifluorfen-methyl	C15H9ClF...	375.01213	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">50594-67-7</a>	<a href="#">82745</a>	Methyl 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nit...	0
Aclonifen	C12ClN2...	264.03017	<input type="checkbox"/>	<input type="checkbox"/>	9.906	<a href="#">74070-46-5</a>	<a href="#">83411</a>	2-Chloro-6-nitro-3-phenoxyaniline	4
Acrinathrin	C26F6NO...	541.13239	<input type="checkbox"/>	<input type="checkbox"/>	13.800	<a href="#">101007-0...</a>	<a href="#">10469290</a>	Cyano(3-phenoxyphenyl)methyl 3-((1Z)-3-((1,1,1,3...	0
ADBI (ABDI) (Celestolide)	C17H24O	244.18272	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">13171-00-1</a>	<a href="#">55495</a>	1-[1,1-Dimethyl-6-(2-methyl-2-propanyl)-2,3-dihydr...	0
Affinin	C14H23NO	221.17796	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">25394-57-4</a>	<a href="#">4509783</a>	(2E,6Z,8E)-N-Isobutyl-2,6,8-decatrienamide	0
AKH-7088	C19H16Cl...	476.05981	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">104459-8...</a>	<a href="#">5005848</a>	Methyl (((1E)-1-[5-[2-chloro-4-(trifluoromethyl)phe...	0
Acibenzolar-S-methyl (CGA 245704)	C8N2OS2...	209.99215	<input type="checkbox"/>	<input type="checkbox"/>	8.490	<a href="#">135158-5...</a>	<a href="#">77928</a>	S-Methyl 1,2,3-benzothiadiazole-7-carbothioate	0
Acifluorfen	C14ClF3N...	360.99648	<input type="checkbox"/>	<input type="checkbox"/>	8.758	<a href="#">50594-66-6</a>	<a href="#">40113</a>	5-[2-Chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenz...	3
Acifluorfen-methyl	C15H9ClF...	375.01213	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">50594-67-7</a>	<a href="#">82745</a>	Methyl 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nit...	0
Aclonifen	C12ClN2...	264.03017	<input type="checkbox"/>	<input type="checkbox"/>	9.906	<a href="#">74070-46-5</a>	<a href="#">83411</a>	2-Chloro-6-nitro-3-phenoxyaniline	4
Acrinathrin	C26F6NO...	541.13239	<input type="checkbox"/>	<input type="checkbox"/>	13.800	<a href="#">101007-0...</a>	<a href="#">10469290</a>	Cyano(3-phenoxyphenyl)methyl 3-((1Z)-3-((1,1,1,3...	0
ADBI (ABDI) (Celestolide)	C17H24O	244.18272	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">13171-00-1</a>	<a href="#">55495</a>	1-[1,1-Dimethyl-6-(2-methyl-2-propanyl)-2,3-dihydr...	0
Affinin	C14H23NO	221.17796	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">25394-57-4</a>	<a href="#">4509783</a>	(2E,6Z,8E)-N-Isobutyl-2,6,8-decatrienamide	0
AKH-7088	C19H16Cl...	476.05981	<input type="checkbox"/>	<input type="checkbox"/>		<a href="#">104459-8...</a>	<a href="#">5005848</a>	Methyl (((1E)-1-[5-[2-chloro-4-(trifluoromethyl)phe...	0

# PCDL – library - spectra

Graphic
Mass List

File Edit View PCDL Links Help

Find Spectra

Single Search Batch Search

Mass  
Precursor ion:

Tolerance: 200 ppm mDa

Collision energy  
Tolerance: 2.0 eV

Spectra for compound: Acetazolamide

Compound Name	Precursor Ion	Collid Energ
Acetazolamide	222.99541	
Acetazolamide	222.99541	

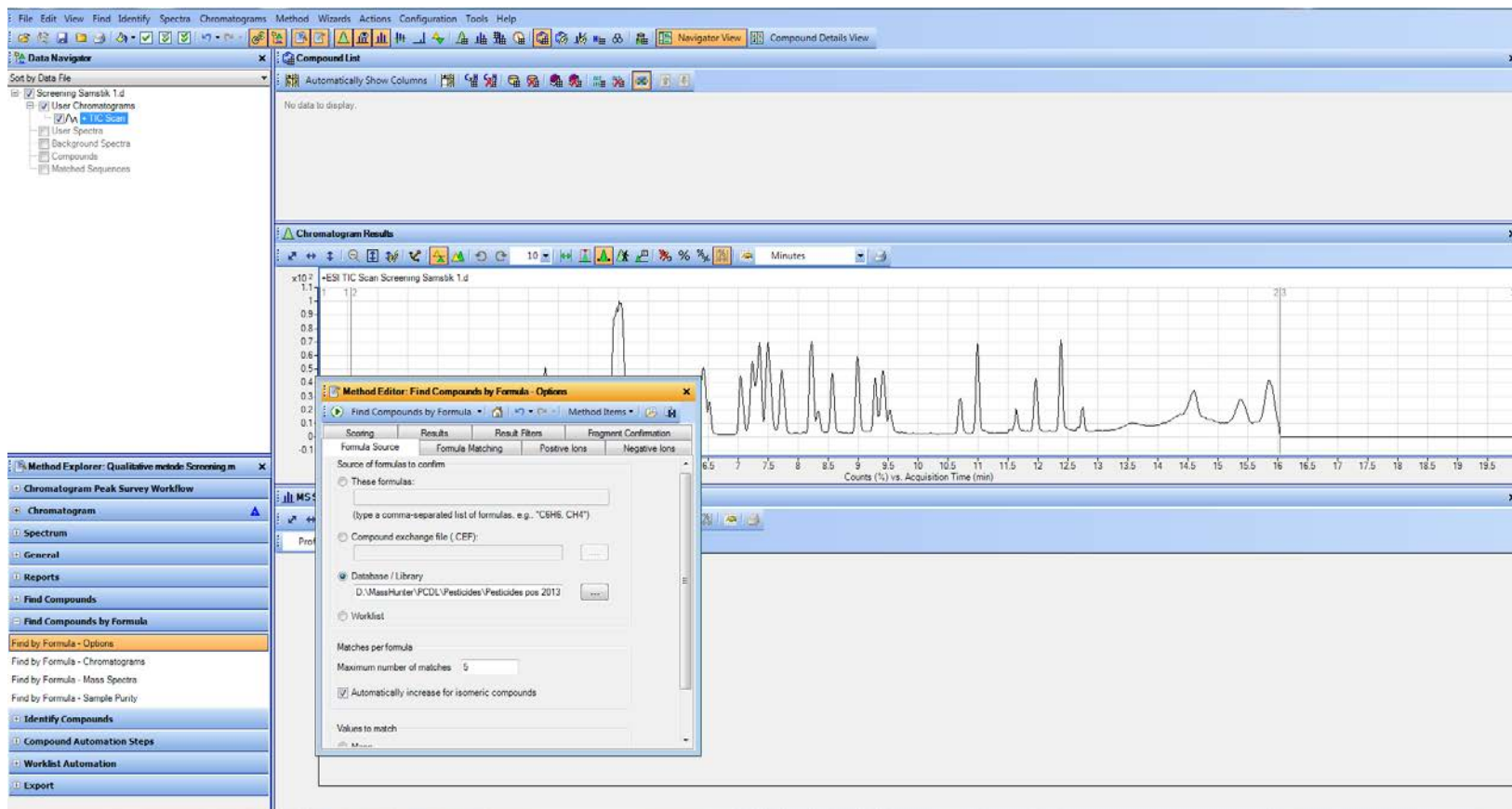
Mass	Rel Abund
180.98484	100.00000
222.99541	52.66977
163.95829	6.56664
205.96886	2.13168

Spectra for compound:

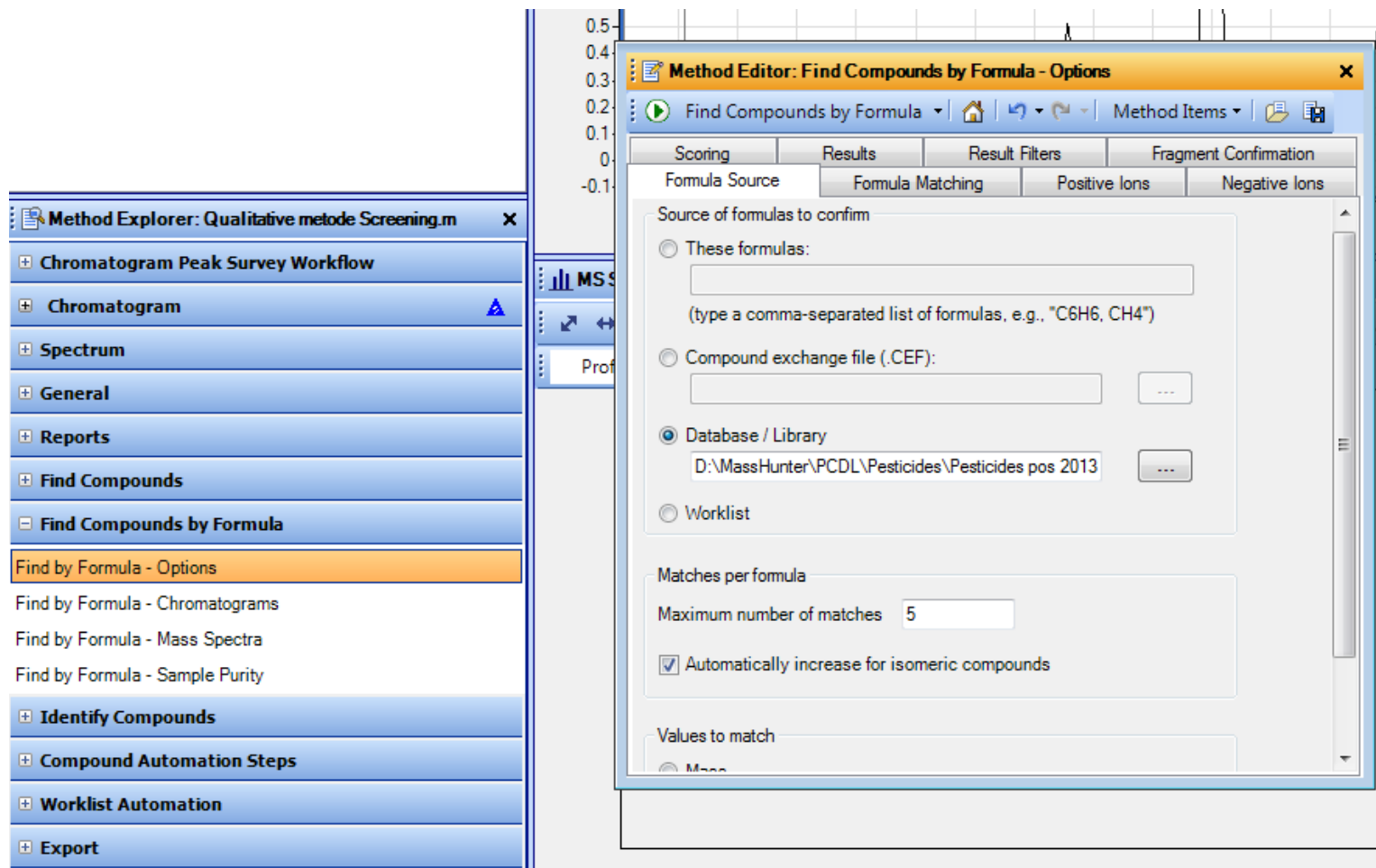
Compound Name	Precursor Ion	Collision Energy	Ion Polarity	Ionization Mode	Instrument Type
Acetazolamide	222.99541	10	Positive	ESI	QTOF
Acetazolamide	222.99541	20	Positive	ESI	QTOF
Acetazolamide	222.99541	40	Positive	ESI	QTOF

# MassHunter Qualitative - Library Search



The screenshot displays the MassHunter Qualitative software interface. The main window shows a chromatogram plot titled "Chromatogram Results" with the x-axis labeled "Counts (%) vs. Acquisition Time (min)" and the y-axis labeled "x10<sup>2</sup> - ESI TIC Scan Screening Samstik 1.d". A peak is visible at approximately 16.5 minutes. Overlaid on the plot is a dialog box titled "Method Editor: Find Compounds by Formula - Options". The dialog box has tabs for "Scoring", "Results", "Result Filters", and "Fragment Confirmation". The "Scoring" tab is active, showing options for "Formula Source" (These formulas, Compound exchange file, Database / Library, or Worklist). The "Database / Library" option is selected, with the path "D:\MassHunter\PCDL\Pesticides\Pesticides pos 2013" displayed. Other options include "Matches per formula" (Maximum number of matches: 5) and a checked box for "Automatically increase for isomeric compounds". The "Values to match" section is partially visible at the bottom.

# Library Search



The screenshot displays a software interface with a sidebar on the left and a main window on the right. The sidebar, titled "Method Explorer: Qualitative metode Screening.m", contains a tree view of methods. The "Find Compounds by Formula" method is selected, and its sub-option "Find by Formula - Options" is highlighted. The main window shows the "Method Editor: Find Compounds by Formula - Options" dialog box. This dialog has tabs for "Scoring", "Results", "Result Filters", and "Fragment Confirmation". The "Formula Matching" sub-tab is active, showing options for the source of formulas to confirm: "These formulas:", "Compound exchange file (.CEF)", "Database / Library" (selected), and "Worklist". The "Database / Library" option is set to "D:\MassHunter\PCDL\Pesticides\Pesticides pos 2013". Below this, the "Matches per formula" section shows "Maximum number of matches" set to 5 and a checked option for "Automatically increase for isomeric compounds".

**Method Explorer: Qualitative metode Screening.m**

- Chromatogram Peak Survey Workflow
- Chromatogram
- Spectrum
- General
- Reports
- Find Compounds
- Find Compounds by Formula
  - Find by Formula - Options
  - Find by Formula - Chromatograms
  - Find by Formula - Mass Spectra
  - Find by Formula - Sample Purity
- Identify Compounds
- Compound Automation Steps
- Worklist Automation
- Export

**Method Editor: Find Compounds by Formula - Options**

Find Compounds by Formula | Method Items

Scoring	Results	Result Filters	Fragment Confirmation
Formula Source	Formula Matching	Positive Ions	Negative Ions

Source of formulas to confirm

- These formulas:  
(type a comma-separated list of formulas, e.g., "C6H6, CH4")
- Compound exchange file (.CEF):
- Database / Library  
D:\MassHunter\PCDL\Pesticides\Pesticides pos 2013
- Worklist

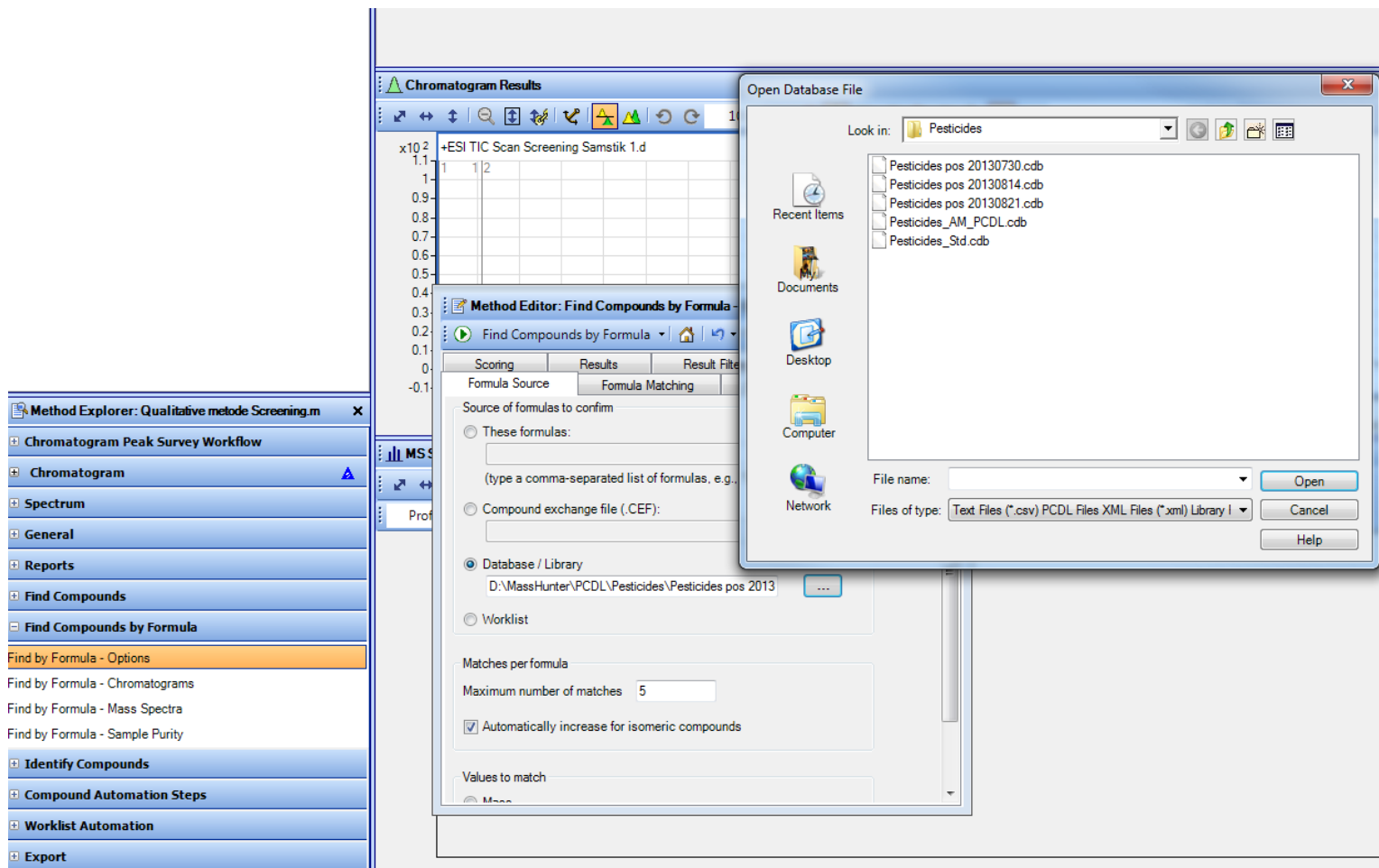
Matches per formula

Maximum number of matches: 5

Automatically increase for isomeric compounds

Values to match

# Library Search

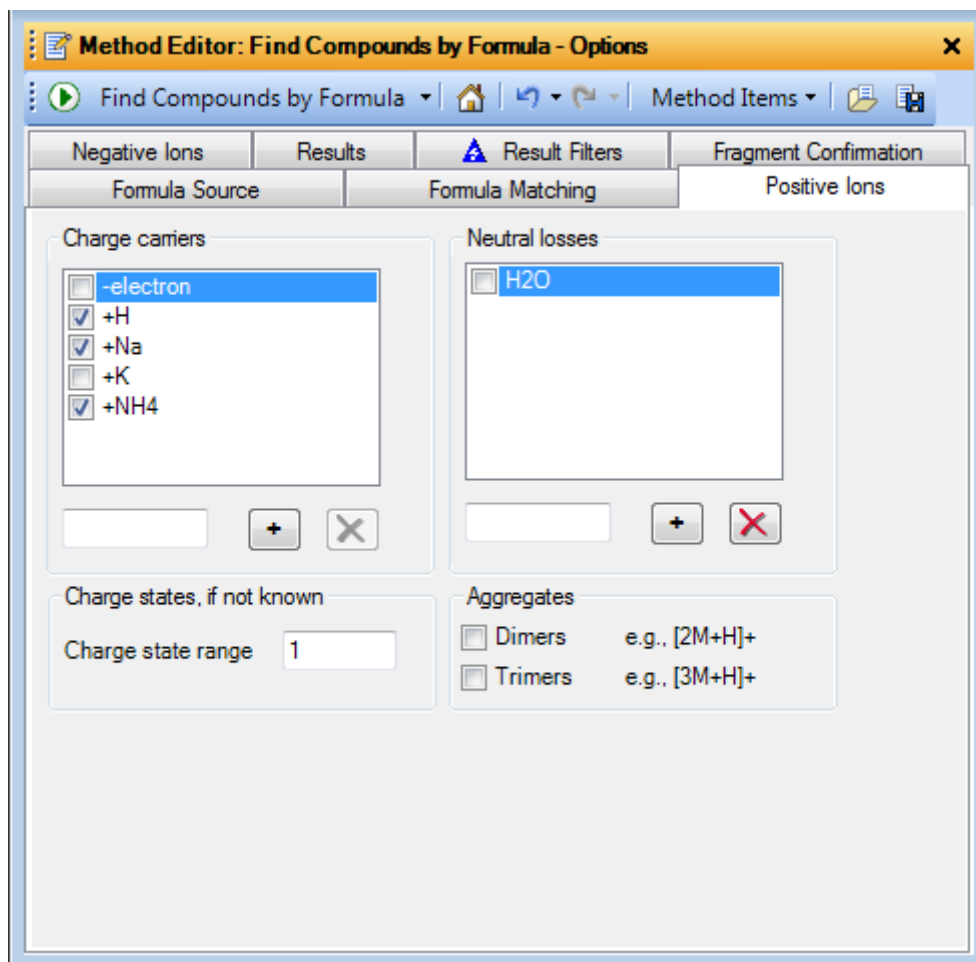


The screenshot displays a software interface for chromatogram analysis. On the left, a sidebar titled "Method Explorer: Qualitative metode Screening.m" contains a tree view with the following items: Chromatogram Peak Survey Workflow, Chromatogram, Spectrum, General, Reports, Find Compounds, Find Compounds by Formula, Find by Formula - Options (highlighted), Find by Formula - Chromatograms, Find by Formula - Mass Spectra, Find by Formula - Sample Purity, Identify Compounds, Compound Automation Steps, Worklist Automation, and Export.

The main window shows a "Chromatogram Results" plot of a Total Ion Chromatogram (TIC) scan. Below the plot is a "Method Editor: Find Compounds by Formula" dialog box. This dialog has tabs for "Scoring", "Results", and "Result Filter". The "Formula Matching" sub-tab is active, showing options for the source of formulas to confirm: "These formulas:", "Compound exchange file (.CEF)", and "Database / Library". The "Database / Library" option is selected, with the path "D:\MassHunter\PCDL\Pesticides\Pesticides pos 2013" displayed. Other settings include "Matches per formula" set to 5 and a checked box for "Automatically increase for isomeric compounds".

An "Open Database File" dialog box is overlaid on the right side of the interface. It shows the "Look in:" directory as "Pesticides" and lists several files: "Pesticides pos 20130730.cdb", "Pesticides pos 20130814.cdb", "Pesticides pos 20130821.cdb", "Pesticides\_AM\_PCDL.cdb", and "Pesticides\_Std.cdb". The "Files of type" dropdown is set to "Text Files (\*.csv) PCDL Files XML Files (\*.xml) Library I".

# Library Search - adducts



**Method Editor: Find Compounds by Formula - Options**

Find Compounds by Formula | Method Items

Negative Ions | Results | **Result Filters** | Fragment Confirmation

Formula Source | **Formula Matching** | Positive Ions

**Charge carriers**

- electron
- +H
- +Na
- +K
- +NH4

**Neutral losses**

- H2O

**Charge states, if not known**

Charge state range:

**Aggregates**

- Dimers e.g., [2M+H]<sup>+</sup>
- Trimers e.g., [3M+H]<sup>+</sup>

# Screening criteria – Match tolerance

**Method Editor: Find Compounds by Formula - Options**

Find Compounds by Formula | Home | Refresh | Method Items | Print

Scoring	Results	Result Filters	Fragment Confirmation
Formula Source	Formula Matching	Positive Ions	Negative Ions

Match tolerance

Masses: +/- 10.00 ppm

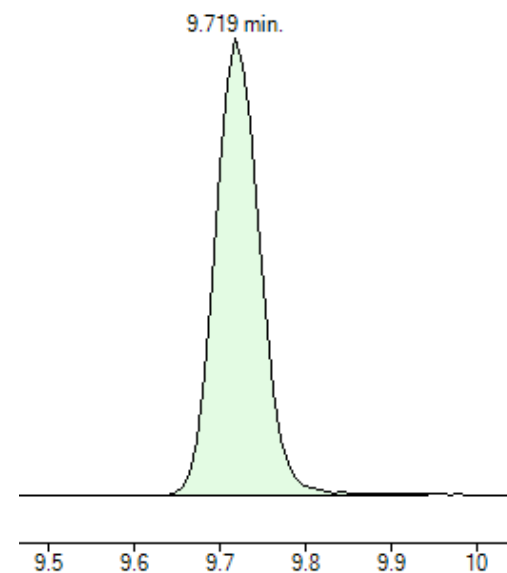
Retention times: +/- 0.35 minutes

Expansion of values for chromatogram extraction

Possible m/z: Symmetric (ppm) +/- 35.0

Limit EIC extraction range

Expected retention time: +/- 1.00 minutes



# Screening criteria – Average scans

**Method Editor: Find Compounds by Formula - Mass Spectra**

Find Compounds by Formula | Home | Back | Forward | Method Items

Peak Spectrum | Peak Location | Charge State

Spectra to include

- At apex of peak
- Average scans >  % of peak height

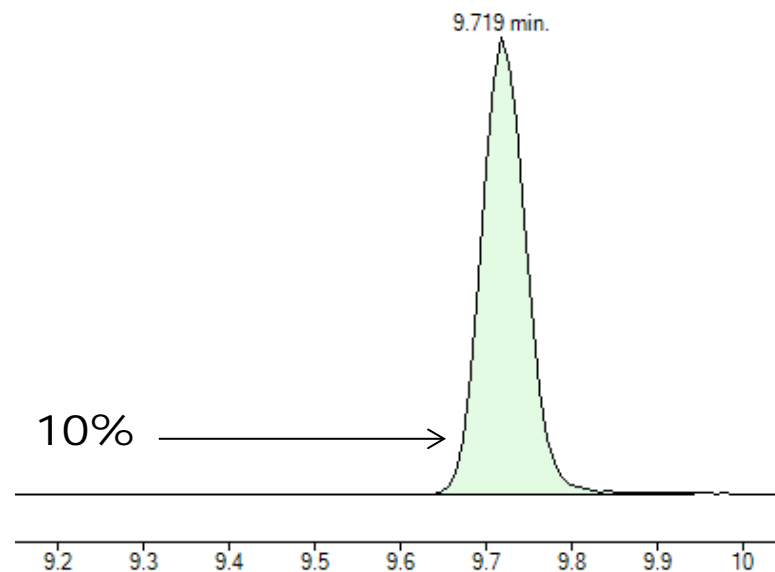
TOF spectra

- Exclude if above  % of saturation
- In the m/z ranges used in the chromatogram
- Anywhere
- In these m/z ranges
- Never return an empty spectrum

Peak spectrum background

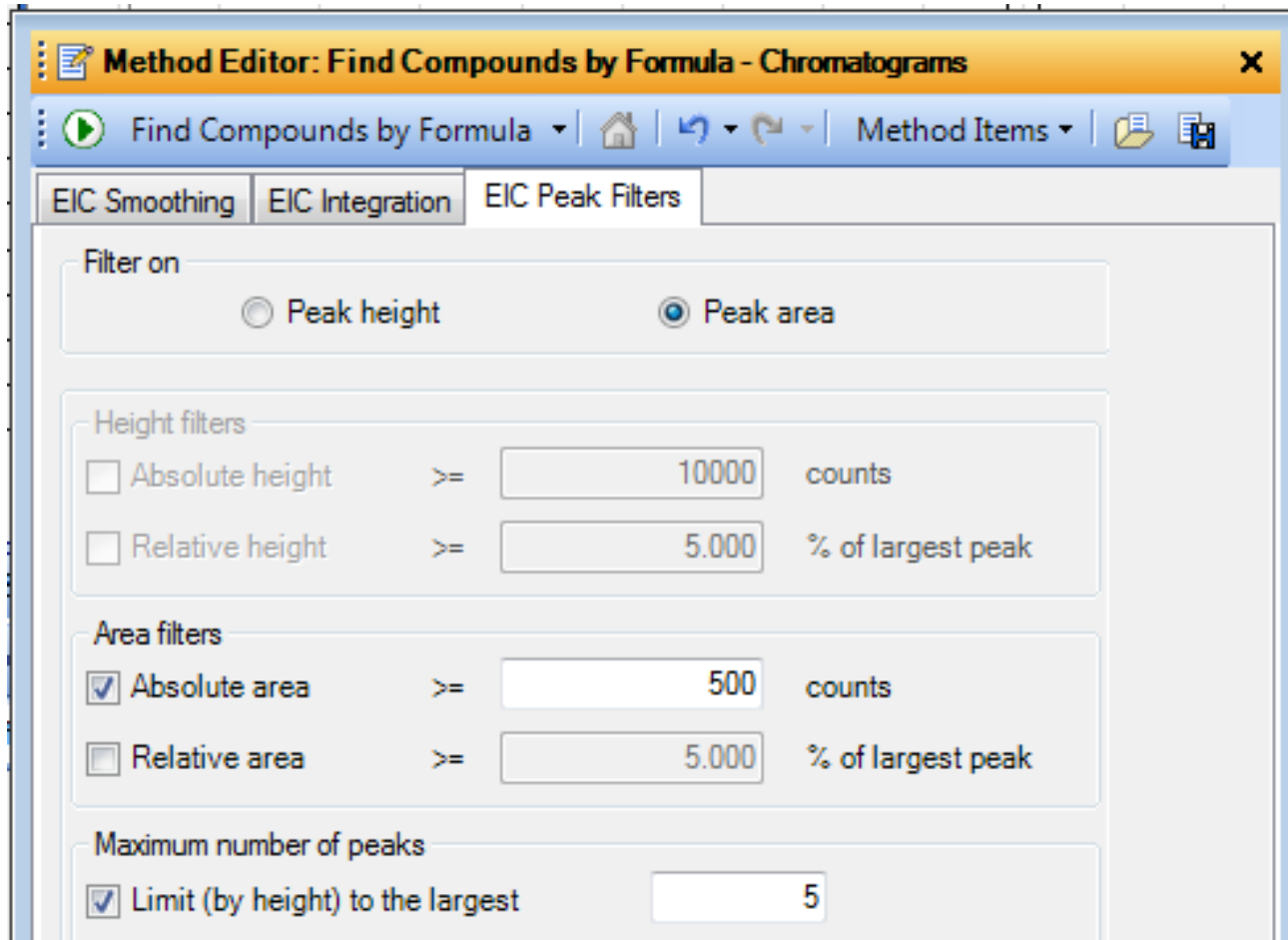
MS

Time range:





# Screening criteria – Match tolerance



The screenshot shows the 'Method Editor: Find Compounds by Formula - Chromatograms' window. The 'EIC Peak Filters' tab is active. The 'Filter on' section has 'Peak area' selected. The 'Height filters' section has 'Absolute height' (>= 10000 counts) and 'Relative height' (>= 5.000 % of largest peak) options, both unchecked. The 'Area filters' section has 'Absolute area' (>= 500 counts) and 'Relative area' (>= 5.000 % of largest peak) options, with 'Absolute area' checked. The 'Maximum number of peaks' section has 'Limit (by height) to the largest' checked with a value of 5.

**Method Editor: Find Compounds by Formula - Chromatograms**

Find Compounds by Formula | Home | Undo | Redo | Method Items | Save | Print

EIC Smoothing | EIC Integration | **EIC Peak Filters**

Filter on

Peak height  Peak area

Height filters

Absolute height >= 10000 counts

Relative height >= 5.000 % of largest peak

Area filters

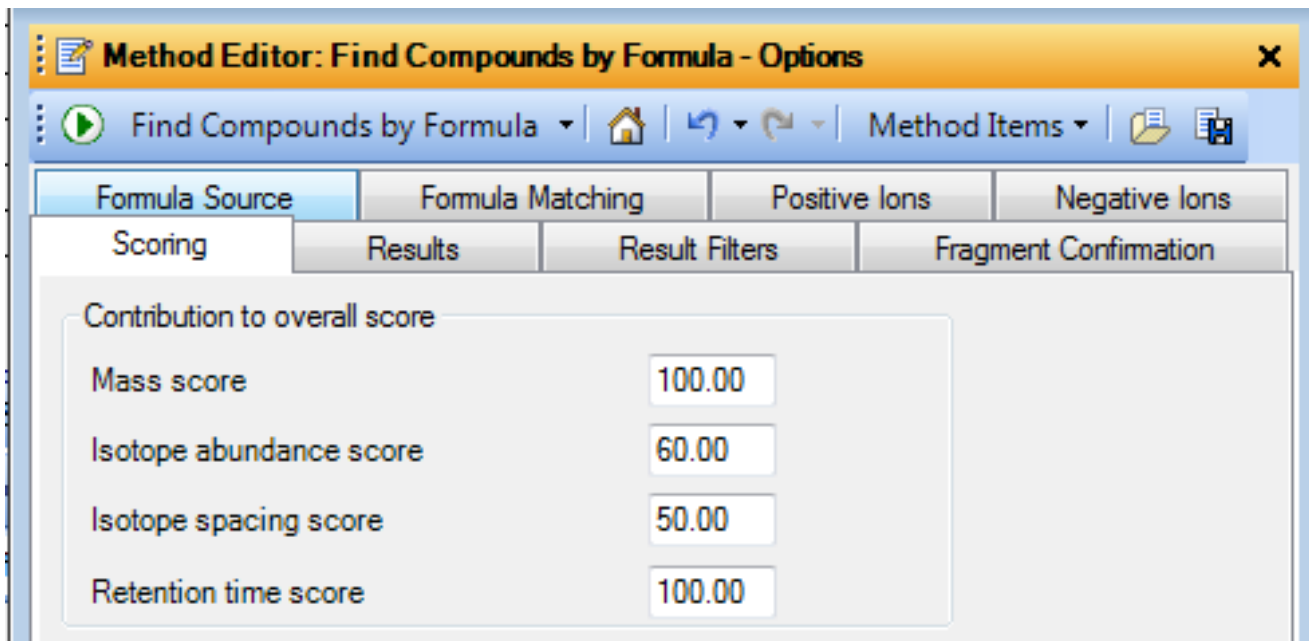
Absolute area >= 500 counts

Relative area >= 5.000 % of largest peak

Maximum number of peaks

Limit (by height) to the largest 5

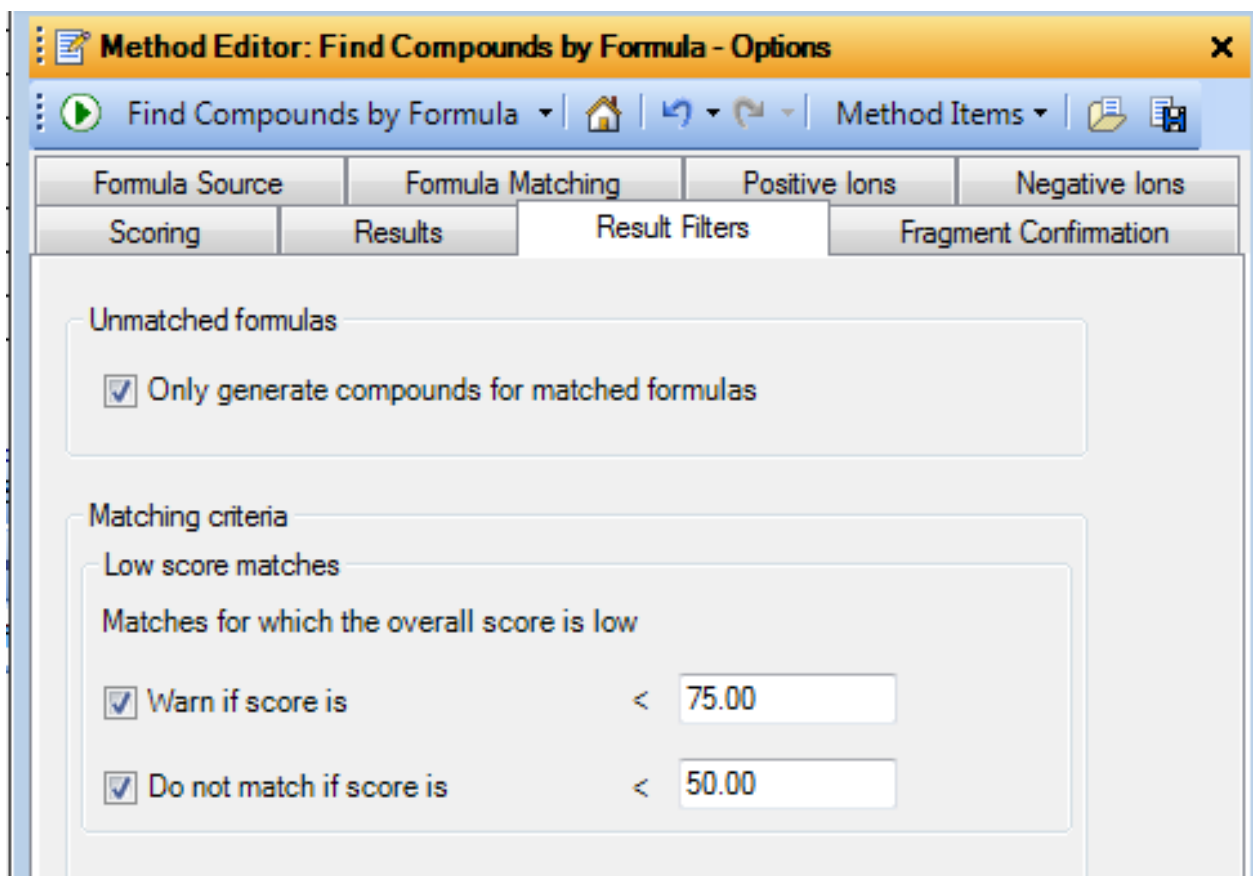
# Library Search - scoring



The screenshot shows a software window titled "Method Editor: Find Compounds by Formula - Options". The window has a toolbar with a play button, a dropdown menu for "Find Compounds by Formula", a home icon, a refresh icon, a "Method Items" dropdown, and file icons. Below the toolbar are four tabs: "Formula Source", "Formula Matching", "Positive Ions", and "Negative Ions". Under "Formula Source", there are four sub-tabs: "Scoring", "Results", "Result Filters", and "Fragment Confirmation". The "Scoring" sub-tab is active, showing a "Contribution to overall score" section with four rows of scores in input fields:

Contribution to overall score	
Mass score	100.00
Isotope abundance score	60.00
Isotope spacing score	50.00
Retention time score	100.00

# Library Search - scoring



**Method Editor: Find Compounds by Formula - Options**

Find Compounds by Formula | Home | Undo | Redo | Method Items | Save | Print

Formula Source	Formula Matching	Positive Ions	Negative Ions
Scoring	Results	Result Filters	Fragment Confirmation

Unmatched formulas

Only generate compounds for matched formulas

Matching criteria

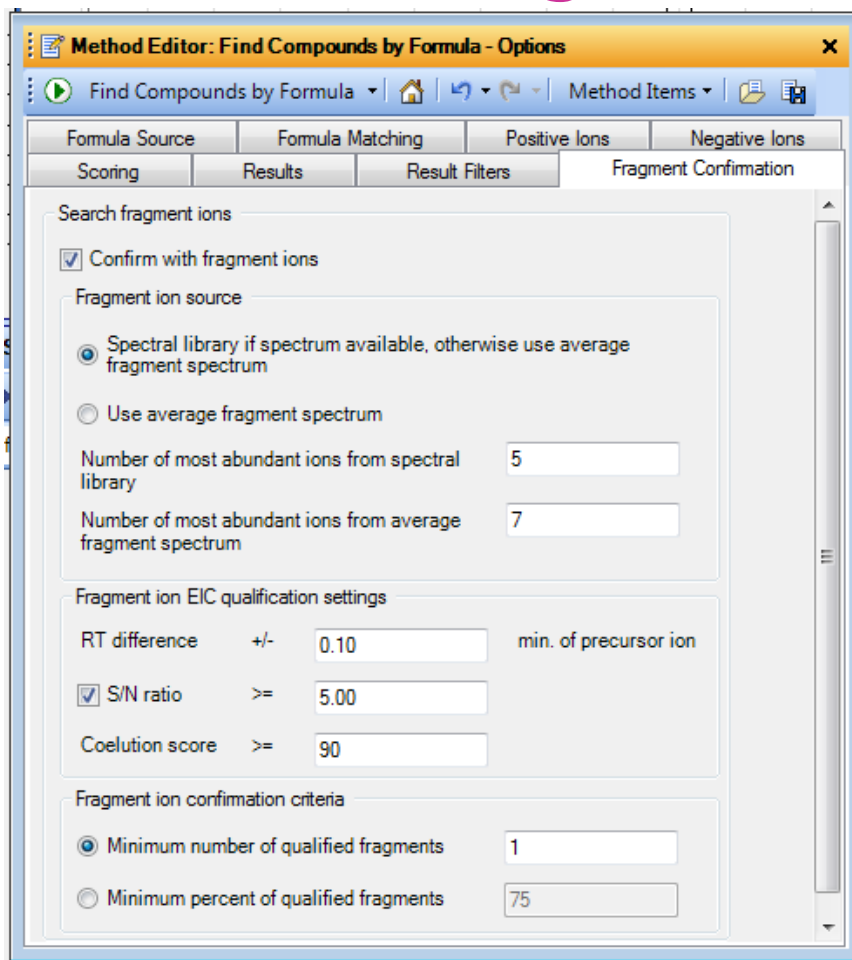
Low score matches

Matches for which the overall score is low

Warn if score is < 75.00

Do not match if score is < 50.00

# Library Search – fragment ions



**Method Editor: Find Compounds by Formula - Options**

Find Compounds by Formula | Method Items

Formula Source | Formula Matching | Positive Ions | Negative Ions

Scoring | Results | Result Filters | **Fragment Confirmation**

Search fragment ions

Confirm with fragment ions

Fragment ion source

Spectral library if spectrum available, otherwise use average fragment spectrum

Use average fragment spectrum

Number of most abundant ions from spectral library: 5

Number of most abundant ions from average fragment spectrum: 7

Fragment ion EIC qualification settings

RT difference +/-: 0.10 min. of precursor ion

S/N ratio >= 5.00

Coelution score >= 90

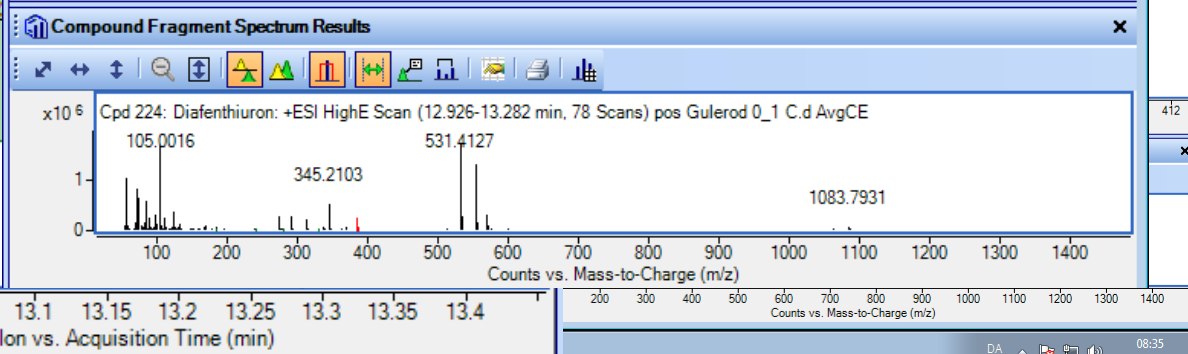
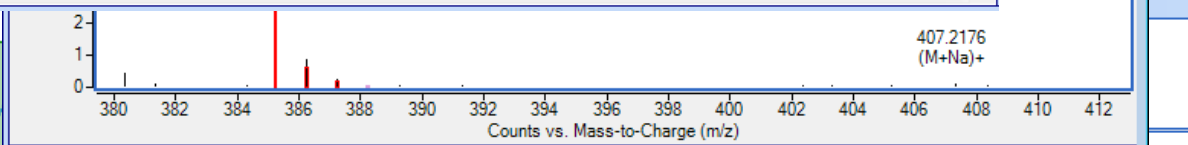
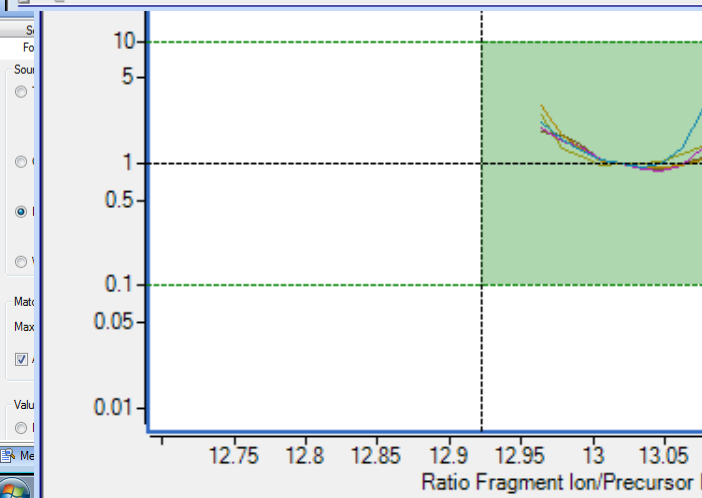
Fragment ion confirmation criteria

Minimum number of qualified fragments: 1

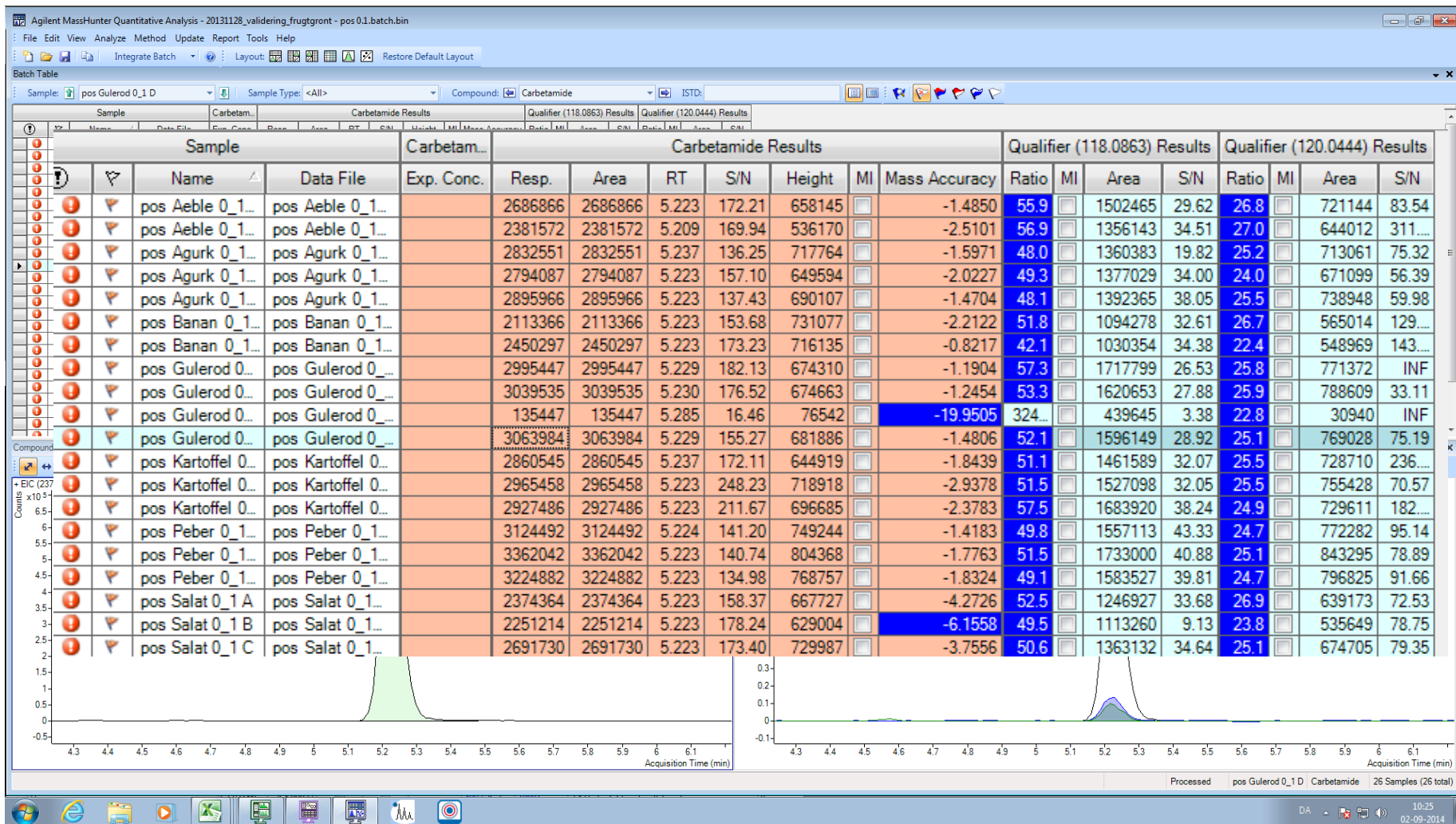
Minimum percent of qualified fragments: 75

# Compounds Detail View

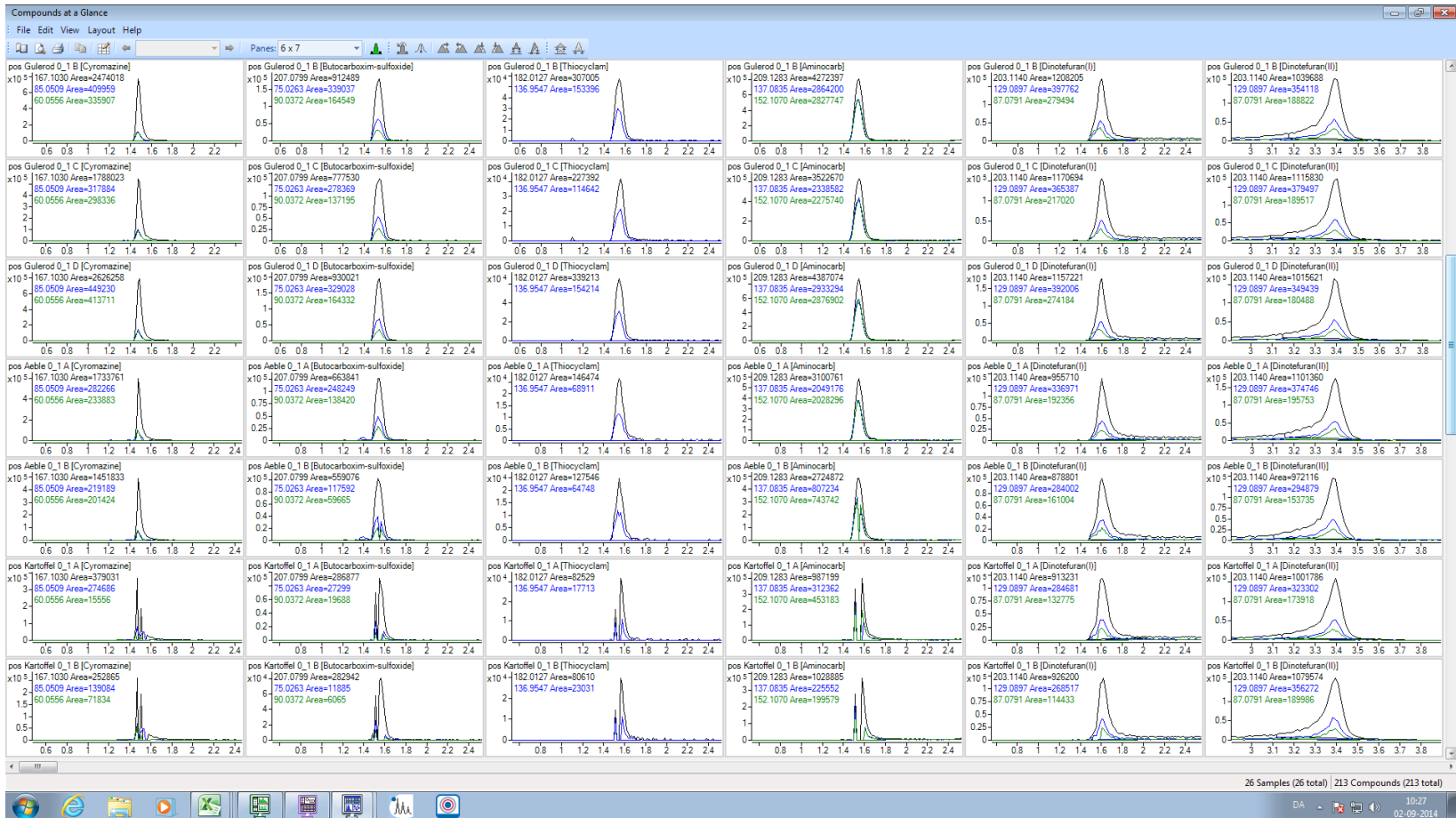
Name	File	Area	Flags (Tgt)	Score (Tgt)	Diff (Tgt, ppm)	RT	Fls Conf. %	Height	Label
Diafenthuron	pos Gulerod 0_1 C.d	3011903	Qualified	98.99	0.97	13.02	100	830295	Cpd 145: Diafenthuron
Dialifos	pos Gulerod 0_1 C.d	57085	low score; No H adduct; Not qualified	72.03	2.23	11.219	0	16335	Cpd 146: Dialifos
Diallate (cis)	pos Gulerod 0_1 C.d	298193	Not qualified	97.87	-2.43	11.666	0	87452	Cpd 147: Diallate (cis)
Diazinon (Dimpylate)	pos Gulerod 0_1 C.d	30298	low score; Not qualified	56.13	6.04	10.479	0	4747	Cpd 148: Diazinon (Dimpylate)
Dichlobutrazol (Diclobutrazol)	pos Gulerod 0_1 C.d	3711540	Qualified	97.82	2.44	8.706	40	1004092	Cpd 176: Dichlobutrazol
Dichlormid	pos Gulerod 0_1 C.d	337115	Qualified	93.67	-0.84	6.96	40	97892	Cpd 177: Dichlormid
Diclofop-methyl	pos Gulerod 0_1 C.d	9445	No H adduct; Not qualified	78.76	-1.79	11.791	0	3691	Cpd 178: Diclofop-methyl
Difenoxuron	pos Gulerod 0_1 C.d	15394443	Qualified	95.6	1.39	6.723	60	3321579	Cpd 179: Difenoxuron
Difenzoquat	pos Gulerod 0_1 C.d	522318	Not qualified	87.74	-3.55	10.241	0	125234	Cpd 180: Difenzoquat
Diflufenzopyr (BAS 65400H)	pos Gulerod 0_1 C.d	35893	Qualified	98.08	-0.54	5.788	20	10322	Cpd 189: Diflufenzopyr (BAS 65400H)
Dikegulac	pos Gulerod 0_1 C.d	100446	Qualified	84.36	-4.08	4.713	20	18756	Cpd 190: Dikegulac
Dimefuron	pos Gulerod 0_1 C.d	198250	Not qualified	89.71	-1.76	7.268	0	46406	Cpd 191: Dimefuron
Dimethenamid (SAN 582H)	pos Gulerod 0_1 C.d	5608712	Qualified	94.91	1.06	8.217	60	1407812	Cpd 105: Dimethenamid (SAN 582H)
Dimethirimol	pos Gulerod 0_1 C.d	5864509	low score; Not qualified	68.81	0.27	3.791	0	515838	Cpd 192: Dimethirimol
Dimethylvinphos	pos Gulerod 0_1 C.d	2496787	Not qualified	96.05	0.96	8.301	0	685828	Cpd 193: Dimethylvinphos
Diniconazole	pos Gulerod 0_1 C.d	1202204	low score; No H adduct; Not qualified	65.62	-8.13	9.306	0	252635	Cpd 194: Diniconazole
Dinotefuran(I)	pos Gulerod 0_1 C.d	1791595	Qualified	95.69	4.92	1.599	60	214284	Cpd 195: Dinotefuran(I)
Dinotefuran(II)	pos Gulerod 0_1 C.d	1648927	Qualified	97.3	0.88	3.4	80	229168	Cpd 196: Dinotefuran(II)



# MassHunter - Quantitative

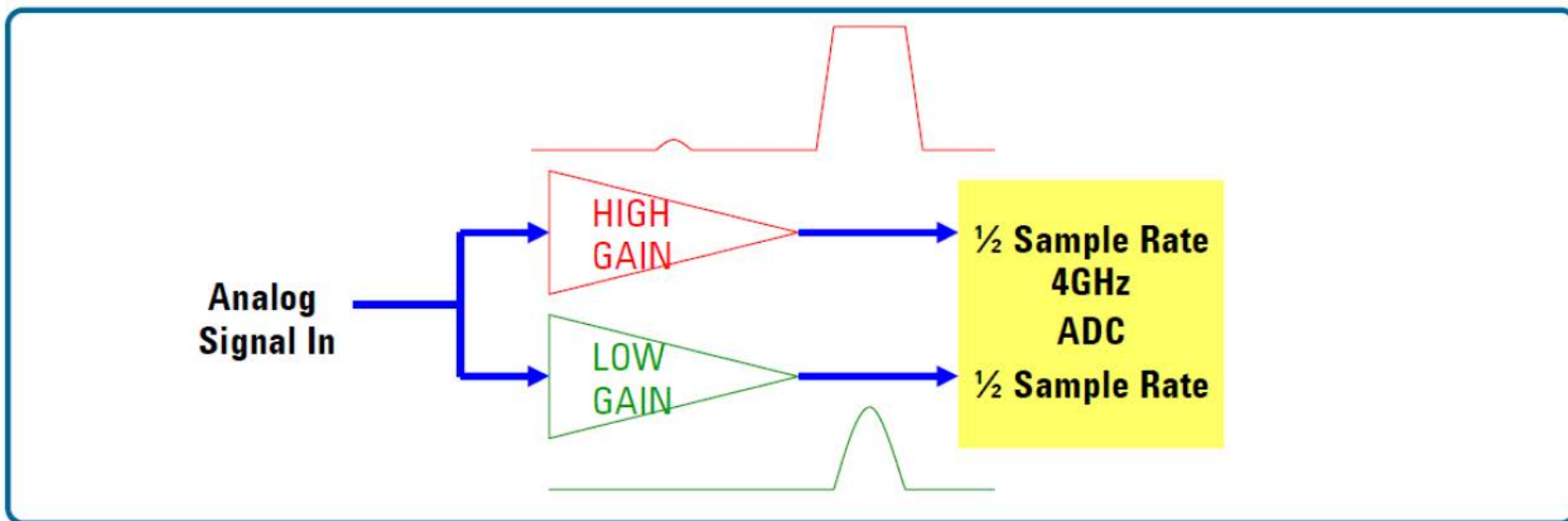


# Compound at a glance



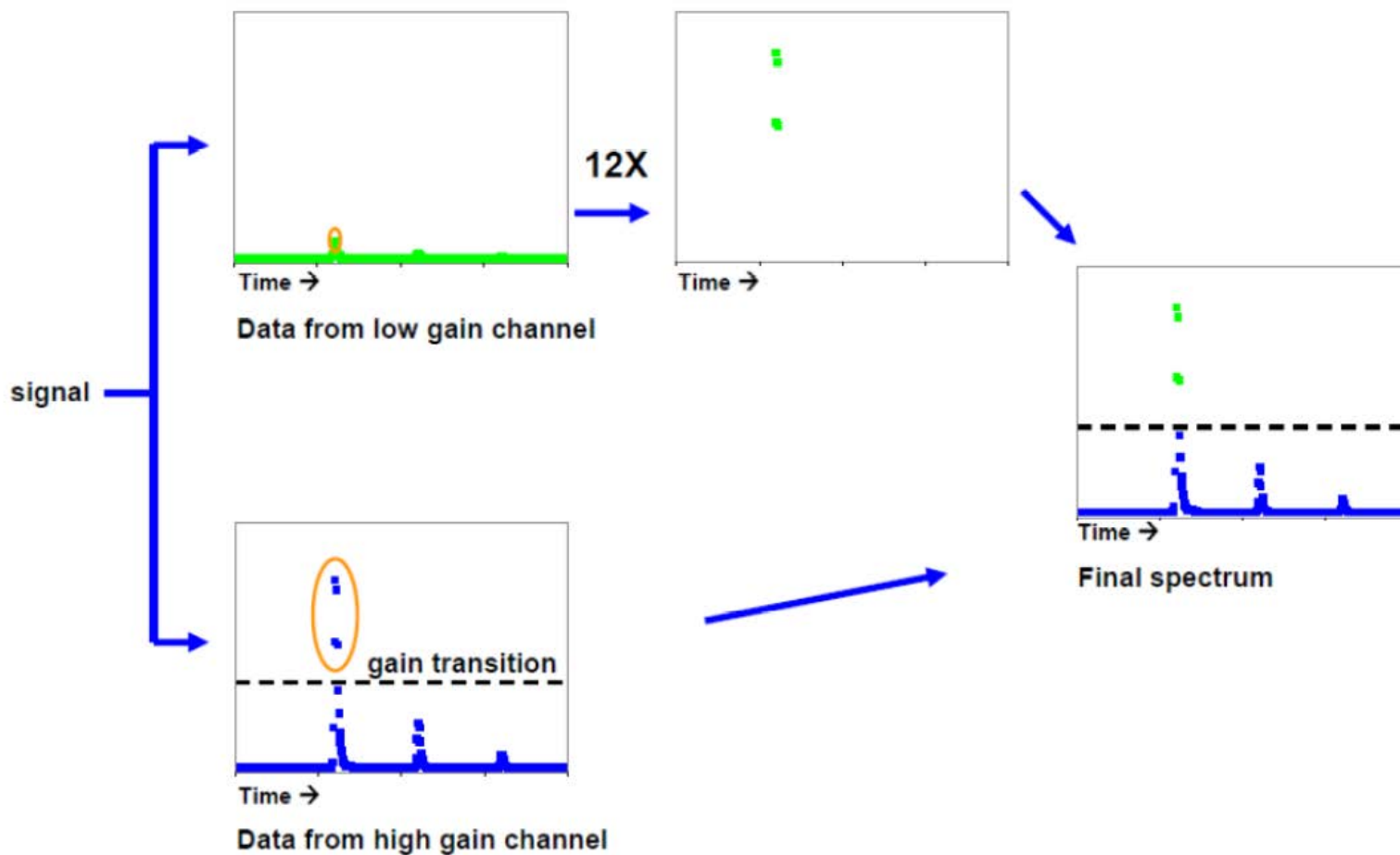


# 2GHz Extended Dynamic Range





# 2GHz Extended Dynamic Range



# Disposition

LC-QTOF screening - MassHunter Qualitative

LC-QTOF - Validation

GC-QTOF screening - MassHunter Quantitative

GC-QTOF - Validation

# Validation

- SANCO/12571/2013:

G9 The validation of a screening method based on a SDL can be focused on detectability. For each commodity group (see Annex 1), a basic validation should involve analysis of at least 20 samples spiked at the estimated SDL. The samples selected should represent multiple commodity categories from the commodity group, with a minimum of two different samples for each commodity category and should be representative for the intended scope of the laboratory. Additional validation data can be collected from on-going AQC-data and method performance verification during routine analysis.

## *Method performance acceptability criteria*

G10 When the screening method is only intended to be used as a qualitative method, there are no requirements with regard to recovery of the analytes. In order to determine the selectivity, the presence of false detects should be verified using non-spiked (preferably "blank") samples. Provided the analytes that are tentatively detected by the screening method are identified and confirmed by a second analysis of the sample using an appropriate confirmatory method, there is no need for a strict criterion for the number of false detects. The SDL of the qualitative screening method is the lowest level at which an analyte has been detected (not necessarily meeting the MS-identification criteria) in at least 95% of the samples (i.e. an acceptable false-negative rate of 5%).

## Validation – LC-QTOF

- We have validated at 3 different concentration levels in rye, oat, barley, wheat and rice.
- Amounts of pesticides (including isomers) validated:

SDL (mg/kg)	Pesticides validated
0.01	246
0.02	41
0.1	39

# Standard mixtures

Mixtures

50-100 pesticides

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Isomers

Avoiding isomers in the mixtures

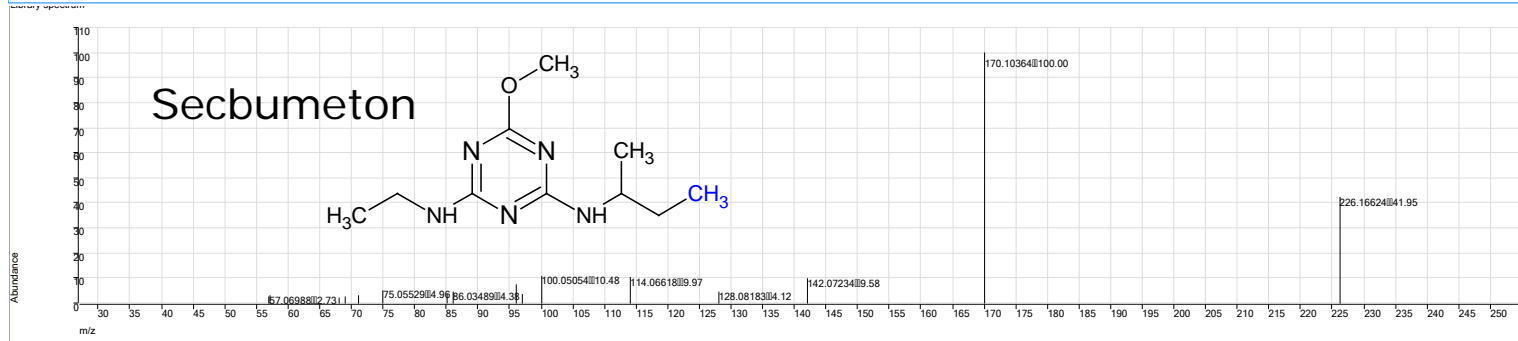
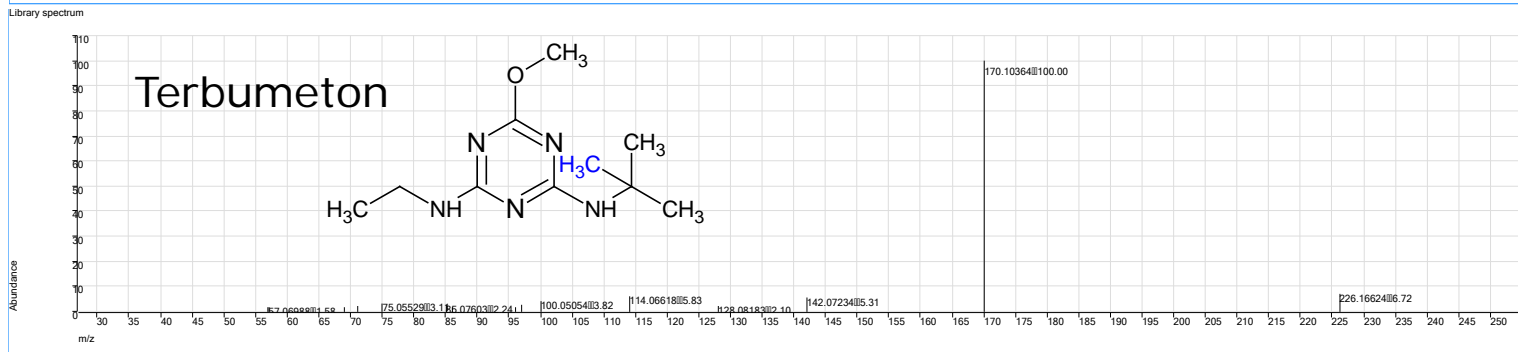
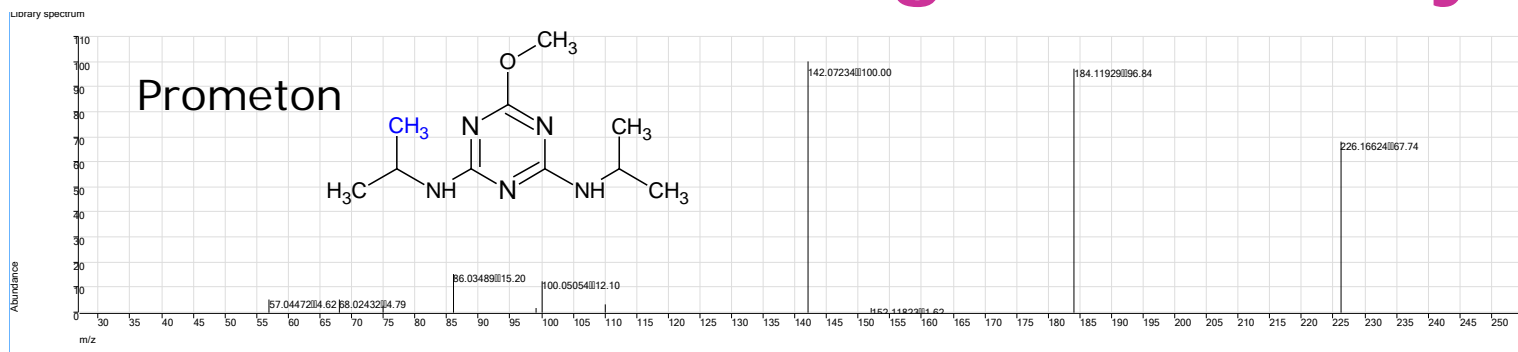
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Validation

2-6 mixtures together

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# Spectra of isomers in Agilents library



# Disposition

LC-QTOF screening - MassHunter Qualitative

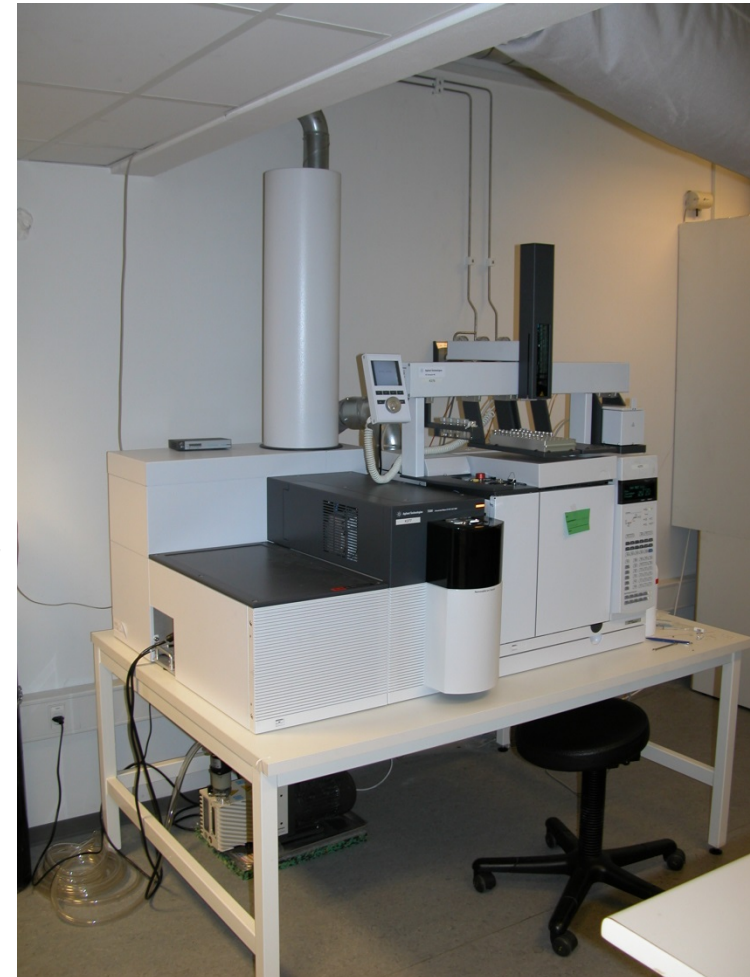
LC-QTOF - Validation

GC-QTOF screening - MassHunter Quantitative

GC-QTOF - Validation

## EURL-CF and GC-QTOF

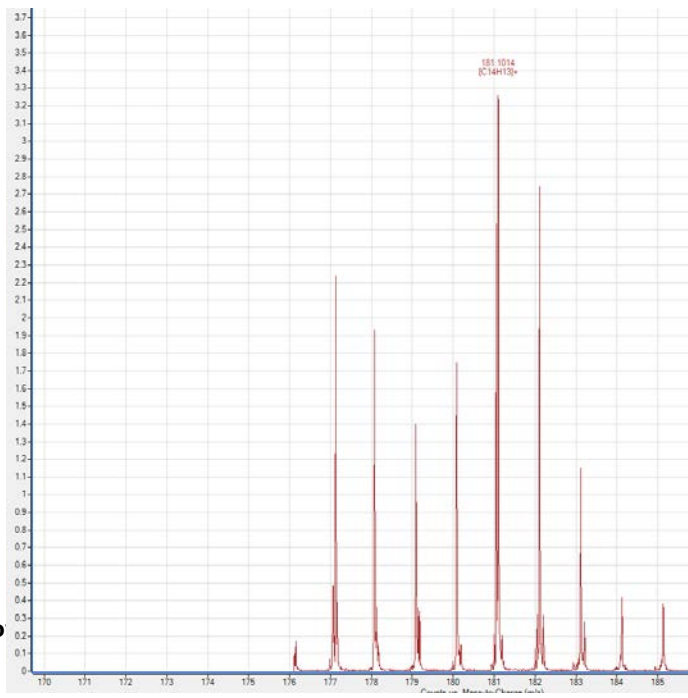
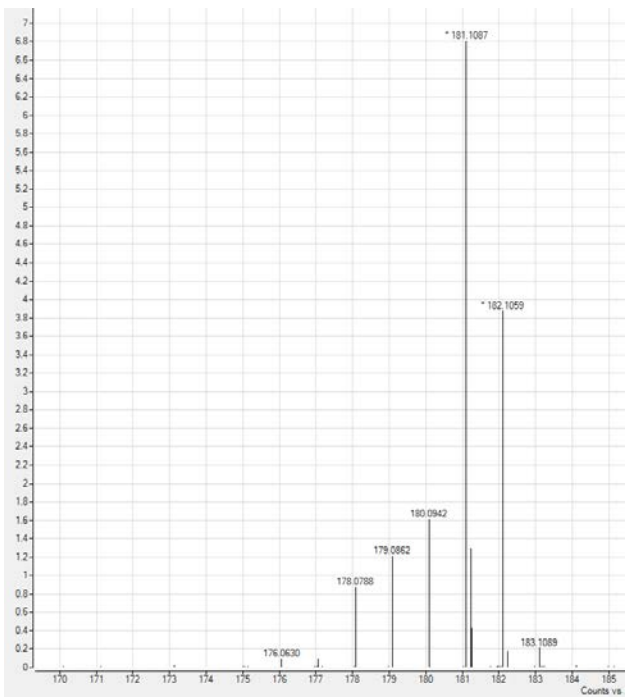
- TOF instrument: 7200 GC/Q-TOF, Agilent Technologies
- GC-system: 7890B, Agilent Technologies
  - back flush,
  - Gerstel PTV injector.
  - Two HP-5MS UI, 15 m, 0.250 mm dia, 0.25 mm filmtickness
  - PAL autosampler system and





# Conditions

- Ionisation mode: EI positive
- Acquisition rate: 4GHz
- Acquisition mode: Centroid or profile
- Source temperature 230 °C
- Software: MassHunter B 06.01.1312,

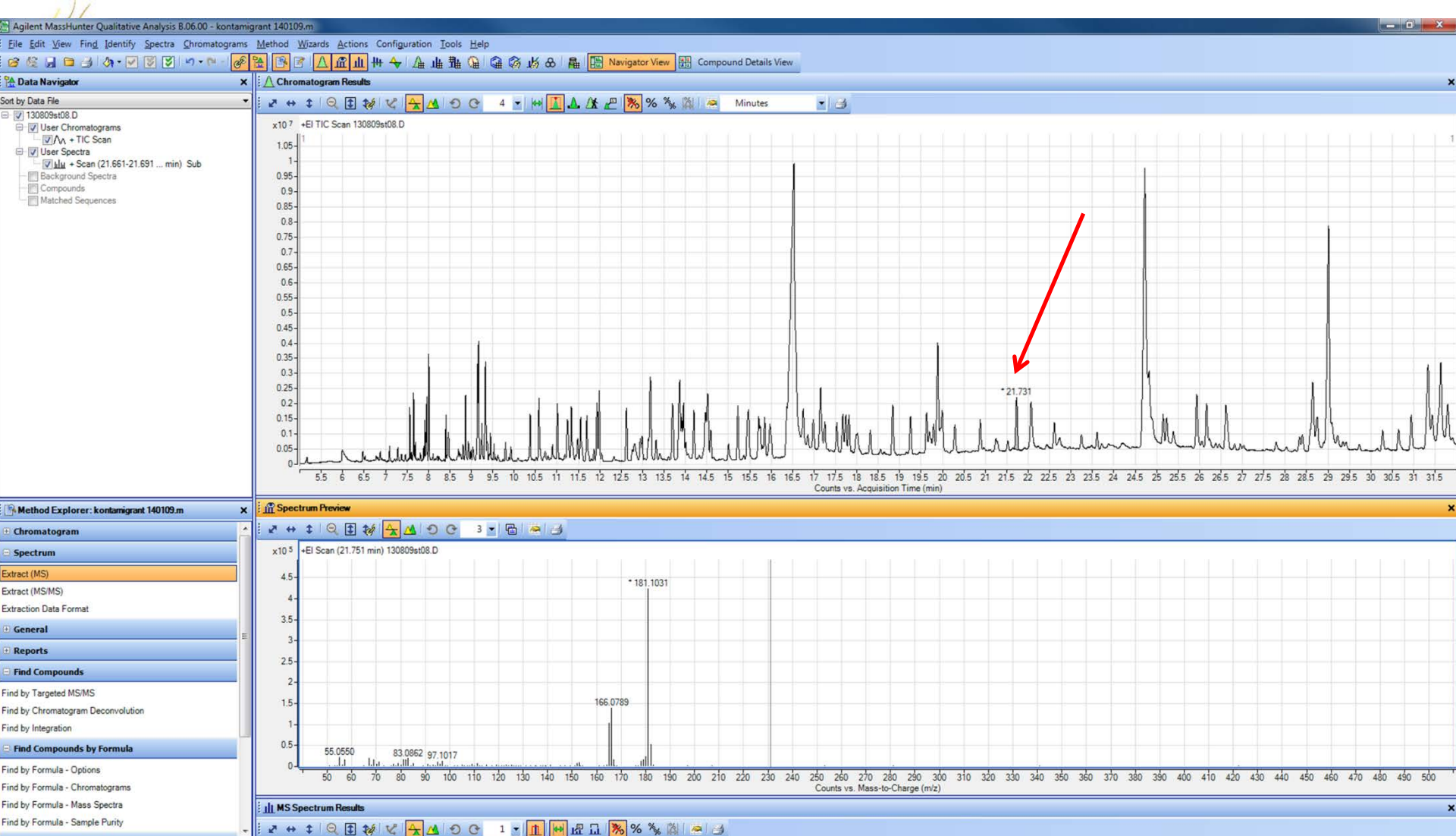


# PCDL library

- Exact masses of pesticides and fragments
- Retention time

	A	B	C	D	E	F	G	H	I	J	K
1	#	Compound database									
2	#										
3	#										
4	#	This is a compound formula database file used by Agilent MassHunter applications.									
5	#	Copy to a different file if you wish to make changes to database contents									
6	#	You can set the version (below) to any string value.									
7	#	We recommend changing it when you update the database contents.									
8	#										
9	#										
10	#	Version: the most recent-one									
11	#										
12	#										
13	#										
14	#	WARNING: User should not change the format of this file.									
15	#										
16	#	Each record in this file contins 5 columns described in the last comment in this comment block.									
17	#	Retention time and Description are optional.									
18	#	Each record should be kept on an individual line.									
19	#	Fields are separated by comma. Use quotes around a field that contains a comma.									
20	#										
21	#	The first two lines have to be comments which start with the '#' character.									
22	#	First line is 'Agilent TOF Formula data store'									
23	#	Second line is 'Version:' followed by a version number									
24	#										
25	#	Additional comments (such as these) may be inserted on individual									
26	#	lines by specifying a '#' character at the beginning of the line									
27	#										
28	#										
29	###	Formula	Retention	Mass	Compound name						
30	#	Formula	RT	Mass	Cpd						
31	C4H7O4P1	6.901	219.9459	Diclorvos							
32	C4H7O4P1	6.901	184.977	Diclorvos F1							
33	C2H6O3P1	6.901	109.0055	Diclorvos F2							
34	C2H3Cl2O	6.901	143.9299	Diclorvos F3							
35	C12H15NO	7.182	221.1052	Carbofuran							
36	C10H12O2	7.182	164.0837	Carbofuran F1							
37	C8H7NO2	7.182	149.0477	Carbofuran F2							
38	C8H5NO	7.182	131.0371	Carbofuran F3							
39	C7H5O2	7.182	121.029	Carbofuran F4							
40	C14H9N2O	7.261	310.0321	Diflubenzuron							
41	C7H5NOF2	7.261	157.0339	Diflubenzuron F1							
42	C7H3OF2	7.261	141.0152	Diflubenzuron F2							
43	C6H3F2	7.261	113.0203	Diflubenzuron F3							
44	C4H10NO2	7.933	183.0119	Acephate							

1	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
2	Formula	Retention Time	Mass	Compound		Description	C	H	D	N	O	P	S	Cl	F	Br	Si
423	C12H7OCl	28.111	202.0185426	Difenoconazole 1 F3	6		12	7			1			1			
424	C19H17N3O3Cl2	28.24	405.0646968	Difenoconazole 2	6		19	17		3	3			2			
425	C16H13O3Cl2	28.24	323.0241747	Difenoconazole 2 F1	6		16	13			3			2			
426	C13H7O2Cl2	28.24	264.9823099	Difenoconazole 2 F2	6		13	7			2			2			
427	C12H7OCl	28.24	202.0185426	Difenoconazole 2 F3	6		12	7			1			1			
428	C22H19NO3Br2	28.385	502.9731687	Deltamethrin 1	6		22	19		1	3					2	
429	C7H9Br2	28.385	250.9071005	Deltamethrin 1 F1	6		7	9								2	
430	C7H9Br	28.385	171.9887629	Deltamethrin 1 F2	6		7	9								1	
431	C22H19NO3Br2	28.776	502.9731687	Deltamethrin 2	6		22	19		1	3					2	
432	C7H9Br2	28.776	250.9071005	Deltamethrin 2 F1	6		7	9								2	
433	C7H9Br	28.776	171.9887629	Deltamethrin 2 F2	6		7	9								1	
434	C12H9NO3Cl2	12.3	284.9959486	Vinclozolin	6		12	9		1	3			2			
435	C7H3NOCl2	12.3	186.9591691	Vinclozolin F1	6		7	3		1	1			2			
436	C9H5NOCl2	12.3	212.9748192	Vinclozolin F2	6		9	5		1	1			2			
437	C10H8NCl2	12.3	212.0033797	Vinclozolin F3	6		10	8		1				2			
438	C10H16O	7.11	152.1201151	Carvone			10	16			1						
439	C10H14O	7.11	150.1044651	Carvone F1			10	14			1						
440	C8H14	7.11	110.1095504	Carvone F2			8	14									
441	C7H11	7.11	95.08607535	Carvone F3			7	11									
442	C20H32N2O3S		380.2133636	Carbosulfan			20	32		2	3		1				
443	C8H18NS		160.1159953	Carbosulfan F1			8	18		1			1				
444	C10H11O2		163.0759046	Carbosulfan F2			10	11			2						
445	C7H3O3		135.008219	Carbosulfan F3			7	3			3						
446	C6H3O2		107.0133043	Carbosulfan F4			6	3			2						
447	C12H8OCl6		377.8706311	Endrin			12	8			1			6			
448	C7H2Cl5		260.8599136	Endrin F1			7	2						5			
449	C5H5O		81.03403978	Endrin F2			5	5			1						
450	C12H8OCl5		342.9017784	Endrin F3			12	8			1			5			
451	C23H26O3		350.1881947	Phenothrin			23	26			3						
452	C13H11O		183.08099	Phenothrin F1			13	11			1						
453	C9H15		123.1173755	Phenothrin F2			9	15									
454			0														
455			0														
456			0														
457			0														
458			0														
459			0														
460			0														



# Exact masses of fragments

NIST MS Search 2.0 - [Simple, Reverse, Presearch Fast, Constrained - 76 spectra]

File Search View Tools Options Window Help

1. +EI Scan (21.037 min) 130823st02.D

Names: Structures

mainlib: replib: 243893 total spectra

#	Lib	Match	R.Match	Name
1	M	923	923	Bifenthrin
...	R			Bifenthrin
...	R			Bifenthrin
2	M	761	797	1,2,3,4-tetrahydro-4-phenanthreneacetic acid
3	M	751	797	1,2,3,4-tetrahydro-4-phenanthreneacetic acid
4	M	743	797	Propionamide, 2,2-diphenyl-N-(2-pyridinyl)-
5	M	755	783	2,6-Dimethyl-N-(2-methylphenyl)phenylamine
6	M	720	768	1-Methylsulfonyl-1,2-diphenylethane
7	M	653	767	7-Methyl-4-azafluorene
8	M	656	761	1,2,4-Triazolidine-3,5-dione, 4-phenyl-1-(9H-fluoren-2-yl)-
9	M	692	758	1,2,4-Triazolidine-3,5-dione, 4-phenyl-1-(1H-indol-3-yl)-
10	M	658	747	8-Methyl-4-azafluorene
11	R	709	736	4,4'-Dimethylbiphenyl
...	R			4,4'-Dimethylbiphenyl
...	R			4,4'-Dimethylbiphenyl
...	R			4,4'-Dimethylbiphenyl
12	M	729	729	Oxylis[α-cyclopropyl-(1-naphthyl)methyl]
13	R	684	728	3,3'-Dimethylbiphenyl
...	R			3,3'-Dimethylbiphenyl
...	M			3,3'-Dimethylbiphenyl
14	M	700	727	2,2-Diphenylpropylamine
15	M	694	725	Benzeneethanol, β-methyl-β-phenyl-
16	R	525	720	9H-Carbazole, 9-methyl-
...	R			9H-Carbazole, 9-methyl-
...	R			9H-Carbazole, 9-methyl-
...	R			9H-Carbazole, 9-methyl-
...	M			9H-Carbazole, 9-methyl-
17	M	524	719	(3S,5S,8aR)-3-Butyl-5-propyloctahydroindolizine
...	M			(3S,5R,8aR)-3-Butyl-5-propyloctahydroindolizine
18	R	680	714	1,1'-Biphenyl, 4-(1-methylethyl)-
...	M			1,1'-Biphenyl, 4-(1-methylethyl)-
19	M	689	708	Benzene, 1,1'-[1-(methylthio)ethylidene]bis-

**Name:** Bifenthrin  
**Formula:** C<sub>23</sub>H<sub>22</sub>ClF<sub>3</sub>O<sub>2</sub>  
**MW:** 422 **Exact Mass:** 422.126041 **CAS#:** 82657-04-3 **NIST#:** 291832 **ID#:** 148729 **DB:** mainlib  
**Other DBs:** RTECS  
**Contributor:** NIST Mass Spectrometry Data Center, 1998.  
**Related CAS#:** 107497-60-9; 92880-79-0; 107538-32-9  
**10 largest peaks:**  
 181 999 | 165 322 | 166 322 | 182 160 | 180 78 |  
 179 64 | 178 56 | 167 53 | 141 46 | 152 38 |  
**Synonyms:**

mainlib: replib: 243893 total spectra

Names: Structures

mainlib: replib: 243893 total spectra

4 Bifenthrin  
 5 Bifenthrine  
 6 Biphenate  
 7 Biphenin  
 8 Bigade  
 9 Capture  
 10 Cyclopropanecarboxylic acid, 3-(1Z)-2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, (2-methyl(1,1'-biphenyl)-3-yl)methyl ester, (1R,3R)-rel-  
 11 Cyclopropanecarboxylic acid, 3-(2-chloro-3,3,3-trifluoro-1-propenyl)-2,2-dimethyl-, (2-methyl[1,1'-biphenyl]-3-yl)methyl ester, [1α,3α(Z)]-  
 12 DeterMite  
 13 Discoiline  
 14 Empower  
 15 Fanfare  
 16 FMC 54800  
 17 TalstarOne

Estimated non-polar retention index (n-alkane scale):  
 Value: 2551 lu  
 Confidence interval (Diverse functional groups): 89(50%) 382(95%) lu

Lib. Search Other Search Names Compare Librarian MSMS

Simple Simple Rev

Bifenthrin - MS Interpreter

File Edit View Options Help

Formula Calculator

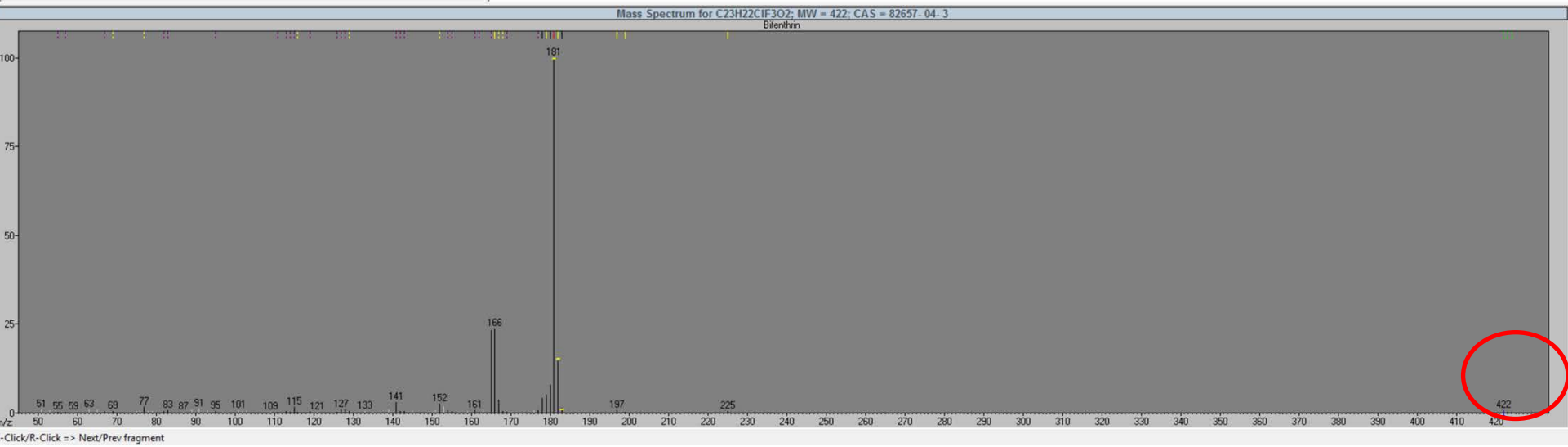
m = 181 C23H22ClF3O2

Calculate Options Parent = 422 Loss = 241

37 Ions	O+E	RDB	Mass	C	H	Cl	F	O
C9ClF2	Even	8.5	180.96566	9	0	1	2	0
C6HClF3O	Even	4.5	180.96680	6	1	1	3	1
C12H2Cl	Even	11.5	180.98450	12	2	1	0	0
C9H3ClFO	Even	7.5	180.98565	9	3	1	1	1
C6H4ClF2O2	Even	3.5	180.98679	6	4	1	2	2
C9F3O	Even	8.5	180.99012	9	0	0	3	1
C7H5ClF3	Even	3.5	181.00319	7	5	1	3	0
C9H6ClO2	Even	6.5	181.00563	9	6	1	0	2
C15H	Even	15.5	181.00783	15	1	0	0	0
C12H2FO	Even	11.5	181.00897	12	2	0	1	1
C9H3F2O2	Even	7.5	181.01011	9	3	0	2	2
C10H7ClF	Even	6.5	181.02203	10	7	1	1	0

Structure, Maximum Dissociation = 98

m/z	mass	formula	loss	type	rate	abund
181 (1/3)	181.101726	C14H13	C9H9ClF3O2	dissociation	0	999



- Bifenthrin – mass 422.126041

Bifenthrin - MS Interpreter

File Edit View Options Help

Formula Calculator

m = 166 C23H22ClF3O2

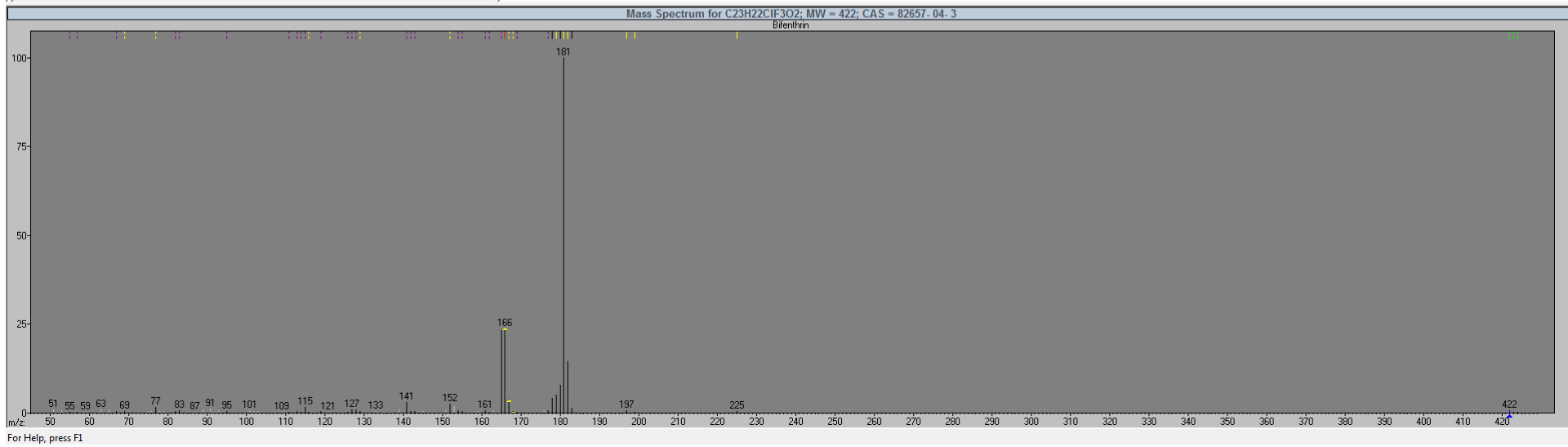
Calculate Options Parent = 422 Loss = 256

32 Ions	O+E	RDB	Mass	C	H	Cl	F	O
C8ClFO	Odd	8	165.96217	8	0	1	1	1
C5HCIF2O2	Odd	4	165.96331	5	1	1	2	2
C6H2CIF3	Odd	4	165.97971	6	2	1	3	0
C8H3ClO2	Odd	7	165.98216	8	3	1	0	2
C8F2O2	Odd	8	165.98664	8	0	0	2	2
C9H4ClF	Odd	7	165.99856	9	4	1	1	0
C6H5ClF2O	Odd	3	165.99970	6	5	1	2	1
C9HF3	Odd	8	166.00303	9	1	0	3	0
C11H2O2	Odd	11	166.00548	11	2	0	0	2
C9H7ClO	Odd	6	166.01854	9	7	1	0	1
C6H8ClFO2	Odd	2	166.01969	6	8	1	1	2
C12H3F	Odd	11	166.02188	12	3	0	1	0

Structure, Maximum Dissociation = 98

m/z	mass	formula	loss	type	rate	abund
166	166.07825	C13H10	C9H9ClF3O2 + CH3	dissociation	0	236

- CH3





Bifenthrin - MS Interpreter

File Edit View Options Help

mz=165 (1/3)

Structure, Maximum Dissociation = 98

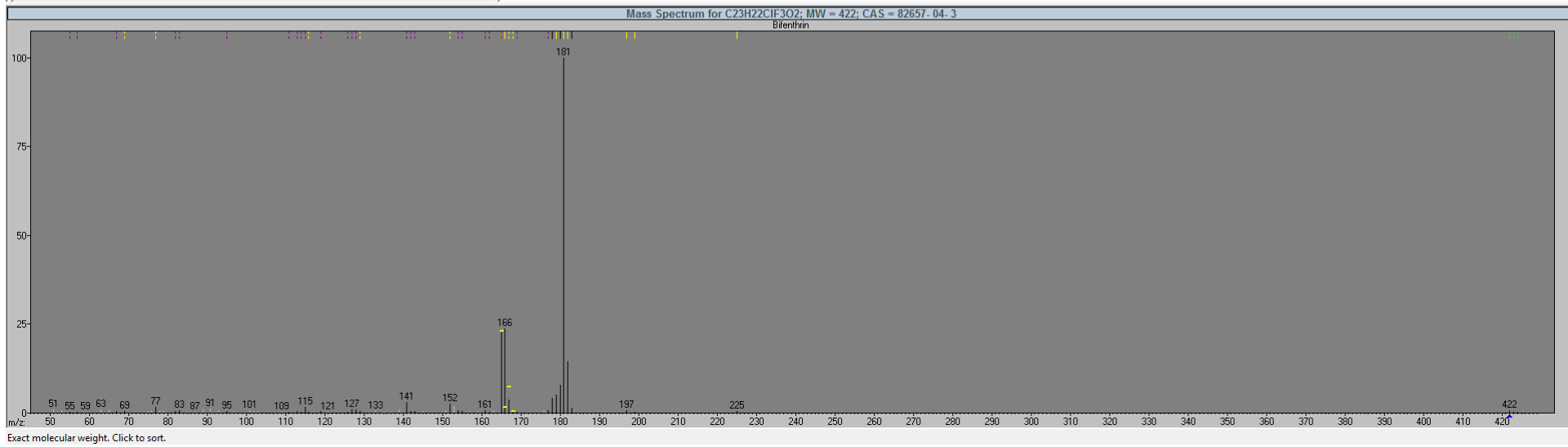
Formula Calculator

m = 165 C23H22ClF3O2

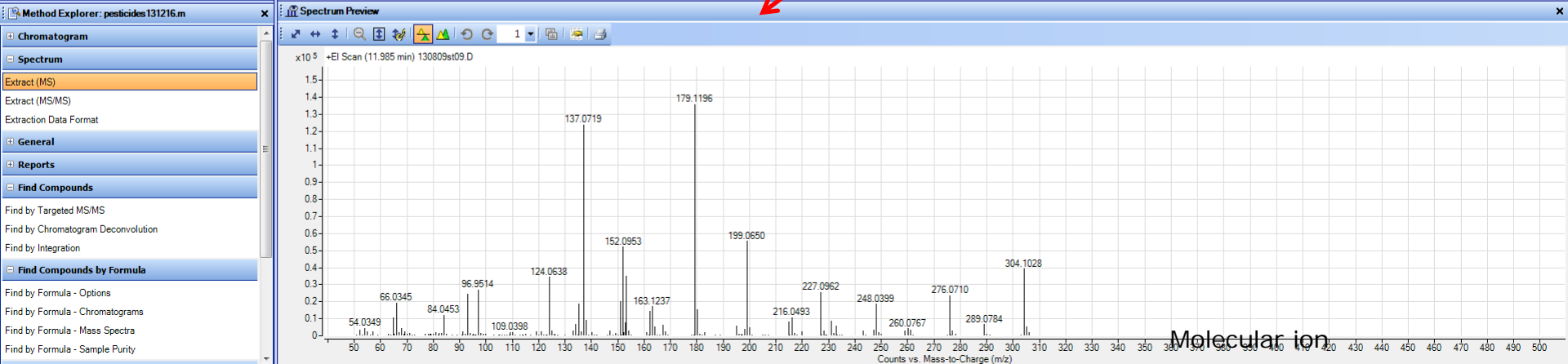
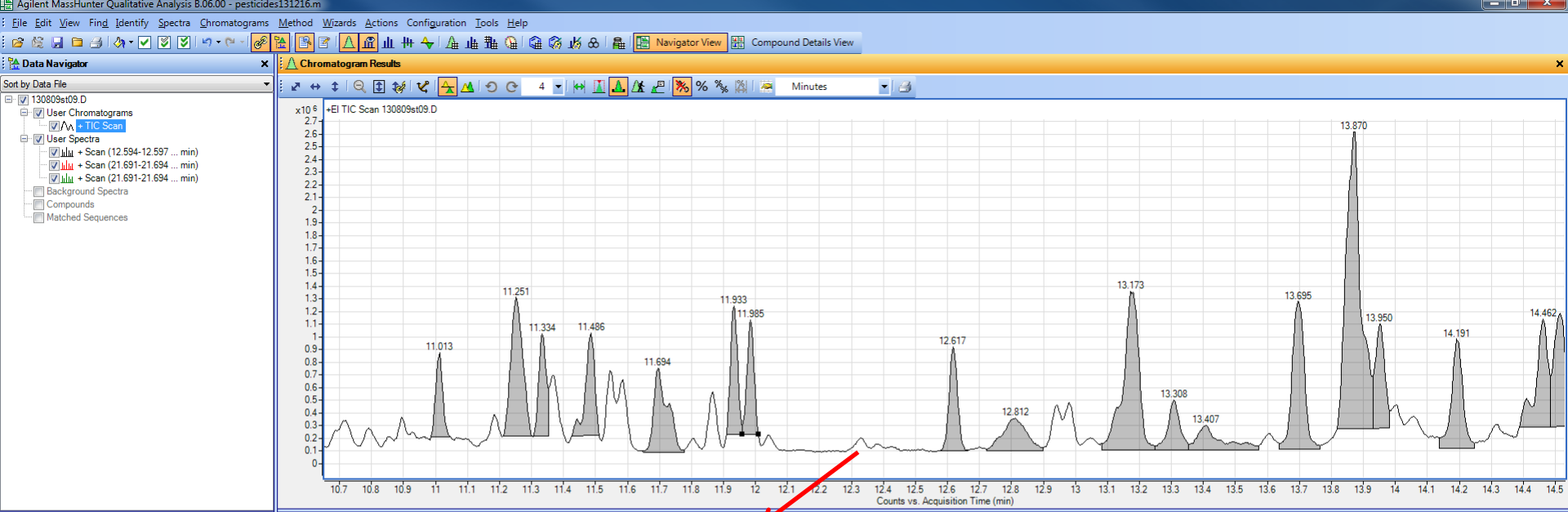
Calculate Options Parent = 422 Loss = 257

34 Ions	O+E	RDB	Mass	C	H	Cl	F	O
C <sub>5</sub> ClF <sub>2</sub> O <sub>2</sub>	Even	4.5	164.95549	5	0	1	2	2
C <sub>6</sub> HClF <sub>3</sub>	Even	4.5	164.97189	6	1	1	3	0
C <sub>8</sub> H <sub>2</sub> ClO <sub>2</sub>	Even	7.5	164.97433	8	2	1	0	2
C <sub>9</sub> H <sub>3</sub> ClF	Even	7.5	164.99073	9	3	1	1	0
C <sub>6</sub> H <sub>4</sub> ClF <sub>2</sub> O	Even	3.5	164.99187	6	4	1	2	1
C <sub>3</sub> H <sub>5</sub> ClF <sub>3</sub> O <sub>2</sub>	+	0	164.99302	3	5	1	3	2
C <sub>9</sub> F <sub>3</sub>	Even	8.5	164.99521	9	0	0	3	0
C <sub>11</sub> HO <sub>2</sub>	Even	11.5	164.99765	11	1	0	0	2
C <sub>9</sub> H <sub>6</sub> ClO	Even	6.5	165.01072	9	6	1	0	1
C <sub>6</sub> H <sub>7</sub> ClFO <sub>2</sub>	Even	2.5	165.01186	6	7	1	1	2
C <sub>12</sub> H <sub>2</sub> F	Even	11.5	165.01405	12	2	0	1	0
C <sub>9</sub> H <sub>3</sub> F <sub>2</sub> O	Even	7.5	165.01520	9	3	0	2	1

m/z	mass	formula	loss	type	rate	abund
165 (1/3)	165.028259	C <sub>7</sub> H <sub>8</sub> ClF <sub>2</sub>	C <sub>16</sub> H <sub>14</sub> FO <sub>2</sub>	unspecified	NA	231







NIST MS Search 2.0 - [Simple, Reverse, Match, Constrained - 85 spectra]

File Search View Tools Options Window Help

1. +EI Scan (11.985 min) 130809st09.D

mainlib; replib: 243893 total spectra

Names Structures Spec List

1000 900 800 700 600 500 400

#	Lib.	Match	R.Match	Name
1	R	967	967	Diazinone
2	M	278	813	2-Acetoxy-5-hydroxyacetophenone
3	R	172	770	1,1'-Biphenyl, 3-nitro-
4	M	280	755	2-Acetoxy-3-hydroxyacetophenone
5	M	184	731	(4S,6R,9aR)-4-Methyl-6-propyloctahydro-1H-quinolizine
6	R	149	727	Acenaphthylene, 1,2-dihydro-5-nitro-
7	M	225	725	1,4,5,6-Tetramethyl-2-pyrimidone
8	M	258	698	1-(4-Dodecyloxy-2-hydroxy-phenyl)-ethanone
9	R	324	680	1,4-Benzenediol, 2,3,5-trimethyl-
10	R	281	677	Resorcinol, 2-acetyl-
11	M	279	673	2,6-Dihydroxyacetophenone, bis(trimethylsilyl) ether
12	R	187	671	6-Mercaptopurine
13	R	175	668	Piperonyl alcohol

Names Structures Hit List

Lib Search Other Search Names Compare Librarian MSMS

Plot of Search Spectrum

Plot of Search Spectrum

Plot of Text of Spec List

Name: +EI Scan (11.985 min) 130809st09.D  
 MW: N/A [ID#]: 3130 [DB]: Text File  
 10 largest peaks:  
 179 991 | 137 908 | 199 407 | 152 382 | 304 287 |  
 153 256 | 124 252 | 97 198 | 227 188 | 93 179 |  
 Synonyms:  
 no synonyms.

Plot of Search Spectrum

Plot of Search Spectrum

Plot of Text of Spec List

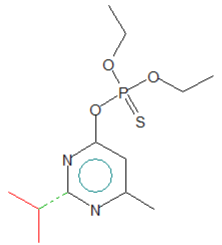
Name: Diazinone  
 Formula: C<sub>12</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub>P  
 MW: 264.34 [Exact Mass]: 304.10105 [CAS#]: 333-41-5 [NIST#]: 378524 [ID#]: 24900 [DB]: replib  
 Other DBs: Fine, TSCA, RTECS, EPA, USP, HODOC, NIH, EINECS, IRDB  
 Contributor: D.G.Hayward MS, Center for Food Safety and Applied Nutrition, FDA, College Park MD.  
 Related CAS#: 30583-38-1; 27936-40-9; 65863-03-8  
 10 largest peaks:  
 179 991 | 137 991 | 152 611 | 199 528 | 153 411 |  
 93 332 | 304 259 | 124 258 | 227 254 | 151 245 |  
 Synonyms:  
 1 Dimpylate  
 2 Phosphorothioic acid, O,O-diethyl O-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester  
 3 Phosphorothioic acid, O,O-diethyl O-(2-isopropyl-6-methyl-4-pyrimidinyl) ester  
 4 Artrigal  
 5 Baudin  
 6 Bazudin  
 7 Ciazinon  
 8 Dacutox  
 9 Dasstox  
 10 Diazinon AG 500  
 11 Dacid  
 12 Dimpylat  
 13 Exodin  
 14 ENT 19,507  
 15 Fyrol  
 16 G 301  
 17 G-24480  
 18 Galesan  
 19 Garden Tox  
 20 Neocidol

Chemical Structure: CCOP(=S)(OCC)Oc1cc(C)c(C)n1

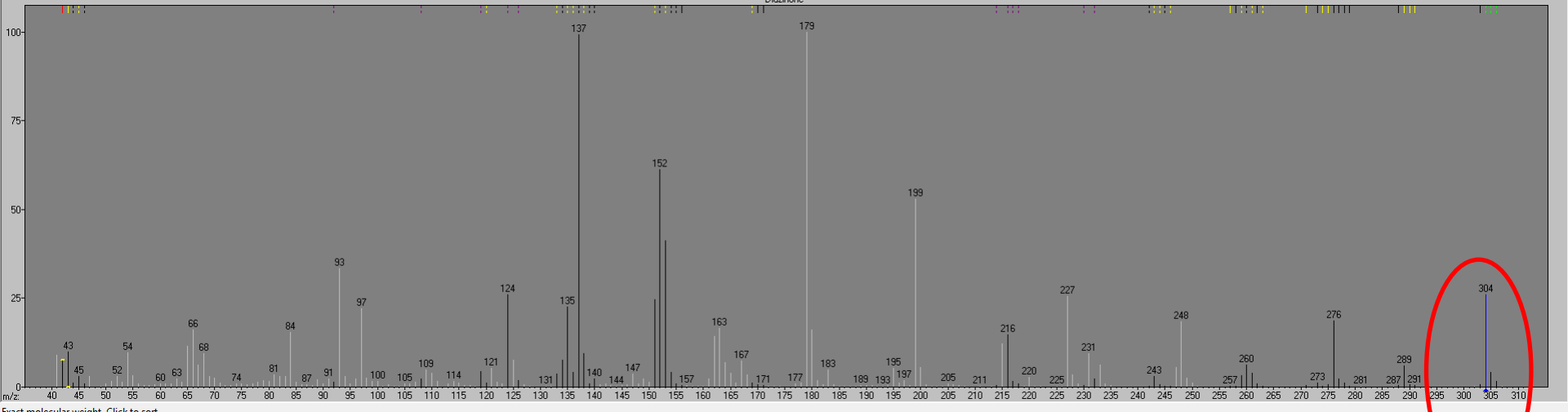
84 Ions	O+E	RDB	Mass	C	H	N	O	P
C7O2PS	Even	8.5-11.5	178.93566	7	0	0	2	1
C6N2OPS	Even	8.5-13.5	178.94690	6	0	2	1	1
C7H2NOPS	Odd	8-12	178.95947	7	2	1	1	1
C6N2O3P	Even	8.5-11.5	178.96465	6	0	2	3	1
C7HNO3S	Odd	8-11	178.96771	7	1	1	3	0
C3H4N2O3PS	Even	3.5-8.5	178.96802	3	4	2	3	1
C11OP	Even	12.5-13.5	178.96868	11	0	0	1	1
C8H4OPS	Even	7.5-10.5	178.97205	8	4	0	1	1
C7H2NO3P	Odd	8-10	178.97723	7	2	1	3	1
C10N2P	Even	12.5-15.5	178.97991	10	0	2	0	1
C8H3O3S	Even	7.5-9.5	178.98029	8	3	0	3	0

m/z	mass	formula	loss	type	H	rate	abund
42	42.04695	C3H6	C9H15N2O3PS	dissociation	-1	-15*	77

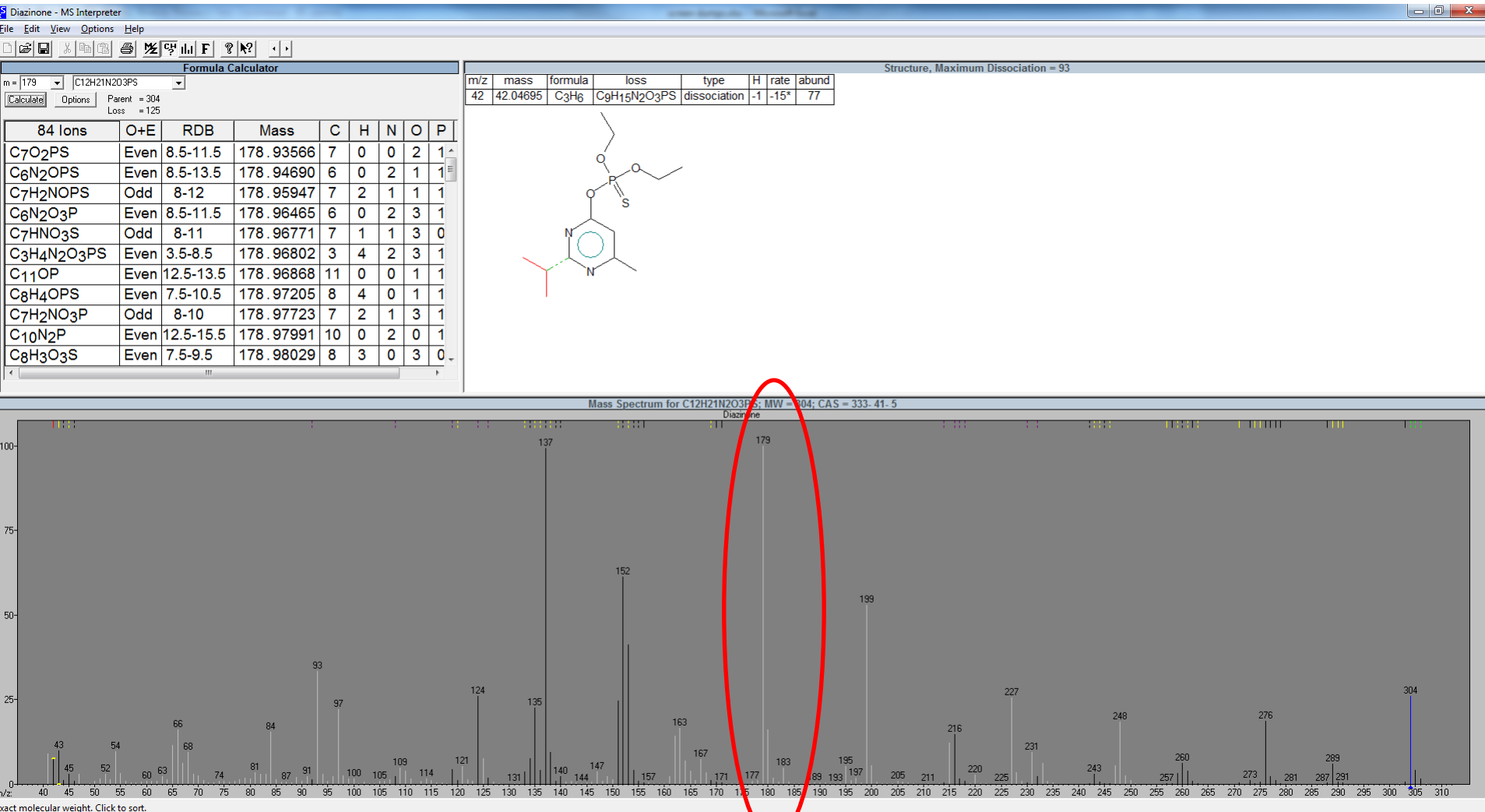
Structure, Maximum Dissociation = 93



Mass Spectrum for C12H21N2O3PS; MW = 304; CAS = 333-41-5



Exact molecular weight. Click to sort.



e - MS Interpreter

View Options Help

Formula Calculator

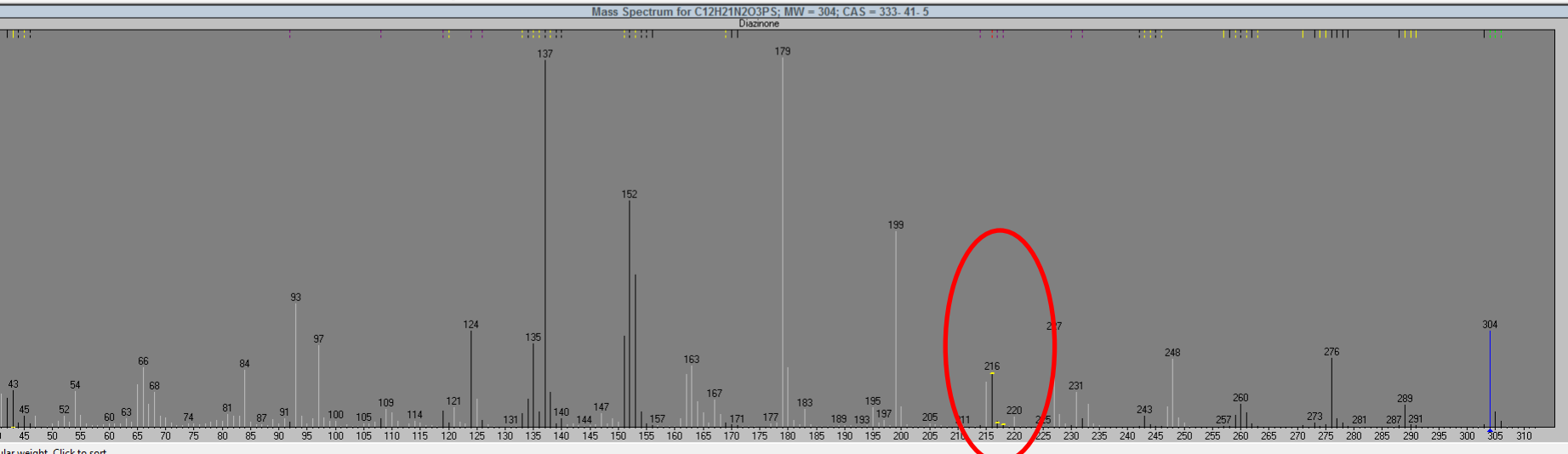
C12H21N2O3PS

Options Parent = 304 Loss = 88

9 Ions	O+E	RDB	Mass	C	H	N	O	P
O2PS	Odd	11-14	215.94349	10	1	0	2	1
O2OPS	Odd	11-16	215.95472	9	1	2	1	1
O3S	Odd	11-15	215.96296	9	0	2	3	0
O3NOPS	Even	10.5-14.5	215.96730	10	3	1	1	1
O2O3P	Odd	11-14	215.97248	9	1	2	3	1
O2NO3S	Even	10.5-13.5	215.97554	10	2	1	3	0
N2O3PS	Odd	6-11	215.97585	6	5	2	3	1
O5OPS	Odd	10-13	215.97987	11	5	0	1	1
O3NO3P	Even	10.5-12.5	215.98505	10	3	1	3	1
O4O3S	Odd	10-12	215.98811	11	4	0	3	0
NO3PS	Even	5.5-9.5	215.98843	7	7	1	3	1

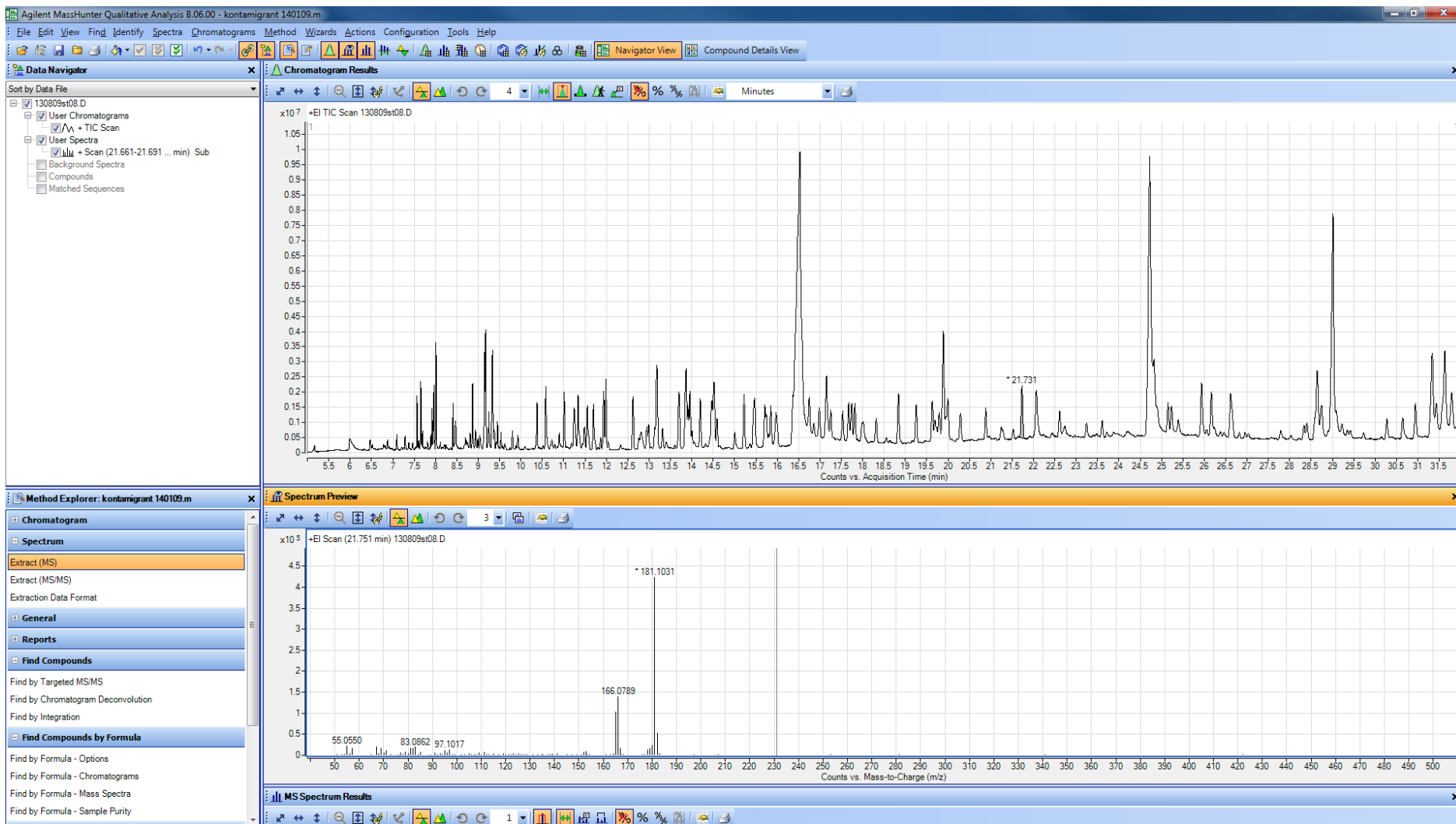
m/z	mass	formula	loss	type	rate	abund
216 (1/2)	216.012236	C7H9N2O2PS	C5H12O	unspecified	N/A	146

Structure, Maximum Dissociation = 93



ular weight. Click to sort.

# Qualitative software



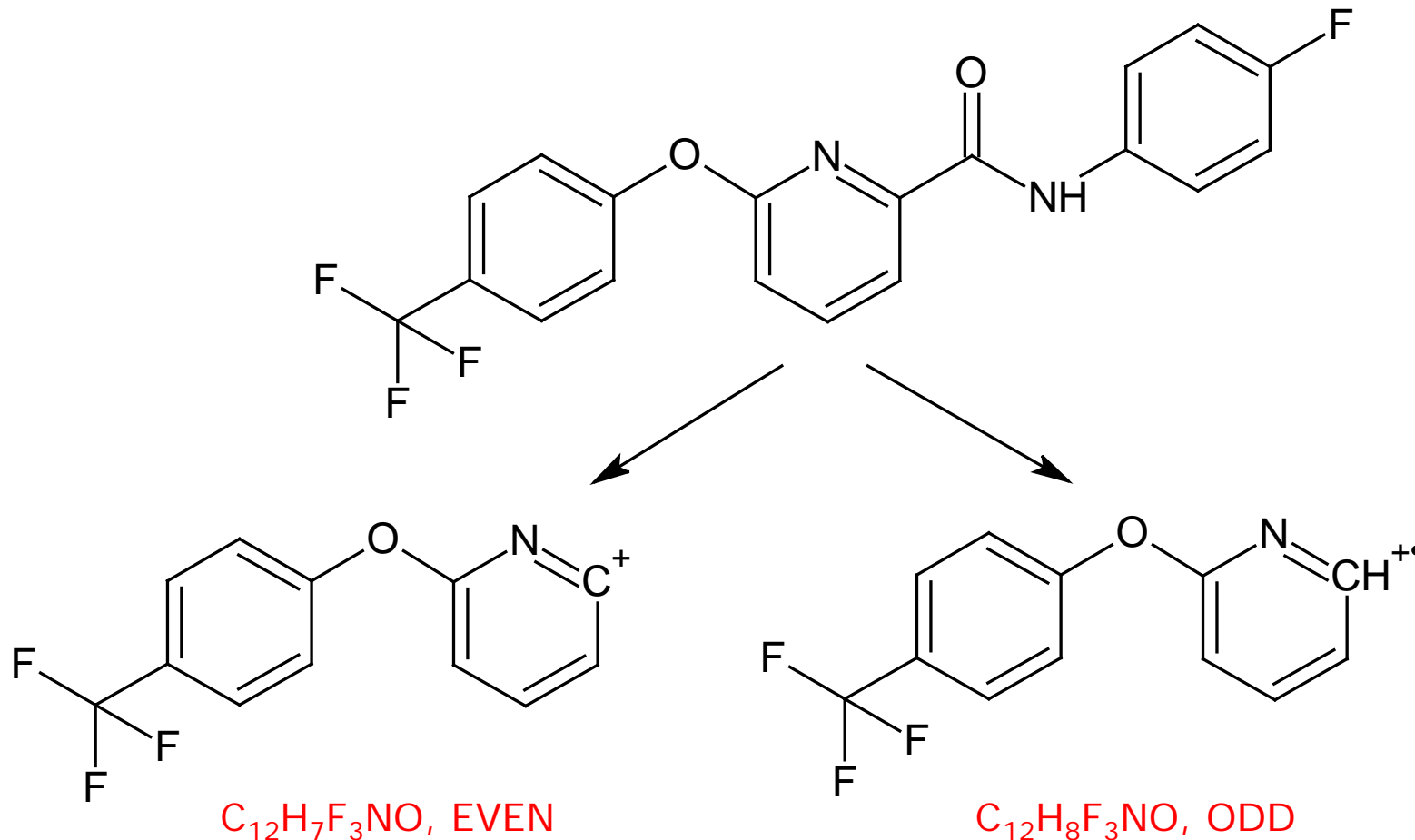
Name	RT (Tgt)	RT	Height	Mass (DB)	Mass	Diff (DB, pp)	Score	Flags (Tgt)	Flag Severity (Tgt)	Formula	Ions	File
Atrazin	10.72	10.71	33758	215.0938	215.0946	-3.69	93.88		Pass	C8 H14 Cl N5	5	130923st0
Atrazin F1	10.72	10.71	66926	200.0703	200.0712	-4.48	96.5		Pass	C7 H11 Cl N5	5	130923st0
Atrazin F2	10.72	10.71	19056	173.0468	173.0462	3.71	76.83		Pass	C5 H8 Cl N5	4	130923st0
Atrazin F3	10.72	10.71	12094	172.039	172.0402	-7.11	59.21	low score; ion count	Warning	C5 H7 Cl N5	1	130923st0
Bromoxynil	10.06	10.038	26297	274.8581	274.8588	-2.55	97.19		Pass	C7 H3 Br2 N O	6	130923st0
Clomazone F1	10.84	10.816	16023	204.1025	204.103	-2.66	97.44		Pass	C12 H14 N O2	3	130923st0
Clomazone F2	10.84	10.812	23311	125.0158	125.0159	-0.84	97.9		Pass	C7 H6 Cl	4	130923st0
Cyfluthrin F1	25.75	25.743	2109	226.0668	226.0673	-2.23	63.63	low score; ion count	Warning	C14 H9 F N O	1	130923st0
Cyfluthrin F2	25.75	25.739	9220	163.0081	163.0087	-3.41	88.91		Pass	C7 H9 Cl2	4	130923st0
Cyfluthrin F3	25.75	25.749	2858	199.0559	199.0572	-6.69	68.13	low score	Warning	C13 H8 F O	2	130923st0
Cyfluthrin F4	25.75	25.759	923	227.0746	227.0741	2.25	74.82	low score	Warning	C14 H10 F N O	2	130923st0
Dieldrin	16.66	16.632	4149	377.8706	377.8708	-0.56	96.55		Pass	C12 H8 Cl6 O	9	130923st0
Dieldrin F1	16.66	16.639	8759	274.8756	274.8761	-2.01	88.88		Pass	C8 H4 Cl5	8	130923st0
Dieldrin F2	16.66	16.639	13372	260.8599	260.8609	-3.68	76.51		Pass	C7 H2 Cl5	4	130923st0
Flufenacet	13.94	13.904	603	363.0665	363.0664	0.22	81.24		Pass	C14 H13 F4 N3 O2 S	2	130923st0
Flufenacet F1	13.94	13.908	9049	210.9789	210.9796	-3.23	95		Pass	C5 H2 F3 N2 O2 S	3	130923st0
Flufenacet F2	13.94	13.904	13296	151.0797	151.08	-2.01	82.03		Pass	C9 H10 F N	2	130923st0
Flufenacet F3	13.94	13.911	5285	136.0563	136.0567	-3.12	77.59		Pass	C8 H7 F N	2	130923st0
Metramitron	16.95	16.92	2588	202.0855	202.0861	-3.31	86.6		Pass	C10 H10 N4 O	2	130923st0
Metramitron F1	16.95	16.923	2201	174.0905	174.0917	-6.75	79.2		Pass	C9 H10 N4	2	130923st0
Metramitron F2	16.95	16.92	3401	104.05	104.0501	-0.44	86.45		Pass	C7 H6 N	2	130923st0
Metramitron F3	16.95	16.917	1061	173.0827	173.0831	-2.34	61.33	low score; ion count	Warning	C9 H9 N4	1	130923st0
Metribuzin F1	12.32	12.287	18809	198.0701	198.0705	-2.02	88.61		Pass	C8 H12 N3 O S	4	130923st0
Metribuzin F2	12.32	12.287	2130	182.0388	182.0393	-2.49	93.63		Pass	C7 H8 N3 O S	3	130923st0
Metribuzin F3	12.32	12.284	1934	144.047	144.0471	-0.75	95.25		Pass	C4 H8 N4 S	3	130923st0
Molinate	8.81	8.802	1185	187.1031	187.1032	-0.38	96.99		Pass	C9 H17 N O S	3	130923st0
Molinate F1	8.81	8.798	11463	126.0919	126.092	-1.19	99.28		Pass	C7 H12 N O	3	130923st0
Molinate F2	8.81	8.805	2809	98.097	98.0972	-2.64	91.37		Pass	C6 H12 N	2	130923st0
Oxamyl F2	8.74	8.719	725	145.0436	145.0445	-6.39	76.35		Pass	C5 H9 N2 O S	3	130923st0
Picolinafen	21	20.974	31497	376.0835	376.0843	-2.13	96.92		Pass	C19 H12 F4 N2 O2	4	130923st0
Picolinafen F1	21	20.971	25213	239.0558	239.0558	-0.05	96.61		Pass	C12 H8 F3 N O	3	130923st0
Picolinafen F2	21	20.971	40926	238.048	238.0489	-3.84	60.18	low score; ion count	Warning	C12 H7 F3 N O	1	130923st0
Prosulfocarb	12.94	12.922	10355	251.1344	251.1352	-3.33	96.32		Pass	C14 H21 N O S	4	130923st0
Prosulfocarb F1	12.94	12.922	3045	160.0796	160.0801	-3.05	92.11		Pass	C7 H14 N O S	3	130923st0
Prosulfocarb F2	12.94	12.922	26712	128.1075	128.1076	-0.86	99		Pass	C7 H14 N O	3	130923st0
Quinoclamine	13.4	13.388	4839	207.0087	207.0108	-9.88	87.71		Pass	C10 H6 Cl N O2	4	130923st0
Quinoclamine F1	13.4	13.392	3570	172.0399	172.0403	-2.83	89.79		Pass	C10 H6 N O2	2	130923st0
Quinoclamine F2	13.4	13.392	983	144.0449	144.0453	-2.36	91.14		Pass	C9 H6 N O	2	130923st0
Triflumizole F1	15.4	15.369	1669	278.056	278.0563	-1.19	92		Pass	C12 H12 Cl F3 N O	3	130923st0
Triflumizole F2	15.4	15.376	1139	287.0437	287.043	2.44	74.8	low score	Warning	C12 H9 Cl F3 N3	3	130923st0
Triflumizole F3	15.4	15.372	1495	205.9984	205.9995	-5.08	59.35	low score; ion count	Warning	C8 H4 Cl F3 N	1	130923st0

# Score system

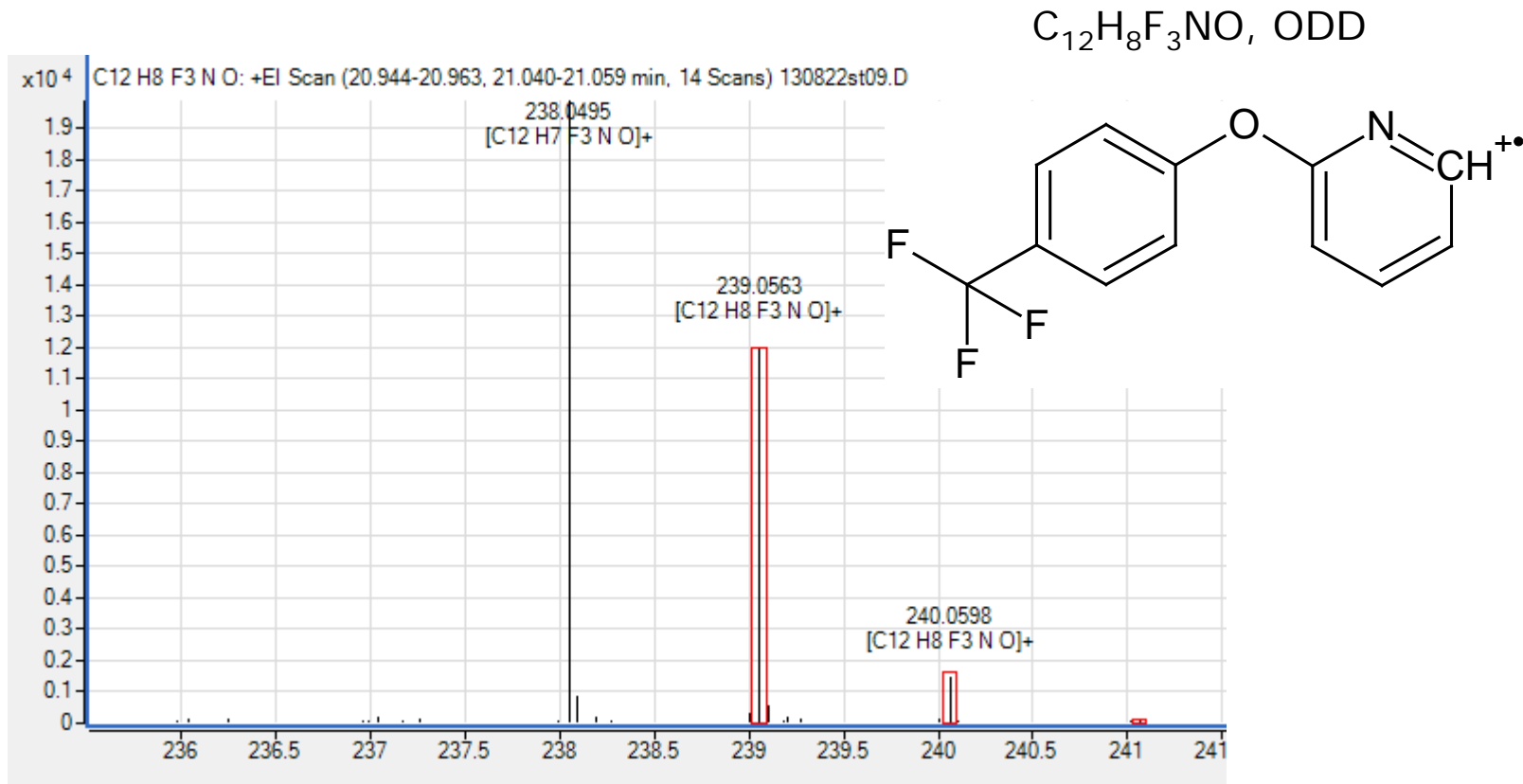
- *Mass Match Score* is the weighted aggregate of the individual metrics calculated when comparing an actual spectrum with a spectrum pattern synthesized from a formula.
  - *Mass Spacing Score*
  - *Mass Accuracy Score*
  - *Mass Abundance Score*
  - *Isotope abundance score*
  - *Isotope spacing score*



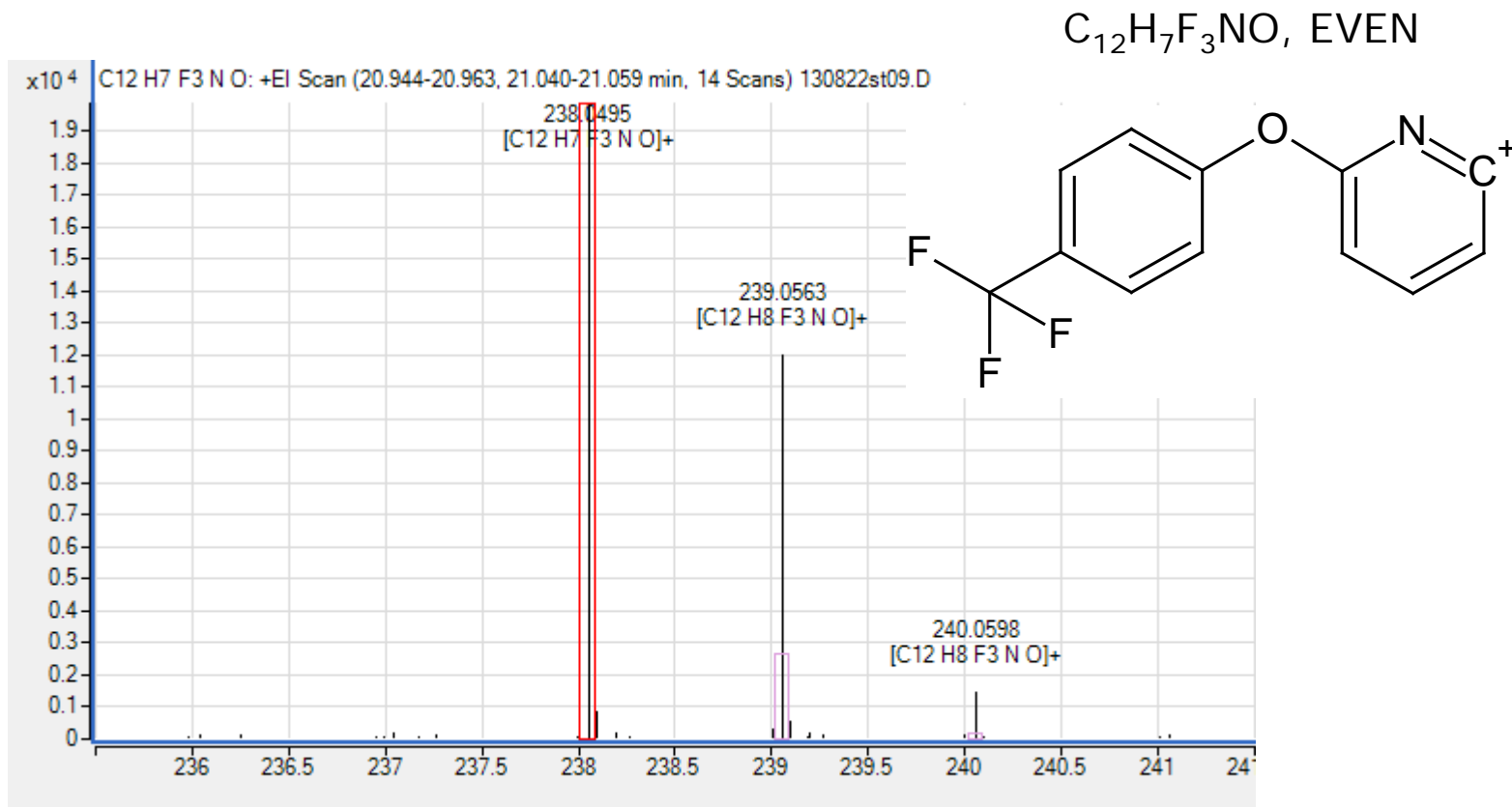
# Picolinafen - overlapping fragments



# Picolinafen - overlapping fragments



# Picolinafen - overlapping fragments



# Low score - poor isotop pattern

Show/Hide	Cpd	Label	Name	Formula	Score	Mass
<input checked="" type="checkbox"/>	1	Cpd 1: Picolinafen	Picolinafen	C <sub>19</sub> H <sub>12</sub> F <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	85.46	376.0863
<input checked="" type="checkbox"/>	2	Cpd 2: Picolinafen F2	Picolinafen F2	C <sub>12</sub> H <sub>7</sub> F <sub>3</sub> N O	54.51	238.05
<input checked="" type="checkbox"/>	3	Cpd 3: Picolinafen F1	Picolinafen F1	C <sub>12</sub> H <sub>8</sub> F <sub>3</sub> N O	93.43	239.0571

# Quantitative processing used qualitative

Agilent MassHunter Quantitative Analysis - 140107 - Validation\_Standard\_A\_0.1\_140218-10ppm.batch.bin

File Edit View Analyze Method Update Report Tools Help

Batch Table

Sample: EUP2-C2 no 059 wheat spk... Sample Type: <All> Compound: Pirimiphos-methyl ISTD:

Sample	Name	Data File	Type	Level	MZ	RT	Pirimiphos-methyl Results				Qualifier (276.0573) Results				Qualifier (305.0962) Results					
							Resp.	Calc. Conc.	Accuracy	Mass Accuracy	Int. Metric	S/N	Ratio	S/N	Mass Accuracy	Int. Metric	Ratio	S/N	Mass Accuracy	Int. Metric
▼	EUP2-C2 no 059 wheat spk. 0.1 ug/ml	140110st06.D	Sample		290.0730	13.1307	39153	0.0264		-3	Accepted	3651	73.0	1279	-2	Accepted	58.8	2716	-2	Accepted
▼	EUP2-SRM6 no 047 rice spk. 0.1 ug/ml	140110st07.D	Sample		290.0730	13.1307	44284	0.0291		-1	Accepted	2847	78.0	1880	-1	Accepted	59.4	892	-1	Accepted
▼	EUP2-C4 no 008 rye spk. 0.1 ug/ml	140110st08.D	Sample		290.0730	13.1307	37952	0.0257		-3	Accepted	4752	75.5	4030	-3	Accepted	60.4	1172	-3	Accepted
▼	EUP2-C6 no 207 barley spk. 0.1 ug/ml	140110st09.D	Sample		290.0730	13.1307	37704	0.0256		-2	Accepted	1807	74.5	1445	-2	Accepted	60.4	1904	-1	Accepted
▼	EUP2-C2 no 059 wheat spk. 0.1 ug/ml	140110st10.D	Sample		290.0730	13.1307	38369	0.0260		-3	Accepted	2324	77.2	1550	-2	Accepted	59.1	1698	-3	Accepted
▼	EUP2-SRM6 no 047 rice spk. 0.1 ug/ml	140110st11.D	Sample		290.0730	13.1307	43437	0.0287		-3	Accepted	3076	75.2	1527	-3	Accepted	59.4	1530	-3	Accepted
▼	EUP2-C4 no 008 rye spk. 0.1 ug/ml	140110st12.D	Sample		290.0730	13.1307	38999	0.0263		-3	Accepted	5074	75.4	912	-3	Accepted	59.5	1270	-3	Accepted
▼	EUP2-C6 no 207 barley spk. 0.1 ug/ml	140110st13.D	Sample		290.0730	13.1307	37058	0.0253		-3	Accepted	4323	74.2	908	-2	Accepted	58.5	1415	-2	Accepted
▼	Standard A Cal 3 - 0.1 ug/ml wheat	140110st14.D	Cal	Cal 3	290.0730	13.1307	183761	0.1040	104.0	-2	Accepted	15200	72.8	4147	-2	Accepted	56.5	9409	-2	Accepted
▼	Blank EUP2-SRM6 no 047 rice spk.	140110st15.D	MatrixBlank		290.0730	13.1307	791	0.0058		-2	Accepted	70	66.8	29	-1	Accepted	58.0	39	-3	Accepted
▼	EUP2-C2 no 059 wheat spk. 0.1 ug/ml	140110st16.D	Sample		290.0730	13.1307	35735	0.0245		-2	Accepted	43	76.5	2034	-2	Accepted	59.2	1322	-2	Accepted
▼	EUP2-SRM6 no 047 rice spk. 0.1 ug/ml	140110st17.D	Sample		290.0730	13.1307	40554	0.0271		-2	Accepted	2174	77.1	3266	-1	Accepted	58.8	394	-1	Accepted
▼	EUP2-C4 no 008 rye spk. 0.1 ug/ml	140110st18.D	Sample		290.0730	13.1307	35724	0.0245		-3	Accepted	1464	78.3	2302	-2	Accepted	58.9	1137	-2	Accepted
▼	EUP2-C6 no 207 barley spk. 0.1 ug/ml	140110st19.D	Sample		290.0730	13.1307	32965	0.0231		-2	Accepted	3527	76.8	2304	-1	Accepted	59.0	1141	-1	Accepted
▼	EUP2-C2 no 059 wheat spk. 0.1 ug/ml	140110st20.D	Sample		290.0730	13.1307	16194	0.0141		-2	Accepted	1459	75.3	441	-3	Accepted	58.6	805	-2	Accepted
▼	EUP2-SRM6 no 047 rice spk. 0.1 ug/ml	140110st21.D	Sample		290.0730	13.1307	37474	0.0255		-2	Accepted	1382	73.7	946	-2	Accepted	57.5	1084	-2	Accepted
▼	EUP2-C4 no 008 rye spk. 0.1 ug/ml	140110st22.D	Sample		290.0730	13.1307	31534	0.0223		-3	Accepted	794	75.8	1525	-4	Accepted	57.5	2125	-3	Accepted
▼	EUP2-C6 no 207 barley spk. 0.1 ug/ml	140110st23.D	Sample		290.0730	13.1307	31810	0.0224		-3	Accepted	4670	77.5	1728	-2	Accepted	57.9	2139	-2	Accepted
▼	Standard A Cal 3 - 0.1 ug/ml wheat	140110st24.D	Cal	Cal 3	290.0730	13.1307	152163	0.0870	87.0	-2	Accepted	13439	74.0	9955	-2	Accepted	57.1	5311	-2	Accepted
▼	Blank EUP2-C4 no 008 rye spk.	140110st25.D	MatrixBlank		290.0730	13.1307	97	0.0054		-4	Accepted	7	50.2	3	17	Accepted	52.1	2	4	Accepted
▼	EUP2-C2 no 059 wheat spk. 0.1 ug/ml	140110st26.D	Sample		290.0730	13.1307	32961	0.0231		-3	Accepted	1384	75.2	2251	-3	Accepted	57.4	2405	-3	Accepted
▼	EUP2-SRM6 no 047 rice spk. 0.1 ug/ml	140110st27.D	Sample		290.0730	13.1307	35014	0.0242		-3	Accepted	2757	79.4	1631	-3	Accepted	61.6	3164	-3	Accepted
▼	EUP2-C4 no 008 rye spk. 0.1 ug/ml	140110st28.D	Sample		290.0730	13.1307	32737	0.0229		-2	Accepted	2502	74.4	3491	-3	Accepted	59.3	1496	-2	Accepted
▼	EUP2-C6 no 207 barley spk. 0.1 ug/ml	140110st29.D	Sample		290.0730	13.1307	31841	0.0225		-3	Accepted	2962	75.6	642	-1	Accepted	60.7	2641	-1	Accepted

Compound Information

Calibration Curve

Y-axis: Counts x10<sup>4</sup>

X-axis: Acquisition Time (min)

Peak at 13.07 min. Ratio = 77.2 (101.0 %), Ratio = 59.1 (99.8 %)

Mass Match Score = 99.6 M+

Peak at 57.0700, 213.1851

Y-axis: Responses x10<sup>5</sup>

X-axis: Concentration (ng)

Equation:  $y = 1862680.590716 * x - 9980.250169$

$R^2 = 0.99640023$

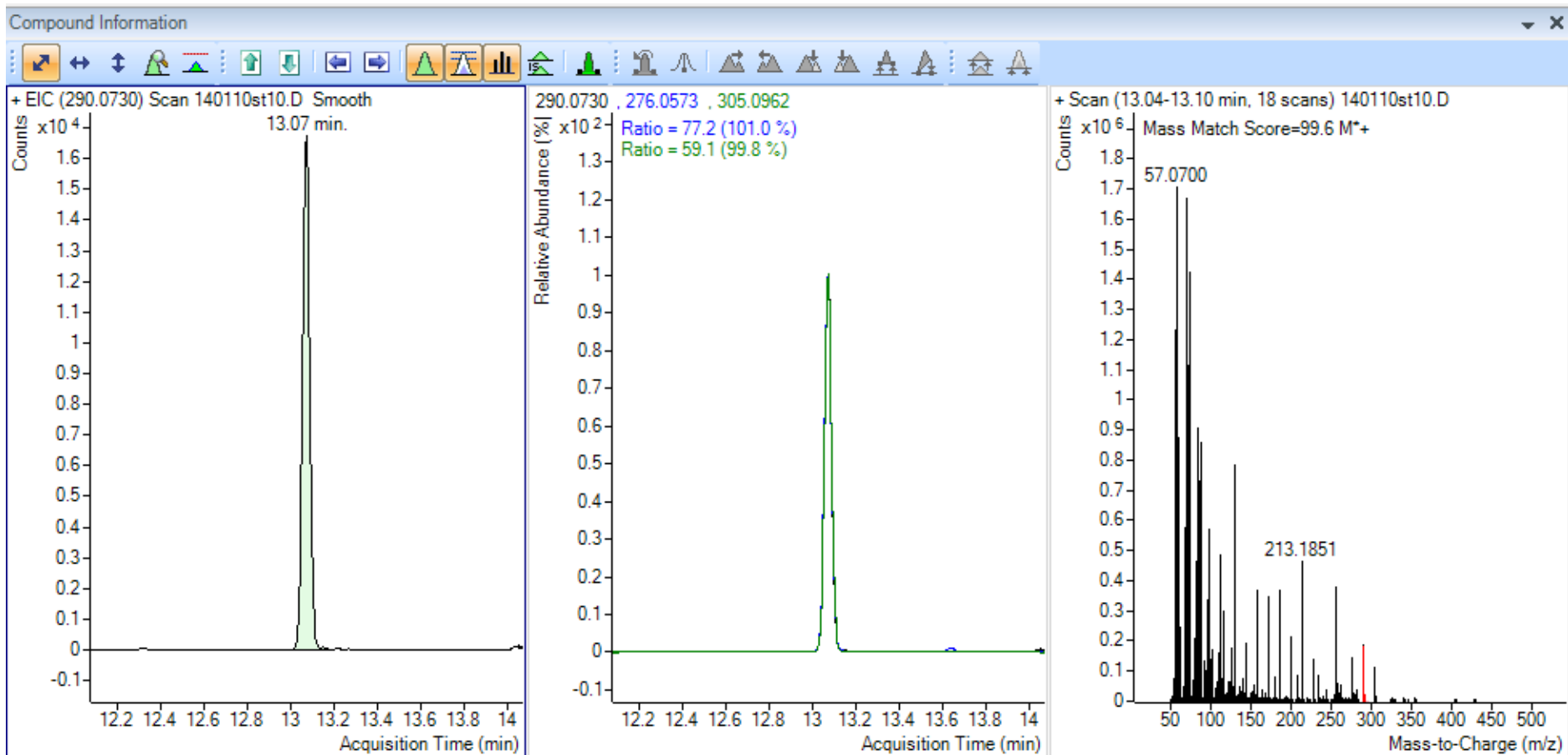
Type: Linear, Origin: Include, Weight: None

Modified EUP2-C2 no 059 wheat spk. 0.1 ug/ml Pirimiphos-methyl 58 Samples (58 to

# Quantitative processing used qualitative

Sample		Pirimiphos-methyl Results										Qualifier (276.0573) Results				Qualifier (305.0962) Results				
Name	Data File	Type	Level	MZ	RT	Resp.	Calc. Conc.	Accuracy	Mass Accuracy	Int. Metric	S/N	Ratio	S/N	Mass Accuracy	Int. Metric	Ratio	S/N	Mass Accuracy	Int. Metric	
EUPT-C2 no 059 wheat spk. 0.1 ug/ml	140110st06.D	Sample		290.0730	13...	39153	0.0264			-3	Accepted	3651	73.0	1279	-2	Accepted	58.8	2716	-2	Accepted
EUPT-SRM6 no 047 rice spk. 0.1 ug/ml	140110st07.D	Sample		290.0730	13...	44284	0.0291			-1	Accepted	2847	78.0	1880	-1	Accepted	59.4	892	-1	Accepted
EUPT-C4 no 008 rye spk. 0.1 ug/ml	140110st08.D	Sample		290.0730	13...	37952	0.0257			-3	Accepted	4752	75.5	4030	-3	Accepted	60.4	1172	-3	Accepted
EUPT-C6 no 207 barley spk. 0.1 ug/ml	140110st09.D	Sample		290.0730	13...	37704	0.0256			-2	Accepted	1807	74.5	1445	-2	Accepted	60.4	1904	-1	Accepted
EUPT-C2 no 059 wheat spk. 0.1 ug/ml	140110st10.D	Sample		290.0730	13...	38369	0.0260			-3	Accepted	2324	77.2	1550	-2	Accepted	59.1	1698	-3	Accepted
EUPT-SRM6 no 047 rice spk. 0.1 ug/ml	140110st11.D	Sample		290.0730	13...	43437	0.0287			-3	Accepted	3076	75.2	1527	-3	Accepted	59.4	1530	-3	Accepted
EUPT-C4 no 008 rye spk. 0.1 ug/ml	140110st12.D	Sample		290.0730	13...	38999	0.0263			-3	Accepted	5074	75.4	912	-3	Accepted	59.5	1270	-3	Accepted
EUPT-C6 no 207 barley spk. 0.1 ug/ml	140110st13.D	Sample		290.0730	13...	37058	0.0253			-3	Accepted	4323	74.2	908	-2	Accepted	58.5	1415	-2	Accepted
Standard A Cal 3 - 0.1 ug/ml wheat	140110st14.D	Cal	Cal 3	290.0730	13...	183761	0.1040	104.0		-2	Accepted	15200	72.8	4147	-2	Accepted	56.5	9409	-2	Accepted
Blank EUPT-SRM6 no 047 rice spk.	140110st15.D	MatrixBlank		290.0730	13...	791	0.0058			-2	Accepted	70	66.8	29	-1	Accepted	58.0	39	-3	Accepted
EUPT-C2 no 059 wheat spk. 0.1 ug/ml	140110st16.D	Sample		290.0730	13...	35735	0.0245			-3	Accepted	43	76.5	2034	-2	Accepted	59.2	1322	-2	Accepted
EUPT-SRM6 no 047 rice spk. 0.1 ug/ml	140110st17.D	Sample		290.0730	13...	40554	0.0271			-2	Accepted	2174	77.1	3266	-1	Accepted	58.8	394	-1	Accepted
EUPT-C4 no 008 rye spk. 0.1 ug/ml	140110st18.D	Sample		290.0730	13...	35724	0.0245			-3	Accepted	1464	78.3	2302	-2	Accepted	58.9	1137	-2	Accepted
EUPT-C6 no 207 barley spk. 0.1 ug/ml	140110st19.D	Sample		290.0730	13...	32965	0.0231			-2	Accepted	3527	76.8	2304	-1	Accepted	59.0	1141	-1	Accepted
EUPT-C2 no 059 wheat spk. 0.1 ug/ml	140110st20.D	Sample		290.0730	13...	16194	0.0141			-2	Accepted	1459	75.3	441	-3	Accepted	58.6	805	-2	Accepted
EUPT-SRM6 no 047 rice spk. 0.1 ug/ml	140110st21.D	Sample		290.0730	13...	37474	0.0255			-2	Accepted	1382	73.7	946	-2	Accepted	57.5	1084	-2	Accepted
EUPT-C4 no 008 rye spk. 0.1 ug/ml	140110st22.D	Sample		290.0730	13...	31534	0.0223			-3	Accepted	794	75.8	1525	-4	Accepted	57.5	2125	-3	Accepted
EUPT-C6 no 207 barley spk. 0.1 ug/ml	140110st23.D	Sample		290.0730	13...	31810	0.0224			-3	Accepted	4670	77.5	1728	-2	Accepted	57.9	2139	-2	Accepted
Standard A Cal 3 - 0.1 ug/ml wheat	140110st24.D	Cal	Cal 3	290.0730	13...	152163	0.0870	87.0		-2	Accepted	13439	74.0	9955	-2	Accepted	57.1	5311	-2	Accepted
Blank EUPT-C4 no 008 rye spk.	140110st25.D	MatrixBlank		290.0730	13...	97	0.0054			-4	Accepted	7	50.2	3	17	Accepted	52.1	2	4	Accepted
EUPT-C2 no 059 wheat spk. 0.1 ug/ml	140110st26.D	Sample		290.0730	13...	32961	0.0231			-3	Accepted	1384	75.2	2251	-3	Accepted	57.4	2405	-3	Accepted
EUPT-SRM6 no 047 rice spk. 0.1 ug/ml	140110st27.D	Sample		290.0730	13...	35014	0.0242			-3	Accepted	2757	79.4	1631	-3	Accepted	61.6	3164	-3	Accepted
EUPT-C4 no 008 rye spk. 0.1 ug/ml	140110st28.D	Sample		290.0730	13...	32737	0.0229			-2	Accepted	2502	74.4	3491	-3	Accepted	59.3	1496	-2	Accepted
EUPT-C6 no 207 barley spk. 0.1 ug/ml	140110st29.D	Sample		290.0730	13...	31841	0.0225			-2	Accepted	2662	75.0	946	-2	Accepted	59.7	2851	-2	Accepted

# Quantitative processing used qualitative



Agilent MassHunter Quantitative Analysis - Method - <F:\GCQTOF-PC Backup\DI\MassHunter\_Data\\_mpou\140107\QuantResults\Validation\_Standard\_A\_0.1\_140218-10ppm.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout: Restore Default Layout

Method Tasks: New / Open Method, Method Setup Tasks, Compound Setup, Retention Time Setup, ISTD Setup, Concentration Setup, Qualifier Setup, Calibration Curve Setup, Globals Setup, Save / Exit, Validate, Save, Save As..., Exit, Manual Setup Tasks, Outlier Setup Tasks, Advanced Tasks

Method Table

Time Segment: <All> Compound: Penconazole Reset Table View

Quantifier Name	TS	Scan	Type	RT
Prirnicarb	1	Scan	Target	11.76
Pririmphos-methyl	1	Scan	Target	13.08
Prochloraz	1	Scan	Target	24.48
Procyimidone	1	Scan	Target	15.08
Propiconazole	1	Scan	Target	18.81
Pyraclostrobin	1	Scan	Target	27.46
Spiroxamin	1	Scan	Target	12.97
Tebuconazole	1	Scan	Target	19.36
Triademel	1	Scan	Target	14.95
Trifloxystrobin	1	Scan	Target	19.08
Trifluralin	1	Scan	Target	9.77
Tribenazoles	1	Scan	Target	21.68
Vinclozolin	1	Scan	Target	12.29

Sample Information

Max # of panes: 2

TIC Scan (140110st14.D)

Scan (16.25-16.25 min, 1 scans) 140110st14.D

Compound Information

EIC (248.0955) Scan 140110st14.D Smooth

248.0955 158.9768 Ratio=94.1

Scan (14.52-14.72 min, 62 scans) 140110st14.D

X 178.2459 Y 62162.828

38 Compounds (38 total) 0 ISTD (0 total)



Agilent MassHunter Quantitative Analysis - Method - <F:\GCQTOF-PC Backup\DI\MassHunter\Data\_m pou\140107\QuantResults\Validation\_Standard\_A\_0.1\_140218-10ppm.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout: Restore Default Layout

Method Tasks

- New / Open Method
- Method Setup Tasks
  - Compound Setup
  - Retention Time Setup
  - ISTD Setup
  - Concentration Setup
  - Qualifier Setup
  - Calibration Curve Setup
  - Globals Setup
  - Save / Exit
  - Validate
  - Save
  - Save As...
  - Exit
- Manual Setup Tasks
- Outlier Setup Tasks
- Advanced Tasks

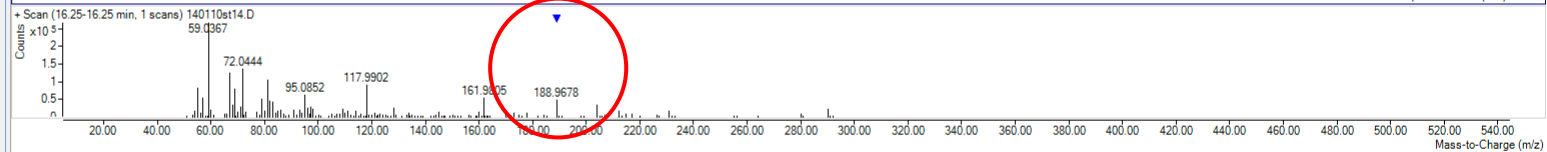
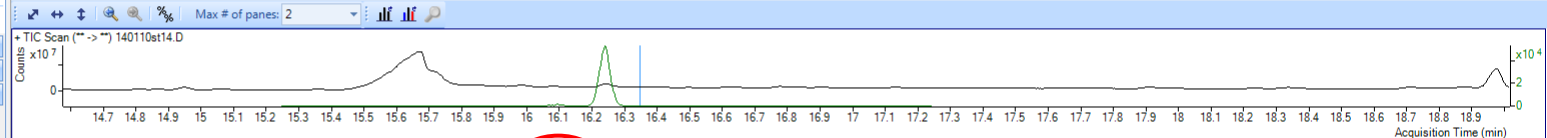
Method Table

Time Segment: <All> Compound: Isoprothiolane Reset Table View

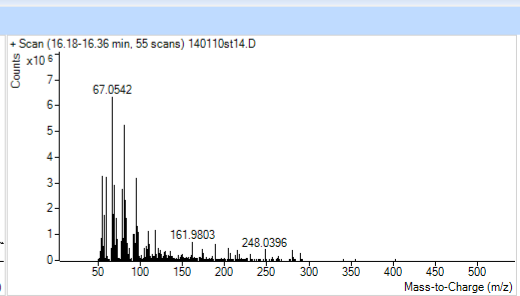
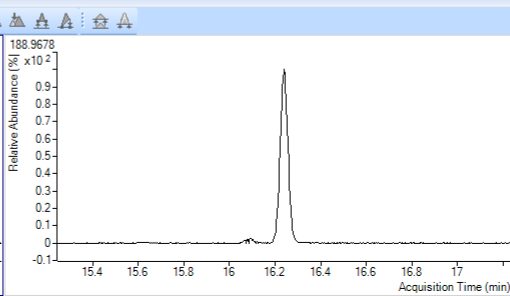
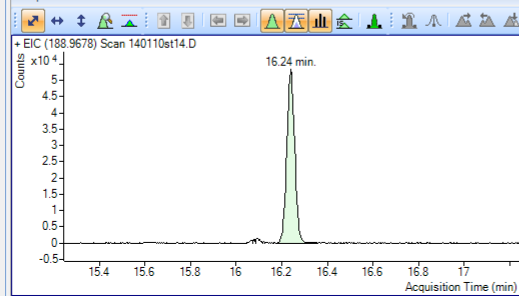
Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Standard A Cal...	140110st14.D	Cal	Cal 3	131216PestFron...	1/11/2014 1:03...	

Quantifier					
Name	TS	Scan	Type	RT	
Isoprothiolane	1	Scan	Target	16.25	
Azinphos-methyl	1	Scan	Target	21.79	
Azoxystrobin	1	Scan	Target	29.31	
Bifenthrin	1	Scan	Target	20.79	
Boscalid	1	Scan	Target	25.68	
Carboxin	1	Scan	Target	16.64	
Chlorpyrifos	1	Scan	Target	13.63	
Chlorpyrifos-met...	1	Scan	Target	12.32	
Cypermethrin	1	Scan	Target	25.89	
Cyfluthrin	1	Scan	Target	14.95	

Sample Information



Compound Information



39 Compounds (39 total) 0 ISTD (0 total)

Agilent MassHunter Quantitative Analysis - Method - <I:\GC\TOF-PC Backup\DI\MassHunter\_Data\mpou\140107\QuantResults\Validation\_Standard\_A\_0.1\_140218-10ppm.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Method Tasks Analyze Batch Layout Restore Default Layout

Method Tasks

New / Open Method

Method Setup Tasks

Compound Setup

Retention Time Setup

ISTD Setup

Concentration Setup

Qualifier Setup

Calibration Curve Setup

Globals Setup

Save / Exit

Validate

Save

Save As...

Exit

Annual Setup Tasks

Outlier Setup Tasks

Advanced Tasks

Method Table

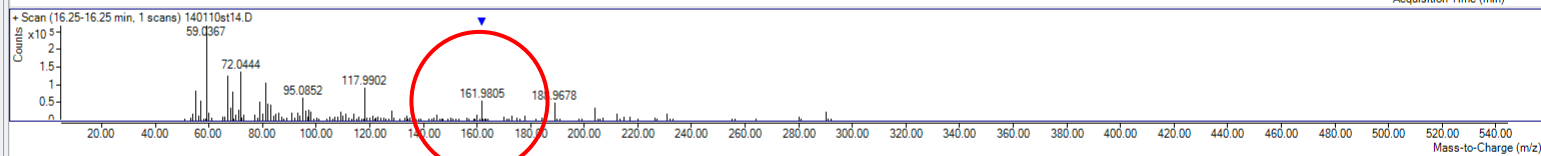
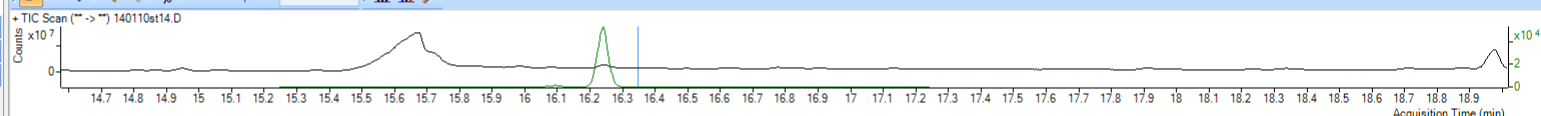
Time Segment: <All> Compound: Isoprothiolane Reset Table View

Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Standard A Cal.	140110st14.D	Cal	Cal 3	131216PestFron.	1/11/2014 1:03	

Quantifier	Name	TS	Scan	Type	RT
	Isoprothiolane	1	Scan	Target	16.25
	Azinphos-methyl	1	Scan	Target	21.79
	Azoxystrobin	1	Scan	Target	29.31
	Bifenthrin	1	Scan	Target	20.79
	Boscalid	1	Scan	Target	25.68
	Carboxin	1	Scan	Target	16.64
	Chlorpyrifos	1	Scan	Target	13.63
	Chlorpyrifos-met.	1	Scan	Target	12.32
	Cypermethrin	1	Scan	Target	25.89
	Cyprothifos	1	Scan	Target	14.26

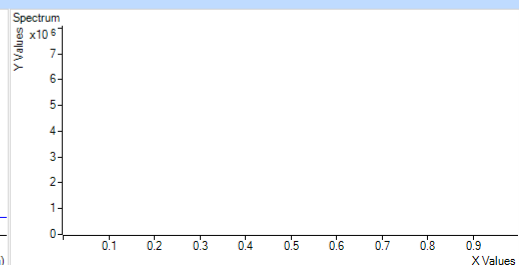
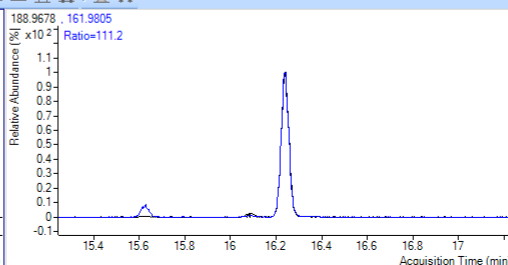
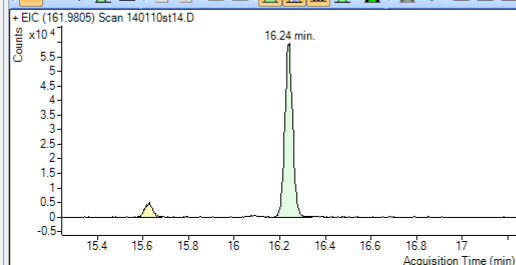
Sample Information

TIC Scan ("\*"") 140110st14.D Max # of panes: 2



Compound Information

EIC (161.9805) Scan 140110st14.D



X 15.6555 Y -1832.397

39 Compounds (39 total) 0 ISTD (0 total)

Agilent MassHunter Quantitative Analysis - Method - <BGCQTOF-PC Backup\DI\MassHunter\Data\\_mpou\140107\QuantResults\Validation\_Standard\_A\_0.1\_140218-10ppm.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout Restore Default Layout

Method Tasks

New / Open Method

Method Setup Tasks

Compound Setup

Retention Time Setup

ISTD Setup

Concentration Setup

Qualifier Setup

Calibration Curve Setup

Global Setup

Save / Exit

Validate

Save

Save As...

Exit

Manual Setup Tasks

New Compound

New Qualifier

New Calibration Level

Delete

Outlier Setup Tasks

Retention Time

Relative Retention Time

Peak Resolution

Peak Symmetry

Peak Full Width Half Maximum

Peak Purity

Signal-to-Noise Ratio

Limit Of Detection

Limit Of Quantitation

Method Detection Limit

Qualifier Ratio

ISTD Response

ISTD Response Percent Deviation

Sample Amount

Sample RSD

Blank Concentration

Blank Response

Method Table

Time Segment: <All> Compound: Isoprothiolane

Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Standard A Cal.	140110st14.D	Cal	Cal 3	1312 For Respon.	1/11/2014 1:03	

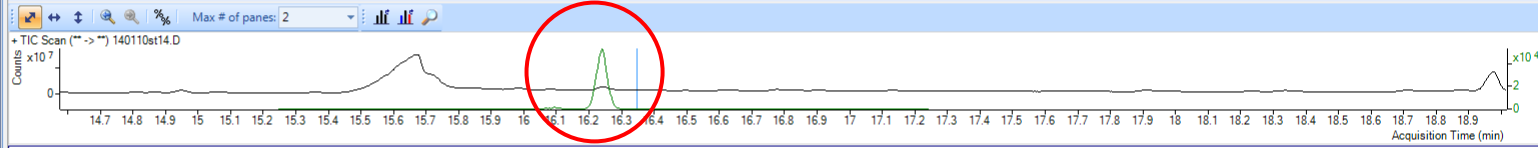
Quantifier	Name	TS	Scan	Type	MZ	RT
Isoprothiolane	161.9805	11.2				
	188.9678			Target	188.9678	16.25

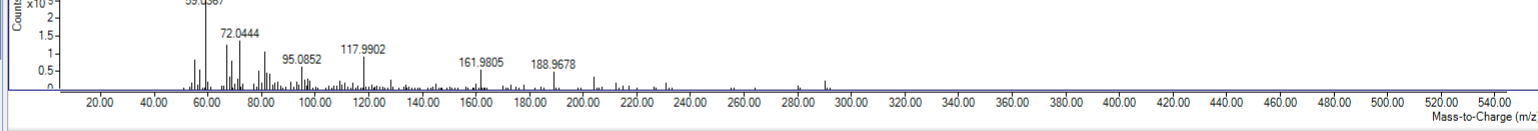
Quantifier	Name	TS	Scan	Type	MZ	RT
Azinphos-methyl		1	Scan	Target	132.0198	21.79

C7H9O2S2	16.36	189.0044	Isoprothiolane F1
C9H11O3S2	16.35	231.015	Isoprothiolane F2
C6H4O4S2	16.35	203.9551	Isoprothiolane F3
C5H6O2S2	16.36	161.9809	Isoprothiolane F4

Sample Information

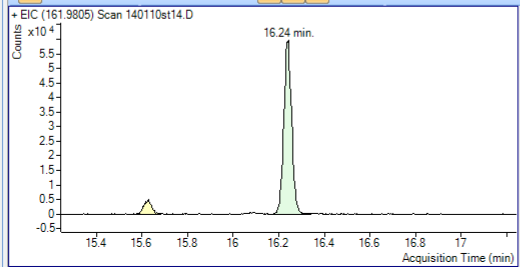


Scan (16.25-16.25 min, 1 scans) 140110st14.D

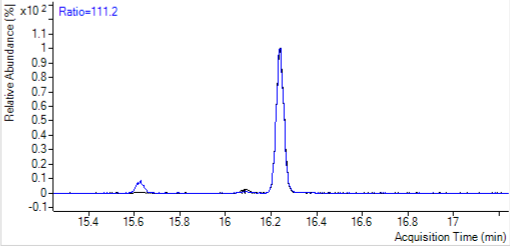


Compound Information

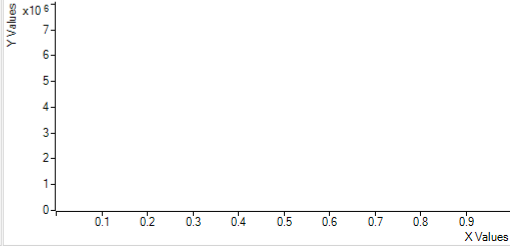
EIC (161.9805) Scan 140110st14.D



188.9678, 161.9805, Ratio=111.2



Spectrum



39 Compounds (39 total) 0 ISTD (0 total)

Agilent MassHunter Quantitative Analysis - Method - <BGCQTOP-PC Backup\DI\MassHunter\Data\_m pou\140107\QuantResults\Validation\_Standard\_A\_0.1\_140218-10ppm.batch.bin>

File Edit View Analyze Method Update Report Tools Help

Analyze Batch Layout Restore Default Layout

- Method Tasks
- New / Open Method
  - Method Setup tasks
    - Compound Setup
    - Retention Time Setup
    - ISTD Setup
    - Concentration Setup
    - Qualifier Setup
    - Calibration Curve Setup
    - Globals Setup
  - Save / Exit
    - Validate
    - Save
    - Save As...
    - Exit
  - Manual Setup Tasks
    - New Compound
    - New Qualifier
    - New Calibration Level
    - Delete
  - Outlier Setup Tasks
    - Retention Time
    - Relative Retention Time
    - Peak Resolution
    - Peak Symmetry
    - Peak Full Width Half Maximum
    - Peak Purity
    - Signal-to-Noise Ratio
    - Limit Of Detection
    - Limit Of Quantitation
    - Method Detection Limit
    - Qualifier Ratio
    - ISTD Response
    - ISTD Response Percent Deviation
    - Sample Amount
    - Sample RSD
    - Blank Concentration
    - Blank Response

Method Table Time Segment: <All> Compound: Isoprothiolane Reset Table View

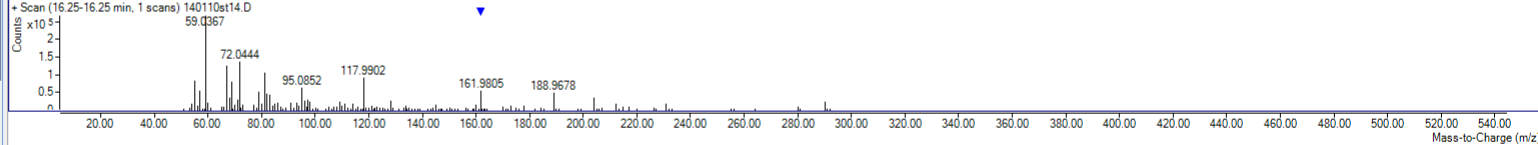
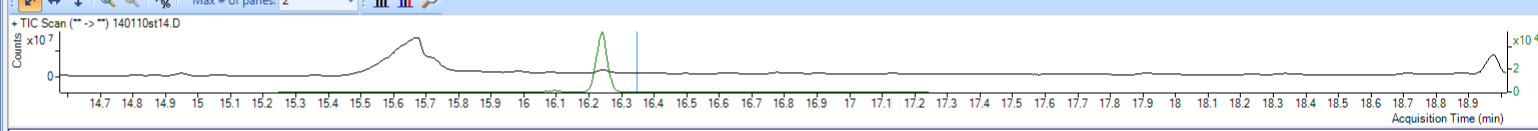
Sample	Name	Data File	Type	Level	Acq. Method File	Acq. Date-Time
Standard A Cal.	140110st14.D	Cal	Cal 3	131216PestFron...	1/11/2014 1:03	

Quantifier	Name	TS	Scan	Type	MZ	RT
	Isoprothiolane	1	Scan	Target	188.9678	16.25

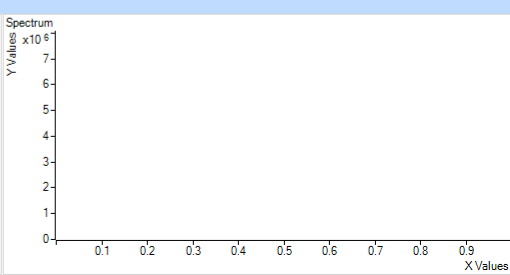
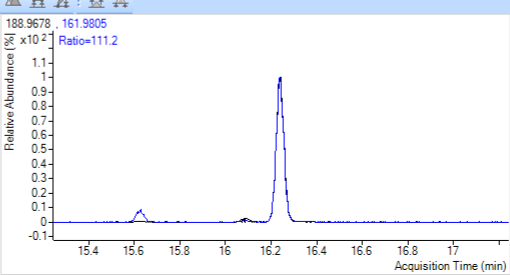
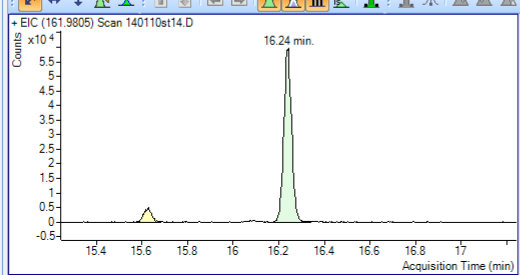
Qualifier	MZ	Rel. Resp.	Area Sum
	161.9805	111.2	

Quantifier	Name	TS	Scan	Type	MZ	RT
	Azinphos-methyl	1	Scan	Target	132.0198	21.79

Sample Information Max # of panes: 2



Compound Information



39 Compounds (39 total) 0 ISTD (0 total)

# Disposition

LC-QTOF screening - MassHunter Qualitative

LC-QTOF - Validation

GC-QTOF screening - MassHunter Quantitative

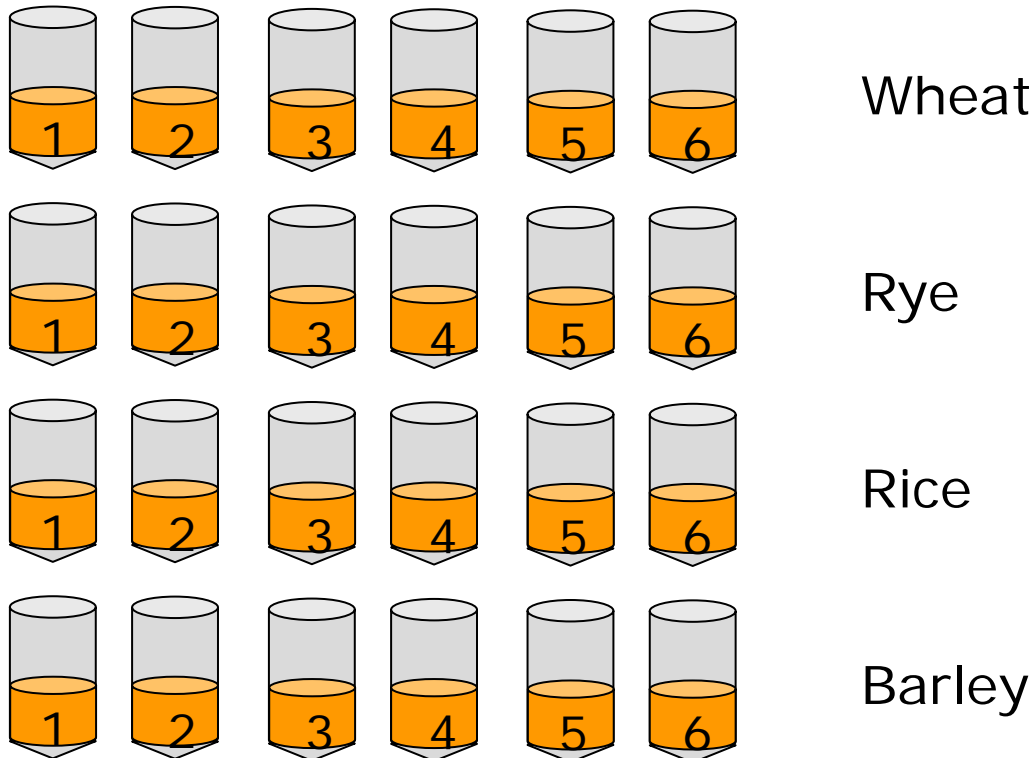
GC-QTOF - Validation

# Validation of screening method

- QuEChERS method combined with a GC-QTOF from Agilent
- The method was validated in cereals two spike levels, 0.01 and 0.05 mg/kg
  
- Purpose:
  - to be familiar with the instrument, be able to analyse and process data, work with well known pesticides.
  - Use the Sanco approach

# Design of validation

- 6 samples of four different types of cereal samples blank EUPT blank test material

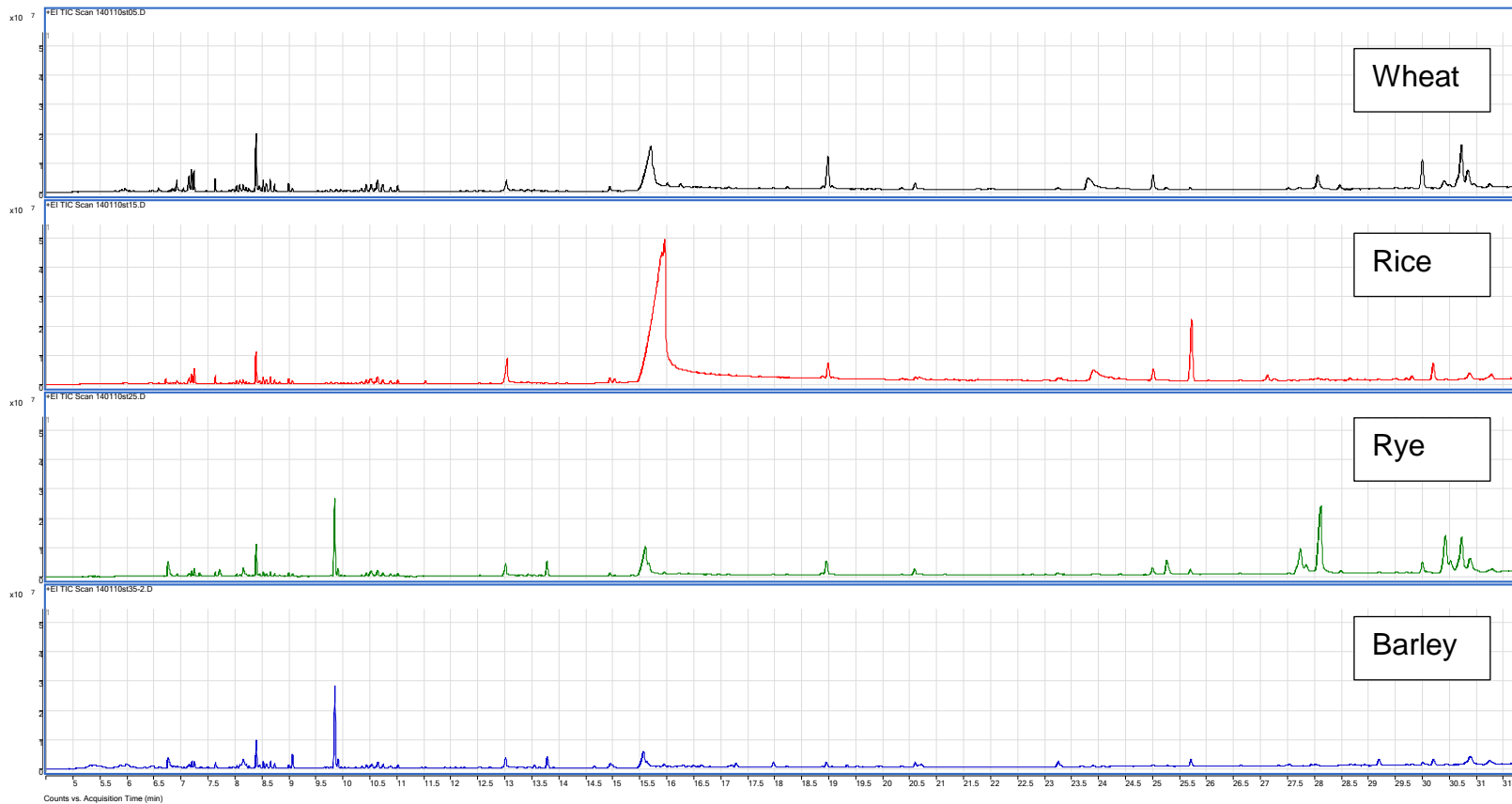


# Design of validation

- Spiked at 0.01 and 0.05 mg/kg
  - 5 standard mixtures called (A, B, C, D and E), containing 356 different compounds altogether.
  - Not all of them can be detected on GC.
- The **24 spiked samples** plus **4 blank cereal** samples and **4 EUPT tests materials** were extracted and cleaned up.
- Only 38 of the compounds have currently been evaluated.
- According to SANCO at least 95% of the samples should be detected (a false-negative rate of 5% is accepted).
  - This means that only 1 out of 20 spiked samples are allowed to be non-detected.



# Matrix



# Screening criteria

- DTU:
  - Retention time (RT):  $\pm 0.1$  min
  - Mass accuracy:
    - 5 ppm for at least 1 fragment ion or
    - 10 ppm for at least 2 fragment ions
  - Signal to noise ratio (S/N): 6
- Sanco:
  - Retention time (RT):  $\pm 0.2$  min
  - Signal to noise ratio (S/N): 3
  - $\geq 2$  diagnostic ions, preferably including the (quasi) molecular ion;
  - mass accuracy  $< 5$  ppm; at least one fragment ion



# Pirimiphos-methyl Results

Qualifier (276.0573) Results

Qualifier (305.0962) Results

Name	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.075	39153	0.0264		3651.28	-3.2	28584	1278.97	-1.8	23008	2716.33	-2
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.072	38369	0.026		2324.2	-3	29625	1550.49	-2.4	22663	1698.24	-3.3
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	35735	0.0245		1343.28	-2.8	27321	2033.78	-2.3	21155	1322.36	-1.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	16194	0.0141		1458.87	-2.2	12195	441.2	-3	9489	804.92	-2.4
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.07	32961	0.0231		1383.74	-3.1	24785	2251.17	-3.3	18905	2404.96	-2.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.074	32121	0.0226		4369.78	-2.3	24485	3114.78	-2	18770	1880.56	-1.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.074	37952	0.0257		4751.72	-2.9	28667	4029.74	-2.5	22921	1172.1	-2.8
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.071	38999	0.0263		5074.47	-3	29420	911.76	-3.1	23221	1270.08	-3.2
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	35724	0.0245		1463.7	-3	27982	2302.36	-1.8	21053	1137	-2.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	31534	0.0223		794.35	-3.5	23890	1524.84	-3.9	18126	2125.3	-2.5
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.076	32737	0.0229		2501.79	-1.6	24351	3491.24	-3	19416	1495.89	-1.9
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	33346	0.0233		2319.11	-2.1	24888	2354.36	-2.1	20084	1222.18	-1.8
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37704	0.0256		1807.3	-1.8	28091	1445.26	-1.8	22763	1903.57	-1.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37058	0.0253		4323.19	-2.8	27506	908.04	-1.8	21677	1415.06	-2.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.075	32965	0.0231		3526.99	-1.5	25306	2304.1	-1.4	19463	1141.04	-0.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.072	31810	0.0224		4670.4	-2.9	24662	1727.86	-1.5	18415	2138.92	-2.3
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.076	31841	0.0225		2065.66	-2.6	23886	846.34	-2	18677	2851.06	-1.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	20225	0.0162		1979.85	-3.3	14795	773.9	-2.6	11817	834.86	-2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	44284	0.0291		2847.2	-1.4	34532	1879.5	-1.3	26325	891.77	-0.8
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	43437	0.0287		3075.92	-3.2	32685	1526.54	-3.1	25795	1530.19	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	40554	0.0271		2173.58	-1.7	31286	3265.97	-1	23856	394.38	-1.2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	37474	0.0255		1382.28	-2.3	27608	945.67	-2	21555	1084.01	-1.7
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	35014	0.0242		2757.14	-2.7	27814	1631.3	-2.9	21560	3163.66	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.077	37104	0.0253		2806.35	-1.6	28705	1403.56	-1.3	22501	2165.39	-0.2
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6854	0.009		683.48	2.2	5144	575.62	2.4	3890	380.68	3.7
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.07	6354	0.0088		722.02	-2.8	4926	227.87	-3.5	3927	367.36	-3.5
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6367	0.0088		765.17	-2.2	5060	200.18	-1.3	3772	252.95	0.6
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.072	6378	0.0088		536.46	-5.4	5183	380.78	-2.2	4120	493.45	-3.3
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6467	0.0088		977.58	-3	5293	595.49	-4.6	4250	464.58	-3.4
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6520	0.0089		568.07	-3.9	5259	610.78	-3.7	4041	475.94	-1.9
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.071	6646	0.0089		947.45	4.2	5286	456.55	3.2	3940	554.06	5.8
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.07	6172	0.0087		650.8	-1	4872	285.24	-2.9	3674	339.2	-1.2
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6930	0.0091		365.33	-4.4	5509	367.1	-3.9	4004	198.03	-3.6
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6828	0.009		983.29	-3.5	5399	486.36	-4.8	4115	315.36	-4.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6420	0.0088		433.69	-4.7	5223	462.55	-4.4	3809	443.77	-3.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6450	0.0088		868.4	-4.1	5035	411.47	-2.4	3625	373.62	-4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.074	6841	0.009		370.19	3.9	5545	146.59	4.6	3964	381.75	5.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6707	0.009		746.95	-2.7	5335	484.64	-1.9	3984	195.52	-2.6
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.073	6509	0.0089		1103.73	-4.6	5089	471.98	-3.6	4150	511.74	-2.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6953	0.0091		511.84	-2.3	5442	723.35	-4.4	3813	551.36	-3.4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.072	6711	0.009		548.35	-6.7	4969	530.79	-2.7	3827	176.45	-4.5
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.076	6531	0.0089		374.2	-4.7	4964	201.78	-5.4	3972	350.87	-5.2
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.075	9614	0.0105		480.15	2.7	7403	544.11	3.5	5949	368.61	2.4
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8835	0.0101		606.26	-2.8	7033	347.19	-2	5247	684.4	-3
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8821	0.0101		684.85	-3.2	6808	452.2	-1.6	5851	387.83	-1.9
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9276	0.0103		972.69	-3.6	6993	326.86	-4	5330	376.24	-1.6
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9958	0.0107		890.19	-3.8	7746	331.17	-3.4	6121	368.32	-3.1
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8784	0.0101		260.19	-2.6	7154	611.4	-2.7	5606	373.43	-1.9





# Pirimiphos-methyl Results

Qualifier (276.0573) Results      Qualifier (305.0962) Results

Name	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.075	39153	0.0264		3651.28	-3.2	28584	1278.97	-1.8	23008	2716.33	-2
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.072	38369	0.026		2324.2	-3	29625	1550.49	-2.4	22663	1698.24	-3.3
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	35735	0.0245		1343.28	-2.8	27321	2033.78	-2.3	21155	1322.36	-1.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	16194	0.0141		1458.87	-2.2	12195	441.2	-3	9489	804.92	-2.4
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.07	32961	0.0231		1383.74	-3.1	24785	2251.17	-3.3	18905	2404.96	-2.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.074	32121	0.0226		4369.78	-2.3	24485	3114.78	-2	18770	1880.56	-1.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.074	37952	0.0257		4751.72	-2.9	28667	4029.74	-2.5	22921	1172.1	-2.8
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.071	38999	0.0263		5074.47	-3	29420	911.76	-3.1	23221	1270.08	-3.2
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	35724	0.0245		1463.7	-3	27982	2302.36	-1.8	21053	1137	-2.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	31534	0.0223		794.35	-3.5	23890	1524.84	-3.9	18126	2125.3	-2.5
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.076	32737	0.0229		2501.79	-1.6	24351	3491.24	-3	19416	1495.89	-1.9
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	33346	0.0233		2319.11	-2.1	24888	2354.36	-2.1	20084	1222.18	-1.8
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37704	0.0256		1807.3	-1.8	28091	1445.26	-1.8	22763	1903.57	-1.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37058	0.0253		4323.19	-2.8	27506	908.04	-1.8	21677	1415.06	-2.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.075	32965	0.0231		3526.99	-1.5	25306	2304.1	-1.4	19463	1141.04	-0.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.072	31810	0.0224		4670.4	-2.9	24662	1727.86	-1.5	18415	2138.92	-2.3
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.076	31841	0.0225		2065.66	-2.6	23886	846.34	-2	18677	2851.06	-1.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	20225	0.0162		1979.85	-3.3	14795	773.9	-2.6	11817	834.86	-2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	44284	0.0291		2847.2	-1.4	34532	1879.5	-1.3	26325	891.77	-0.8
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	43437	0.0287		3075.92	-3.2	32685	1526.54	-3.1	25795	1530.19	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	40554	0.0271		2173.58	-1.7	31286	3265.97	-1	23856	394.38	-1.2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	37474	0.0255		1382.28	-2.3	27608	945.67	-2	21555	1084.01	-1.7
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	35014	0.0242		2757.14	-2.7	27814	1631.3	-2.9	21560	3163.66	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.077	37104	0.0253		2806.35	-1.6	28705	1403.56	-1.3	22501	2165.39	-0.2
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6854	0.009		683.48	2.2	5144	575.62	2.4	3890	380.68	3.7
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.07	6354	0.0088		722.02	-2.8	4926	227.87	-3.5	3927	367.36	-3.5
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6367	0.0088		765.17	-2.2	5060	200.18	-1.3	3772	252.95	0.6
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.072	6378	0.0088		536.46	-5.4	5183	380.78	-2.2	4120	493.45	-3.3
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6467	0.0088		977.58	-3	5293	595.49	-4.6	4250	464.58	-3.4
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6520	0.0089		568.07	-3.9	5259	610.78	-3.7	4041	475.94	-1.9
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.071	6646	0.0089		947.45	4.2	5286	456.55	3.2	3940	554.06	5.8
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.07	6172	0.0087		650.8	-1	4872	285.24	-2.9	3674	339.2	-1.2
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6930	0.0091		365.33	-4.4	5509	367.1	-3.9	4004	198.03	-3.6
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6828	0.009		983.29	-3.5	5399	486.36	-4.8	4115	315.36	-4.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6420	0.0088		433.69	-4.7	5223	462.55	-4.4	3809	443.77	-3.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6450	0.0088		868.4	-4.1	5035	411.47	-2.4	3625	373.62	-4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.074	6841	0.009		370.19	3.9	5545	146.59	4.6	3964	381.75	5.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6707	0.009		746.95	-2.7	5335	484.64	-1.9	3984	195.52	-2.6
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.073	6509	0.0089		1103.73	-4.6	5089	471.98	-3.6	4150	511.74	-2.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6953	0.0091		511.84	-2.3	5442	723.35	-4.4	3813	551.36	-3.4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.072	6711	0.009		548.35	-6.7	4969	530.79	-2.7	3827	176.45	-4.5
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.076	6531	0.0089		374.2	-4.7	4964	201.78	-5.4	3972	350.87	-5.2
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.075	9614	0.0105		480.15	2.7	7403	544.11	3.5	5949	368.61	2.4
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8835	0.0101		606.26	-2.8	7033	347.19	-2	5247	684.4	-3
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8821	0.0101		684.85	-3.2	6808	452.2	-1.6	5851	387.83	-1.9
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9276	0.0103		972.69	-3.6	6993	326.86	-4	5330	376.24	-1.6
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9958	0.0107		890.19	-3.8	7746	331.17	-3.4	6121	368.32	-3.1
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8784	0.0101		260.19	-2.6	7154	611.4	-2.7	5606	373.43	-1.9





# Pirimiphos-methyl Results

Qualifier (276.0573) Results      Qualifier (305.0962) Results

Name	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.075	39153	0.0264		3651.28	-3.2	28584	1278.97	-1.8	23008	2716.33	-2
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.072	38369	0.026		2324.2	-3	29625	1550.49	-2.4	22663	1698.24	-3.3
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	35735	0.0245		1343.28	-2.8	27321	2033.78	-2.3	21155	1322.36	-1.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	16194	0.0141		1458.87	-2.2	12195	441.2	-3	9489	804.92	-2.4
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.07	32961	0.0231		1383.74	-3.1	24785	2251.17	-3.3	18905	2404.96	-2.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.074	32121	0.0226		4369.78	-2.3	24485	3114.78	-2	18770	1880.56	-1.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.074	37952	0.0257		4751.72	-2.9	28667	4029.74	-2.5	22921	1172.1	-2.8
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.071	38999	0.0263		5074.47	-3	29420	911.76	-3.1	23221	1270.08	-3.2
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	35724	0.0245		1463.7	-3	27982	2302.36	-1.8	21053	1137	-2.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	31534	0.0223		794.35	-3.5	23890	1524.84	-3.9	18126	2125.3	-2.5
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.076	32737	0.0229		2501.79	-1.6	24351	3491.24	-3	19416	1495.89	-1.9
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	33346	0.0233		2319.11	-2.1	24888	2354.36	-2.1	20084	1222.18	-1.8
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37704	0.0256		1807.3	-1.8	28091	1445.26	-1.8	22763	1903.57	-1.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37058	0.0253		4323.19	-2.8	27506	908.04	-1.8	21677	1415.06	-2.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.075	32965	0.0231		3526.99	-1.5	25306	2304.1	-1.4	19463	1141.04	-0.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.072	31810	0.0224		4670.4	-2.9	24662	1727.86	-1.5	18415	2138.92	-2.3
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.076	31841	0.0225		2065.66	-2.6	23886	846.34	-2	18677	2851.06	-1.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	20225	0.0162		1979.85	-3.3	14795	773.9	-2.6	11817	834.86	-2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	44284	0.0291		2847.2	-1.4	34532	1879.5	-1.3	26325	891.77	-0.8
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	43437	0.0287		3075.92	-3.2	32685	1526.54	-3.1	25795	1530.19	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	40554	0.0271		2173.58	-1.7	31286	3265.97	-1	23856	394.38	-1.2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	37474	0.0255		1382.28	-2.3	27608	945.67	-2	21555	1084.01	-1.7
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	35014	0.0242		2757.14	-2.7	27814	1631.3	-2.9	21560	3163.66	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.077	37104	0.0253		2806.35	-1.6	28705	1403.56	-1.3	22501	2165.39	-0.2
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6854	0.009		683.48	2.2	5144	575.62	2.4	3890	380.68	3.7
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.07	6354	0.0088		722.02	-2.8	4926	227.87	-3.5	3927	367.36	-3.5
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6367	0.0088		765.17	-2.2	5060	200.18	-1.3	3772	252.95	0.6
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.072	6378	0.0088		536.46	-5.4	5183	380.78	-2.2	4120	493.45	-3.3
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6467	0.0088		977.58	-3	5293	595.49	-4.6	4250	464.58	-3.4
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6520	0.0089		568.07	-3.9	5259	610.78	-3.7	4041	475.94	-1.9
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.071	6646	0.0089		947.45	4.2	5286	456.55	3.2	3940	554.06	5.8
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.07	6172	0.0087		650.8	-1	4872	285.24	-2.9	3674	339.2	-1.2
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6930	0.0091		365.33	-4.4	5509	367.1	-3.9	4004	198.03	-3.6
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6828	0.009		983.29	-3.5	5399	486.36	-4.8	4115	315.36	-4.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6420	0.0088		433.69	-4.7	5223	462.55	-4.4	3809	443.77	-3.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6450	0.0088		868.4	-4.1	5035	411.47	-2.4	3625	373.62	-4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.074	6841	0.009		370.19	3.9	5545	146.59	4.6	3964	381.75	5.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6707	0.009		746.95	-2.7	5335	484.64	-1.9	3984	195.52	-2.6
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.073	6509	0.0089		1103.73	-4.6	5089	471.98	-3.6	4150	511.74	-2.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6953	0.0091		511.84	-2.3	5442	723.35	-4.4	3813	551.36	-3.4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.072	6711	0.009		548.35	-6.7	4969	530.79	-2.7	3827	176.45	-4.5
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.076	6531	0.0089		374.2	-4.7	4964	201.78	-5.4	3972	350.87	-5.2
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.075	9614	0.0105		480.15	2.7	7403	544.11	3.5	5949	368.61	2.4
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8835	0.0101		606.26	-2.8	7033	347.19	-2	5247	684.4	-3
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8821	0.0101		684.85	-3.2	6808	452.2	-1.6	5851	387.83	-1.9
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9276	0.0103		972.69	-3.6	6993	326.86	-4	5330	376.24	-1.6
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9958	0.0107		890.19	-3.8	7746	331.17	-3.4	6121	368.32	-3.1
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8784	0.0101		260.19	-2.6	7154	611.4	-2.7	5606	373.43	-1.9

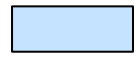




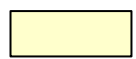
# Pirimiphos-methyl Results

Qualifier (276.0573) Results      Qualifier (305.0962) Results

Name	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.075	39153	0.0264		3651.28	-3.2	28584	1278.97	-1.8	23008	2716.33	-2
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.072	38369	0.026		2324.2	-3	29625	1550.49	-2.4	22663	1698.24	-3.3
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	35735	0.0245		1343.28	-2.8	27321	2033.78	-2.3	21155	1322.36	-1.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.073	16194	0.0141		1458.87	-2.2	12195	441.2	-3	9489	804.92	-2.4
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.07	32961	0.0231		1383.74	-3.1	24785	2251.17	-3.3	18905	2404.96	-2.6
EUPT-C2 no 059 wheat spk. 0.05 ug/ml	13.074	32121	0.0226		4369.78	-2.3	24485	3114.78	-2	18770	1880.56	-1.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.074	37952	0.0257		4751.72	-2.9	28667	4029.74	-2.5	22921	1172.1	-2.8
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.071	38999	0.0263		5074.47	-3	29420	911.76	-3.1	23221	1270.08	-3.2
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	35724	0.0245		1463.7	-3	27982	2302.36	-1.8	21053	1137	-2.3
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	31534	0.0223		794.35	-3.5	23890	1524.84	-3.9	18126	2125.3	-2.5
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.076	32737	0.0229		2501.79	-1.6	24351	3491.24	-3	19416	1495.89	-1.9
EUPT-C4 no 008 rye spk. 0.05 ug/ml	13.073	33346	0.0233		2319.11	-2.1	24888	2354.36	-2.1	20084	1222.18	-1.8
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37704	0.0256		1807.3	-1.8	28091	1445.26	-1.8	22763	1903.57	-1.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	37058	0.0253		4323.19	-2.8	27506	908.04	-1.8	21677	1415.06	-2.5
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.075	32965	0.0231		3526.99	-1.5	25306	2304.1	-1.4	19463	1141.04	-0.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.072	31810	0.0224		4670.4	-2.9	24662	1727.86	-1.5	18415	2138.92	-2.3
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.076	31841	0.0225		2065.66	-2.6	23886	846.34	-2	18677	2851.06	-1.6
EUPT-C6 no 207 barley spk. 0.05 ug/ml	13.073	20225	0.0162		1979.85	-3.3	14795	773.9	-2.6	11817	834.86	-2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	44284	0.0291		2847.2	-1.4	34532	1879.5	-1.3	26325	891.77	-0.8
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	43437	0.0287		3075.92	-3.2	32685	1526.54	-3.1	25795	1530.19	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	40554	0.0271		2173.58	-1.7	31286	3265.97	-1	23856	394.38	-1.2
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.073	37474	0.0255		1382.28	-2.3	27608	945.67	-2	21555	1084.01	-1.7
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.075	35014	0.0242		2757.14	-2.7	27814	1631.3	-2.9	21560	3163.66	-2.9
EUPT-SRM6 no 047 rice spk. 0.05 ug/ml	13.077	37104	0.0253		2806.35	-1.6	28705	1403.56	-1.3	22501	2165.39	-0.2
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6854	0.009		683.48	2.2	5144	575.62	2.4	3890	380.68	3.7
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.07	6354	0.0088		722.02	-2.8	4926	227.87	-3.5	3927	367.36	-3.5
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6367	0.0088		765.17	-2.2	5060	200.18	-1.3	3772	252.95	0.6
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.072	6378	0.0088		536.46	-5.4	5183	380.78	-2.2	4120	493.45	-3.3
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.074	6467	0.0088		977.58	-3	5293	595.49	-4.6	4250	464.58	-3.4
EUPT-C2 no 059 wheat spk. 0.01 ug/ml	13.073	6520	0.0089		568.07	-3.9	5259	610.78	-3.7	4041	475.94	-1.9
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.071	6646	0.0089		947.45	4.2	5286	456.55	3.2	3940	554.06	5.8
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.07	6172	0.0087		650.8	-1	4872	285.24	-2.9	3674	339.2	-1.2
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6930	0.0091		365.33	-4.4	5509	367.1	-3.9	4004	198.03	-3.6
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6828	0.009		983.29	-3.5	5399	486.36	-4.8	4115	315.36	-4.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.074	6420	0.0088		433.69	-4.7	5223	462.55	-4.4	3809	443.77	-3.1
EUPT-C4 no 008 rye spk. 0.01 ug/ml	13.075	6450	0.0088		868.4	-4.1	5035	411.47	-2.4	3625	373.62	-4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.074	6841	0.009		370.19	3.9	5545	146.59	4.6	3964	381.75	5.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6707	0.009		746.95	-2.7	5335	484.64	-1.9	3984	195.52	-2.6
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.073	6509	0.0089		1103.73	-4.6	5089	471.98	-3.6	4150	511.74	-2.9
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.075	6953	0.0091		511.84	-2.3	5442	723.35	-4.4	3813	551.36	-3.4
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.072	6711	0.009		548.35	-6.7	4969	530.79	-2.7	3827	176.45	-4.5
EUPT-C6 no 207 barley spk. 0.01 ug/ml	13.076	6531	0.0089		374.2	-4.7	4964	201.78	-5.4	3972	360.87	-5.2
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.075	9614	0.0105		480.15	2.7	7403	544.11	3.5	5949	368.61	2.4
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8835	0.0101		606.26	-2.8	7033	347.19	-2	5247	684.4	-3
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8821	0.0101		684.85	-3.2	6808	452.2	-1.6	5851	387.83	-1.9
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9276	0.0103		972.69	-3.6	6993	326.86	-4	5330	376.24	-1.6
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.074	9958	0.0107		890.19	-3.8	7746	331.17	-3.4	6121	368.32	-3.1
EUPT-SRM6 no 047 rice spk. 0.01 ug/ml	13.073	8784	0.0101		260.19	-2.6	7154	611.4	-2.7	5606	373.43	-1.9



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Spike level, mg/kg		0.01	0.01	0.05	0.05	
No. of detects with mass accuracy						
Mass accuracy difference	Molecular or fragment ion*					SDL, mg/kg
		≤5ppm	≤10ppm	≤5ppm	≤10ppm	
Pirimiphos-methyl	1	22	24	24	24	0.01
Pirimiphos-methyl	2	23	24	24	24	
Pirimiphos-methyl	3	21	24	24	24	

Spike level, mg/kg		0.01	0.01	0.05	0.05	
No. of detects with mass accuracy						
Mass accuracy difference	Molecular or fragment ion*					SDL, mg/kg
		≤5ppm	≤10ppm	≤5ppm	≤10ppm	
Pirimiphos-methyl	1	22	24	24	24	0.01
Pirimiphos-methyl	2	23	24	24	24	
Pirimiphos-methyl	3	21	24	24	24	



Spike level, mg/kg		0.01	0.01	0.05	0.05	
		No. of detects with mass accuracy				
Mass accuracy difference	Molecular or fragment ion*	≤5ppm	≤10ppm	≤5ppm	≤10ppm	SDL, mg/kg
Pirimiphos-methyl	1	22	24	24	24	0.01
Pirimiphos-methyl	2	23	24	24	24	
Pirimiphos-methyl	3	21	24	24	24	

Spike level, mg/kg		0.01	0.01	0.05	0.05	
No. of detects with mass accuracy						
Mass accuracy difference	Molecular or fragment ion*					SDL, mg/kg
		≤5ppm	≤10ppm	≤5ppm	≤10ppm	
Pirimiphos-methyl	1	22	24	24	24	0.01
Pirimiphos-methyl	2	23	24	24	24	
Pirimiphos-methyl	3	21	24	24	24	

Spike level, mg/kg		0.01	0.01	0.05	0.05	
No. of detects with mass accuracy						
Mass accuracy difference	Molecular or fragment ion*					SDL, mg/kg
		≤5ppm	≤10ppm	≤5ppm	≤10ppm	
Pirimiphos-methyl	1	22	24	24	24	0.01
Pirimiphos-methyl	2	23	24	24	24	
Pirimiphos-methyl	3	21	24	24	24	

# Validation results – spike experiments

- SDL = 0.01 mg/kg (17)
  - Bifenthrin, Chlorpyrifos, Chlorpyrifos-methyl, Diazinon, Fenitrothion, Fipronil, Flutriafol, Iprodione, Krexoxim-methyl, Malathion, Methacrifos, Penconazole, Pirimicarb, Pirimiphos-methyl, Propiconazole, Trifluralin and Vinclozolin
- SDL = 0.05 mg/kg (19)
  - Azoxystrobin, Boscalid, Carboxin, Cypermethrin, Cyprodinil, Diclorvos, Difenoconazole, Epoxiconazole, Fenbuconazole, Lambda-cyhalothrin, Pendimethanil, Prochloraz, Procymidone, Pyraclostrobin, Spiroxamin, Tebuconazole, Triademenol, Trifloxystrobin, Triticonazole
- Not validated (2)
  - Azinphos-methyl, Metconazole

## Validation results – PT test material

- The test materials contained 46 residues of 27 different pesticides.
- All pesticides were detected apart from one residue of lambda-cyhalothrin.
  - assigned value = 0.25 mg/kg; SDL = 0.05 mg/kg
- No false positive results were seen.

# Validation results – PT test material

Name	Pirimiphos-methyl Results						Qualifier (276.0573) Results			Qualifier (305.0962) Results		
	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
EUPT-C2 no 003 wheat	13.07	158	0.0054		10.99	13.6	164	10.79	7.7	99	9.59	5.2
EUPT-S5 no 105	13.077	26638	0.0197		2974.89	0.7	20537	2572.68	1.6	15978	1740.4	0.4
EUPT-C4 no 143 rye	13.076	32283	0.0227		2519.07	2.4	23981	3377.95	4.1	18355	2167.42	4.1
EUPT-C6 no 032 barleyspk	12.634	20	0.0054		0.17	-79.9	13	0.21	-8.4	10	0.6	99.5



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# Validation results – PT test material

Name	Pirimiphos-methyl Results						Qualifier (276.0573) Results			Qualifier (305.0962) Results		
	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
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# Validation results – PT test material

Name	Pirimiphos-methyl Results						Qualifier (276.0573) Results			Qualifier (305.0962) Results		
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# Validation results – PT test material

Name	Pirimiphos-methyl Results						Qualifier (276.0573) Results			Qualifier (305.0962) Results		
	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
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# Validation results – PT test material

Name	Pirimiphos-methyl Results					Qualifier (276.0573) Results			Qualifier (305.0962) Results			
	RT	Area	Final Conc	Accuracy	S/N	Mass Accu	Area	S/N	Mass Accu	Area	S/N	Mass Accu
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EUPT-C6 no 032 barleyspk	12.634	20	0.0054		0.17	-79.9	13	0.21	-8.4	10	0.6	99.5



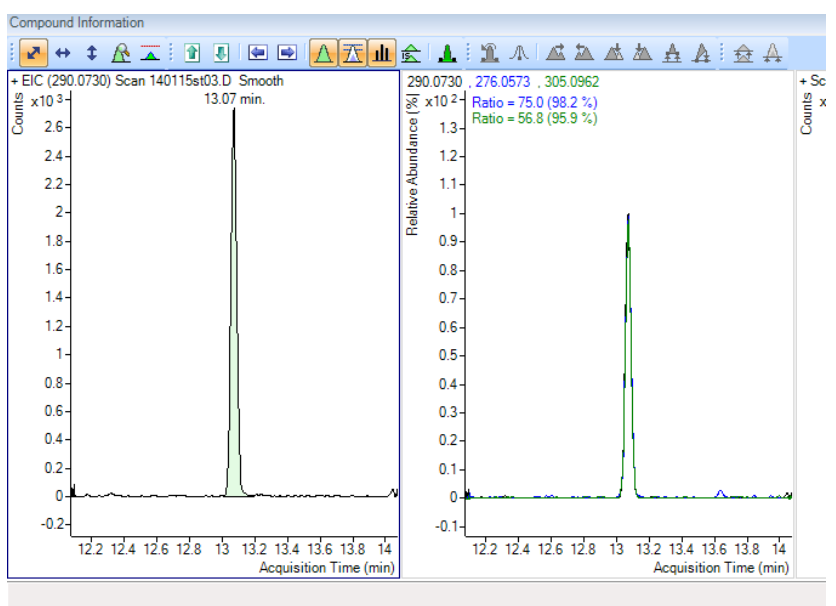
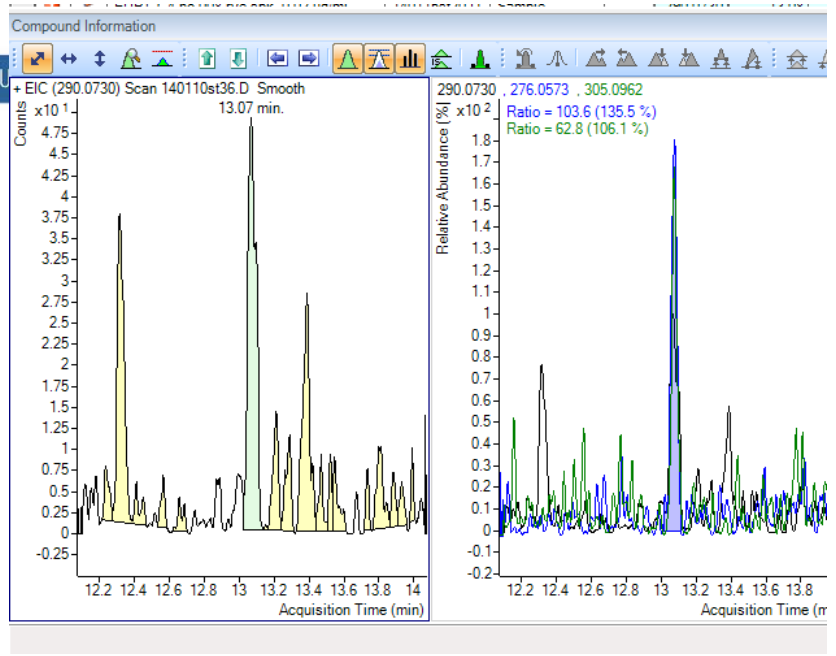
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**Thank you for your attention**

