

Agilent E-seminar on Emerging Contaminants

9 to 12 March @ 11am Singapore time

NOW AVAILABLE:

AUDIO BROADCAST - Audio will be broadcasted through your computer speakers, please un-mute your speaker settings.

AUDIO over the telephone, please dial one of the phone numbers listed.

PASSCODE: AGILENT

International Telephone Number for Singapore: +65-6622 1044 or Toll Free 8008 523 396			
International Telephone Number for Hong Kong: +852 3006 8101			
Toll Free International Numbers:			
Australia	1800 999 130	New Zealand	0800 450 755
China	800 876 5011	Malaysia	1800 807 180
Indonesia*	0018 038 526 350	Taiwan	0080 185 5735
Thailand*	0018 008 526 361	South Korea	0079 885 214 717
Philippines*	1800 185 50065	Vietnam*	120 650 065

* Not accessible from Mobile Phones. Must be IDD enabled.

Choosing the Best LC/MS Solution for your Environmental Laboratory

Dr. Christopher Tye

Chemical Analysis Group
Business Manager

March 2010



Agilent Technologies

The Agilent LC/MS portfolio

What's in my sample?

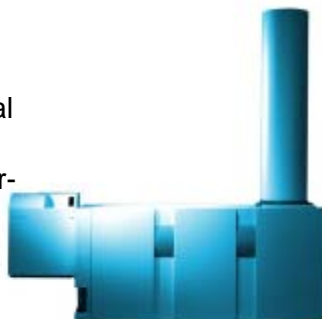
How much is in my sample?

Qualitative

Quantitative

6500 QTOF Series

Sensitive, Accurate-Mass MS and MS/MS Analyses
Superior data quality and advanced analytical capabilities for profiling, identifying, characterizing, and quantifying low molecular-weight compounds and biomolecules with confidence.



6400 Triple Quadrupole Series

High sensitivity MS/MS system for targeted quantitative analysis in environmental measurements



6200 TOF Series

High throughput walk up accurate mass system for compound screening and confirmation



All Powered by: New 1200 Series LC and Rapid Resolution System



6100 Series Single Quad

Easy to use high selectivity MS system for routine quantification and use in QC/QA



Agilent Technologies

Agilent's New 6540 Ultra High Definition QTOF

Research Performance in a Benchtop Format

- 40,000 Resolving Power
- <1 ppm MS <3 ppm MS/MS Mass Accuracy
- 20 Spectra/s
- 2 pg – 50:1 Reserpine S/N
- 5 Decades in Spectrum Dynamic Range
- Excellent Linearity and Isotopic Fidelity
- Supports Standard ESI, Agilent Jet Stream and HPLC-Chip

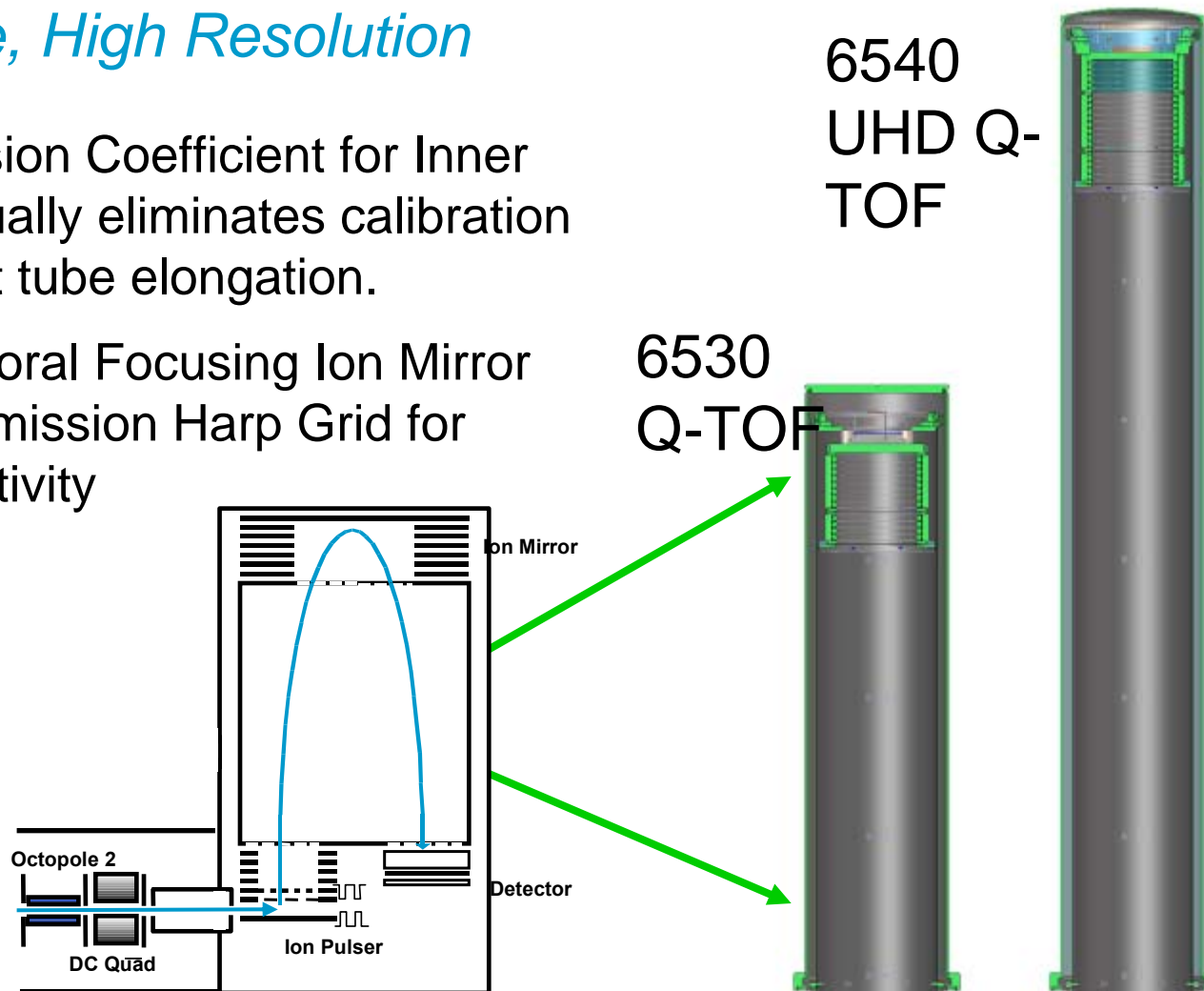


Unsurpassed Analytical Capacity in a Benchtop
The result of *RELENTLESS INNOVATION*

Enhanced Ion Flight Tube and Mirror Technology

Stable, Sensitive, High Resolution

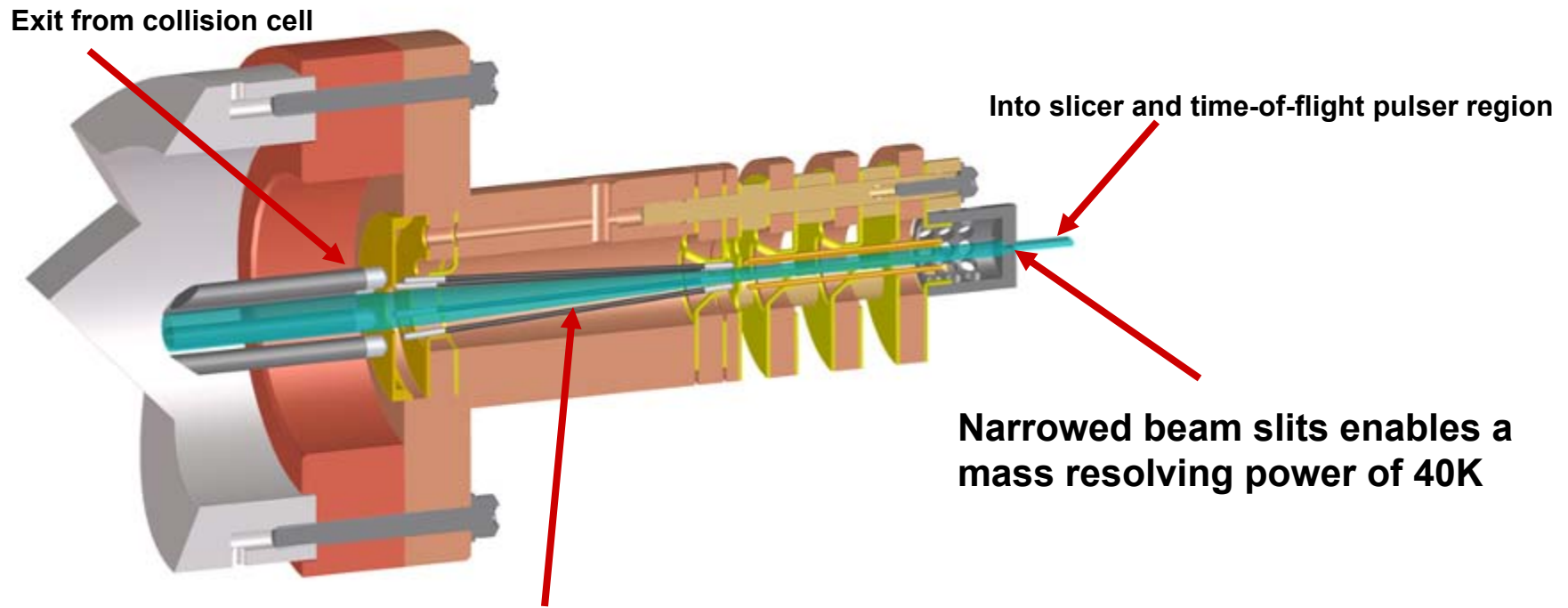
- 1ppm/C Expansion Coefficient for Inner Flight Tube virtually eliminates calibration drift due to flight tube elongation.
- 2nd Order Temporal Focusing Ion Mirror uses high transmission Harp Grid for maximum sensitivity



Ion Beam Compression (IBC)* Technology

Drives Higher Resolution

Active Ion Beam Compression simultaneously maximizes ion transmission and reduces beam divergence



Active Ion Beam Compression is achieved with Agilent's Axial Ion Acceleration Technology applied to a tapered ion guide design.

* Patent pending

LC/MS Ion Sources

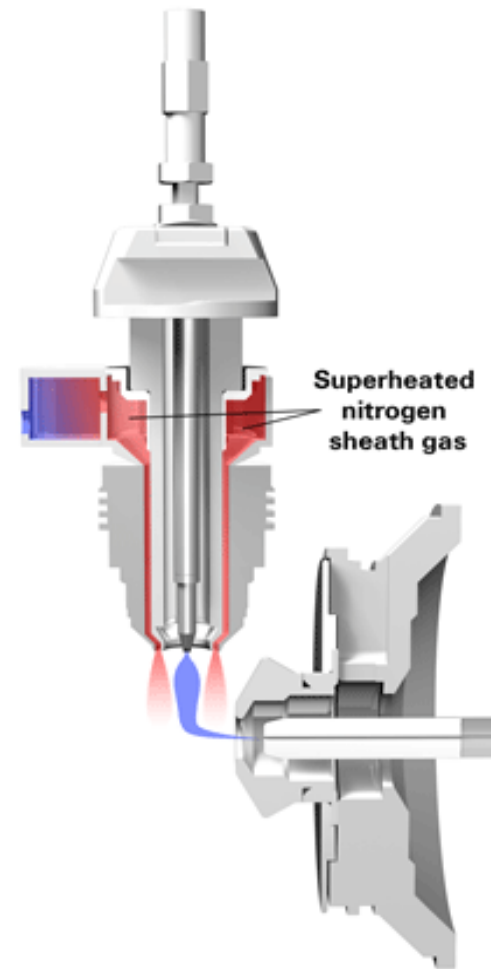
- Widest choice of sources from any manufacturer
 - Dual electrospray (ESI)
 - Agilent Jet Stream Thermal Focusing Technology
 - Dual nanospray
 - APCI
 - APPI
 - CE-TOF
 - PDF-MALDI
- Interchangeable between MS platforms
- Multimode Source
 - ESI and APCI combined in one source
 - Simultaneous operation
- HPLC-Chip/MS
 - Nanospray made ease
 - Reproducible results
 - Sample processing on chip



Ionize Anything!



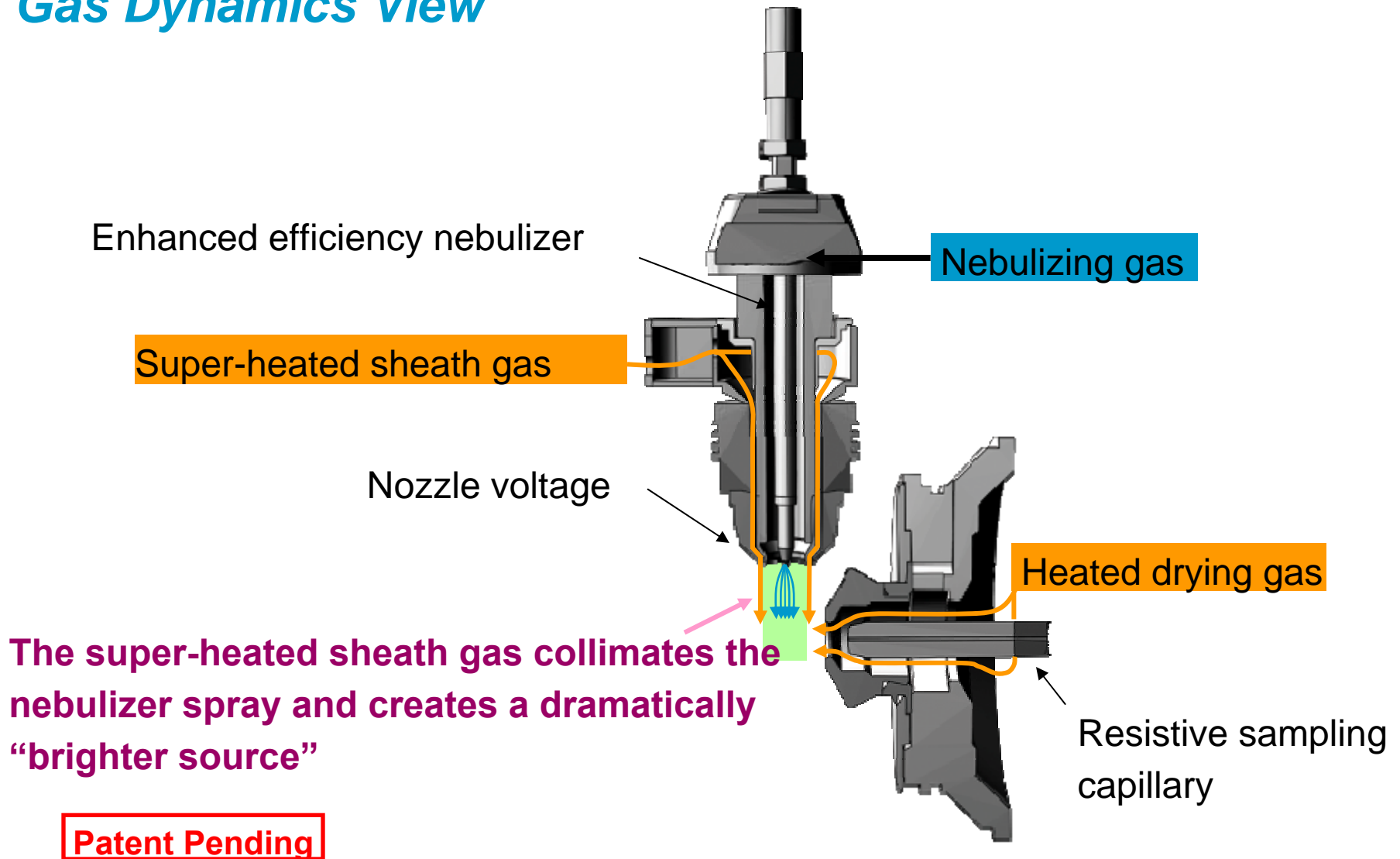
Agilent Technologies



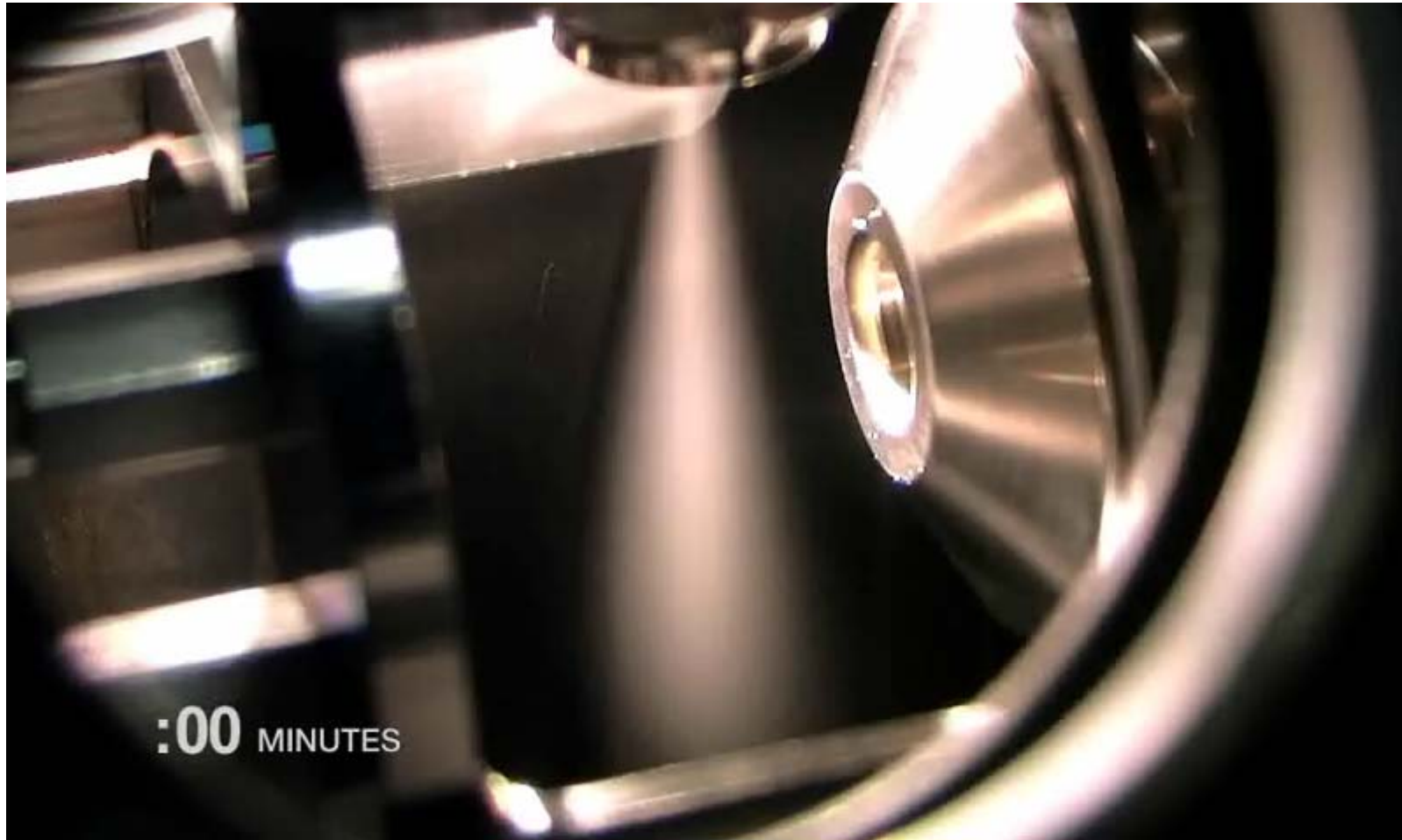
•Agilent Jet Stream Technology

Agilent Jet Stream Ion Generation

Gas Dynamics View



Agilent Jet Stream: Thermal Gradient Focussing



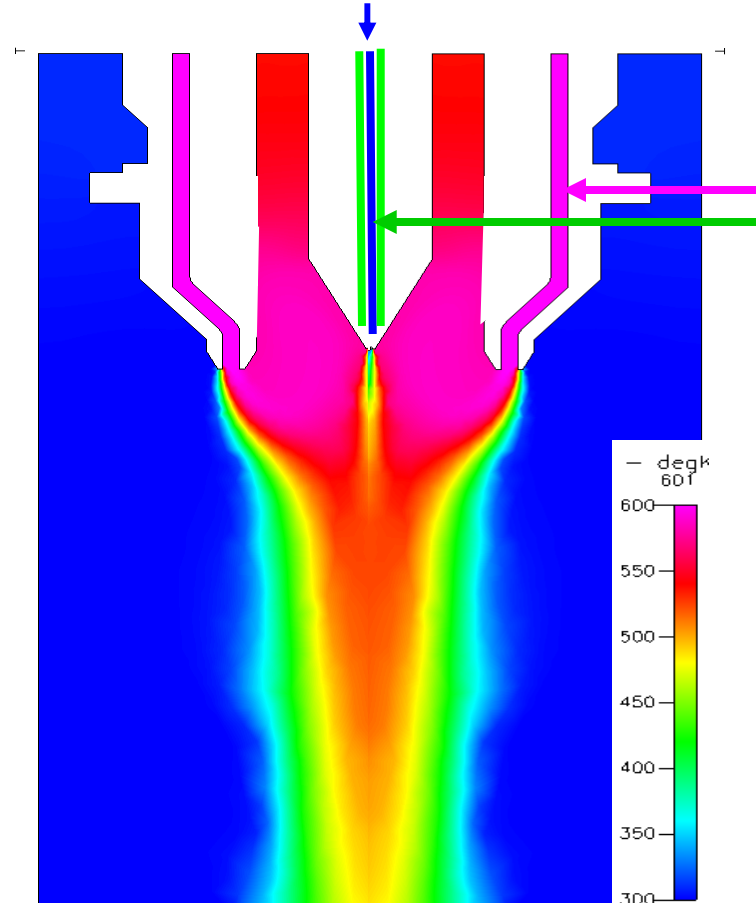
Agilent Jet Stream Ion Generation

Thermal Dynamics View

This plot is a simulation showing the **thermal profile** of Agilent Jet Stream Technology

LC flow

Thermal focusing produces the most efficient desolvation and ion generation possible!

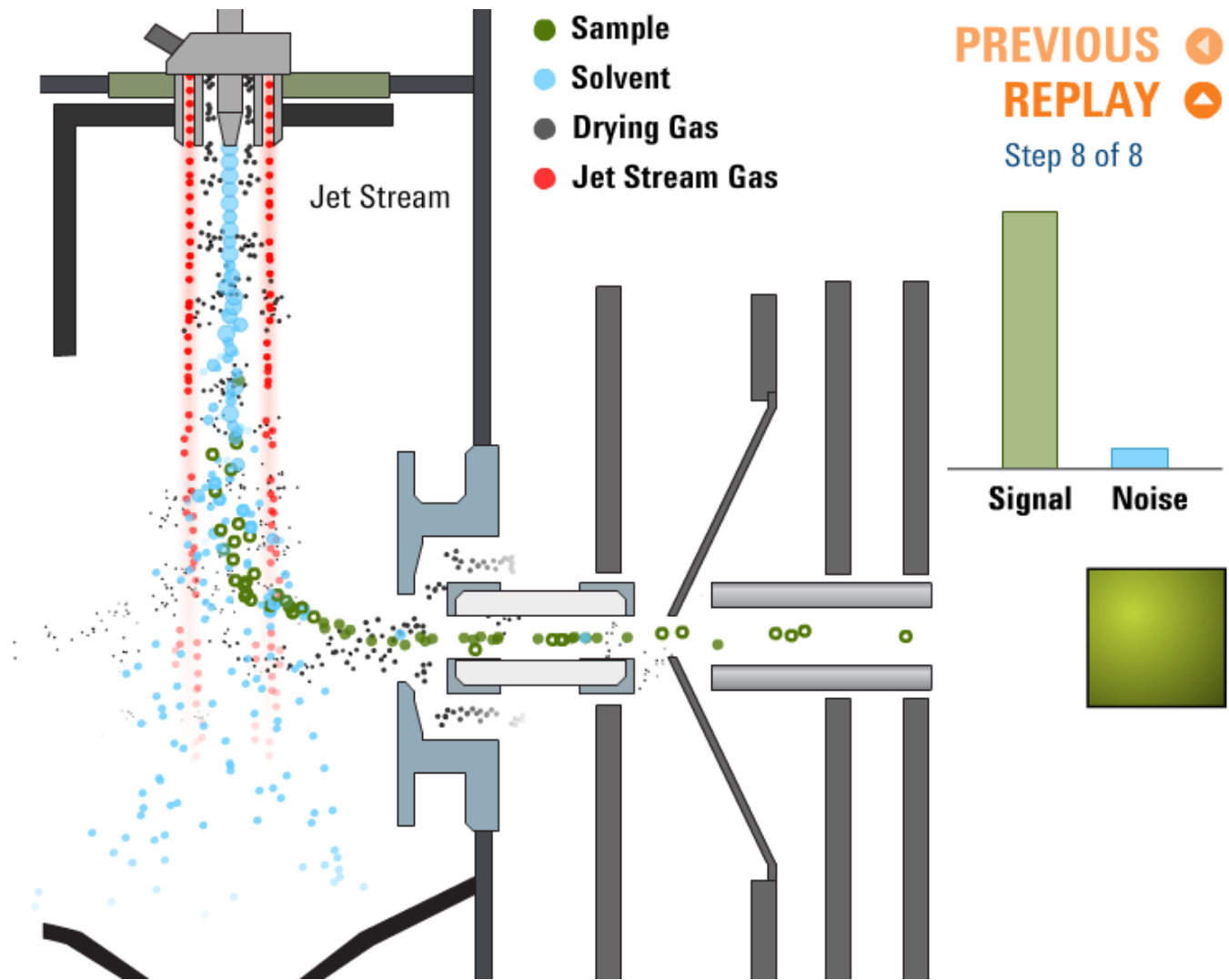


Super-heated N₂ sheath gas

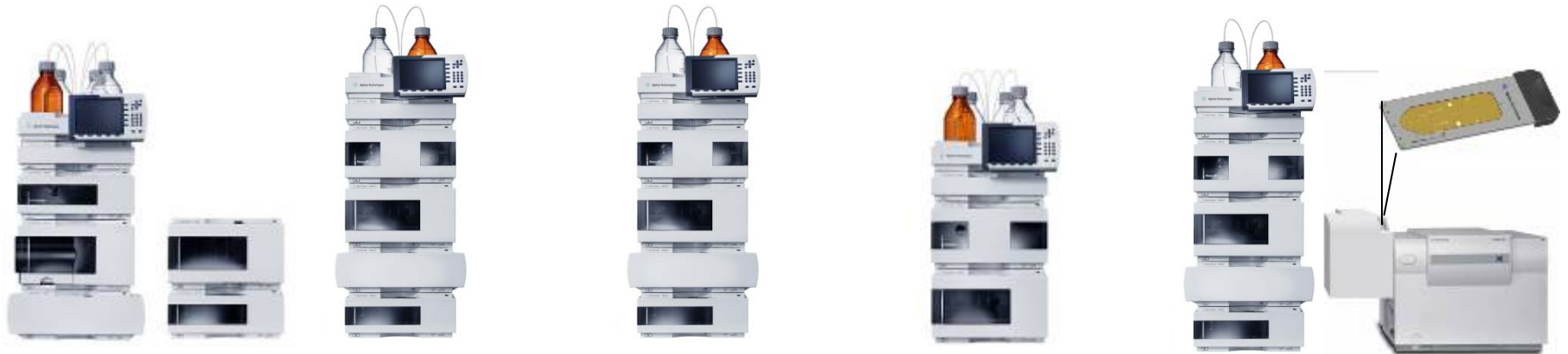
Nebulizer N₂ gas (near sonic velocity)

Patent Pending

How Does Agilent Jet Stream Work?



Agilent High Performance 1200 Series LC: Best in Class “Front End” Systems for MS



Preparative LC

Standard LC

Rapid Resolution
LC

Capillary &
Nano LC

High Sensitivity
HPLC-Chip/MS

***Chose from the industry's most comprehensive LC
portfolio to configure an integrated LC/MS system***



Agilent Technologies

Agilent 1290 Infinity LC

- *Infinite possibilities*

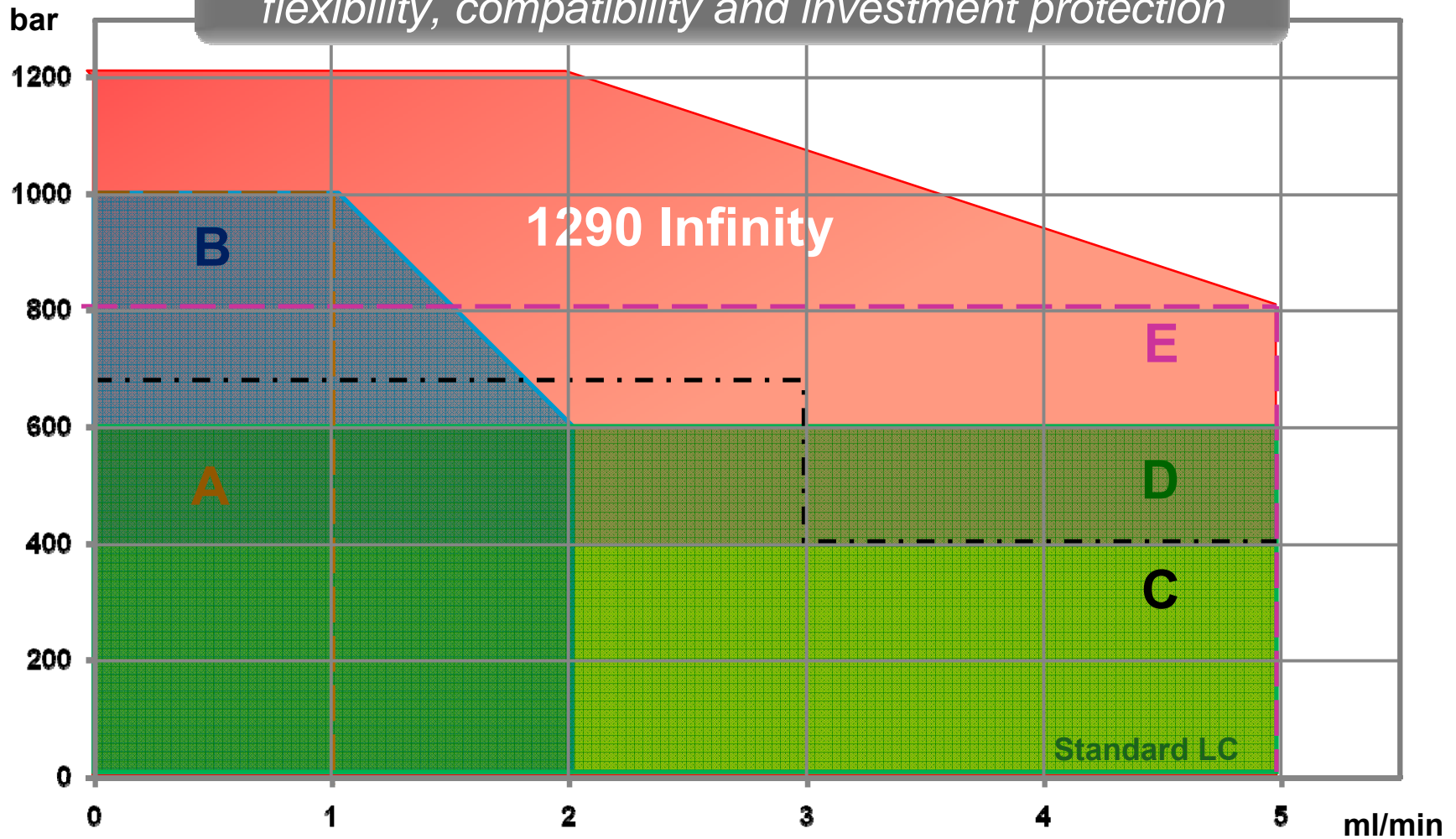


- **New** 1290 Infinity Binary Pump with integrated degasser
- **New** 1290 Infinity Autosampler
- **New** 1290 Infinity FlexCube (extend the autosampler possibilities)
- **New** 1290 Infinity TCC
- **New** 1290 Infinity Diode-Array Detector
- **New** Chemstation Software Control
- **New** MassHunter Software Control
- **New** Third party SW control
- **New** High pressure STM columns
- **New** Diagnostics capabilities



1290 Infinity – Compatible with any HPLC and UHPLC

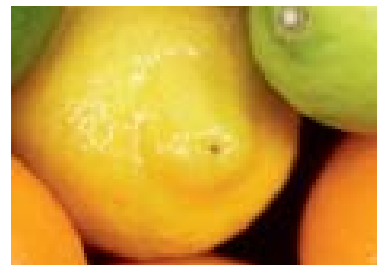
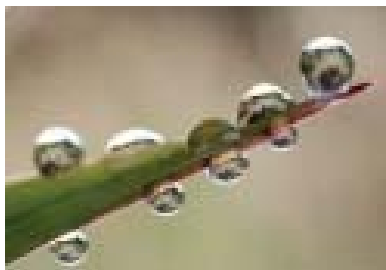
A new power range providing maximum performance, flexibility, compatibility and investment protection



Pesticides application kits

Fast and easy through your toughest problems

- Reduce the costs of implementing new technologies
- Increase confidence in your first results
- Reduce the time to technical mastery



Agilent Technologies



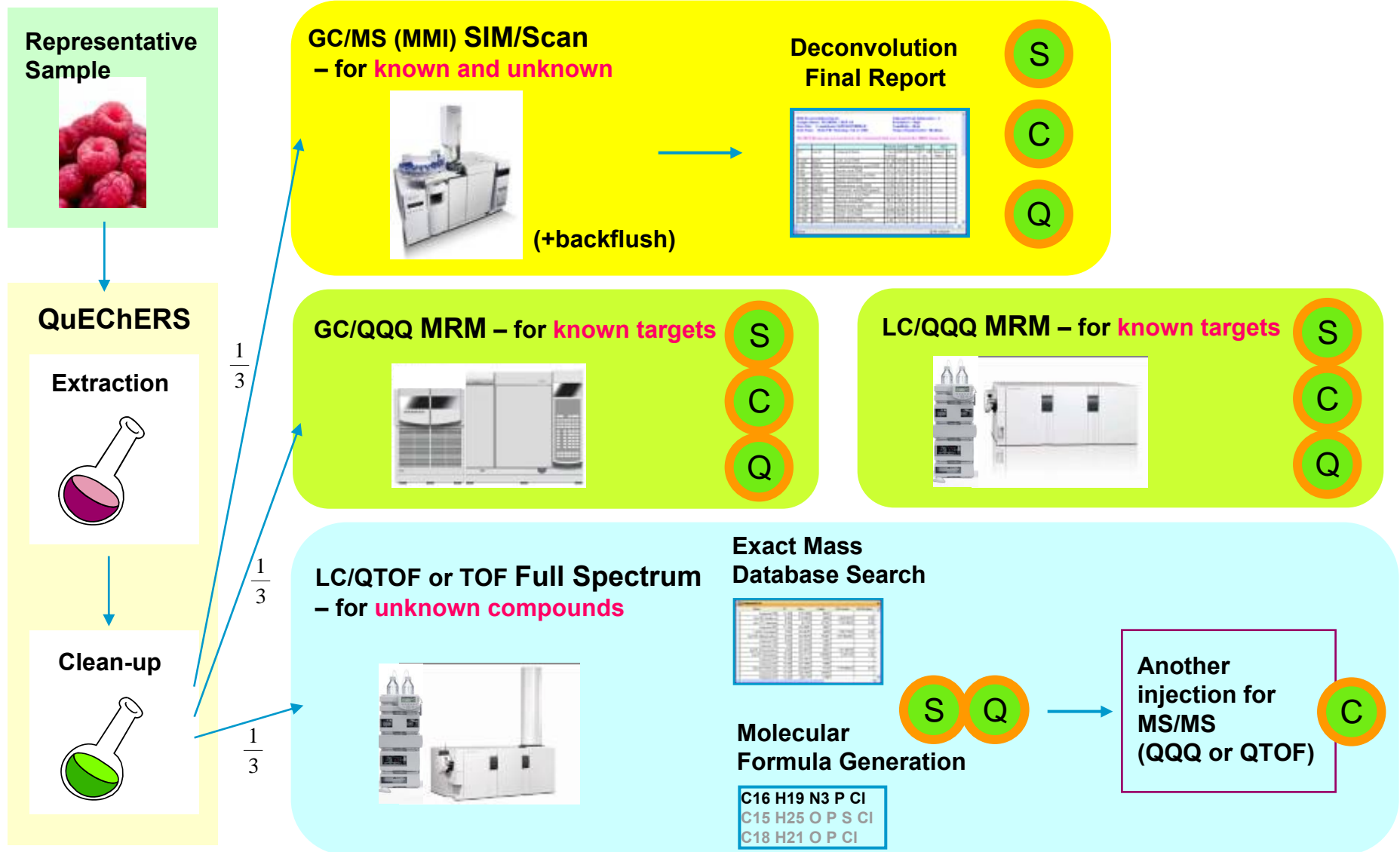
Get started quickly

Application kit

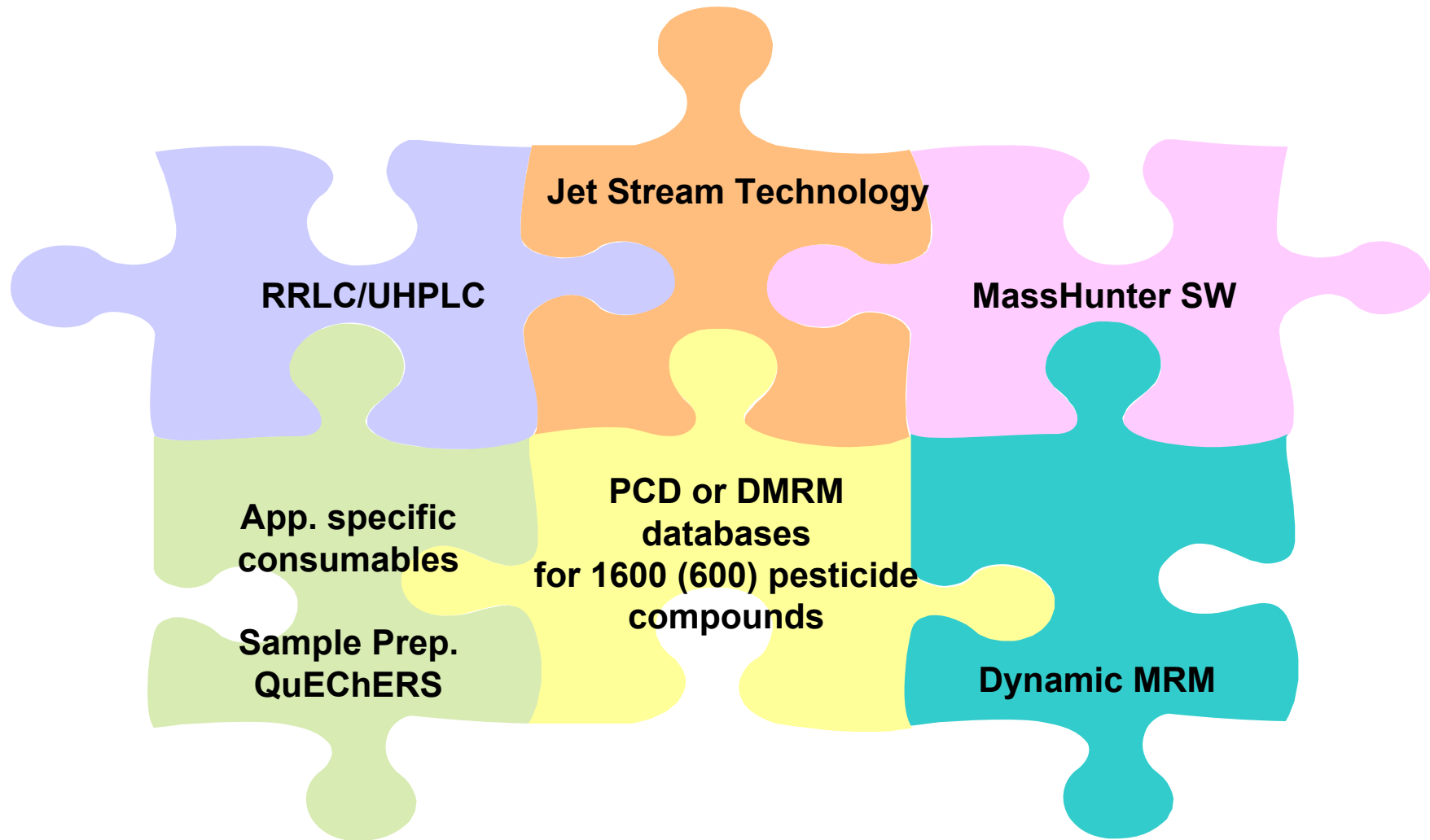
Columns, consumables & test mix
Application Note and Quick start guide
CD with method parameters
PCD and DMRM LCMS databases for fast screening

* Contents may vary based upon the application. Ask your Account Manager about the details for your application of interest.

Pesticide Workflow: Screen **S**, Confirm **C** and Quantify **Q**



State-of-the-Art Technologies to Improve Pesticide Screening with Agilent LC/MS



SUMMARY



Agilent is a Mass Spec Company

- A complete portfolio of Analyzers and inlets
- Continuous Innovations



Agilent is a Chromatography Company

- A complete portfolio of LC components
- Continuous Innovations



Agilent Solutions with Pesticide Application Kits

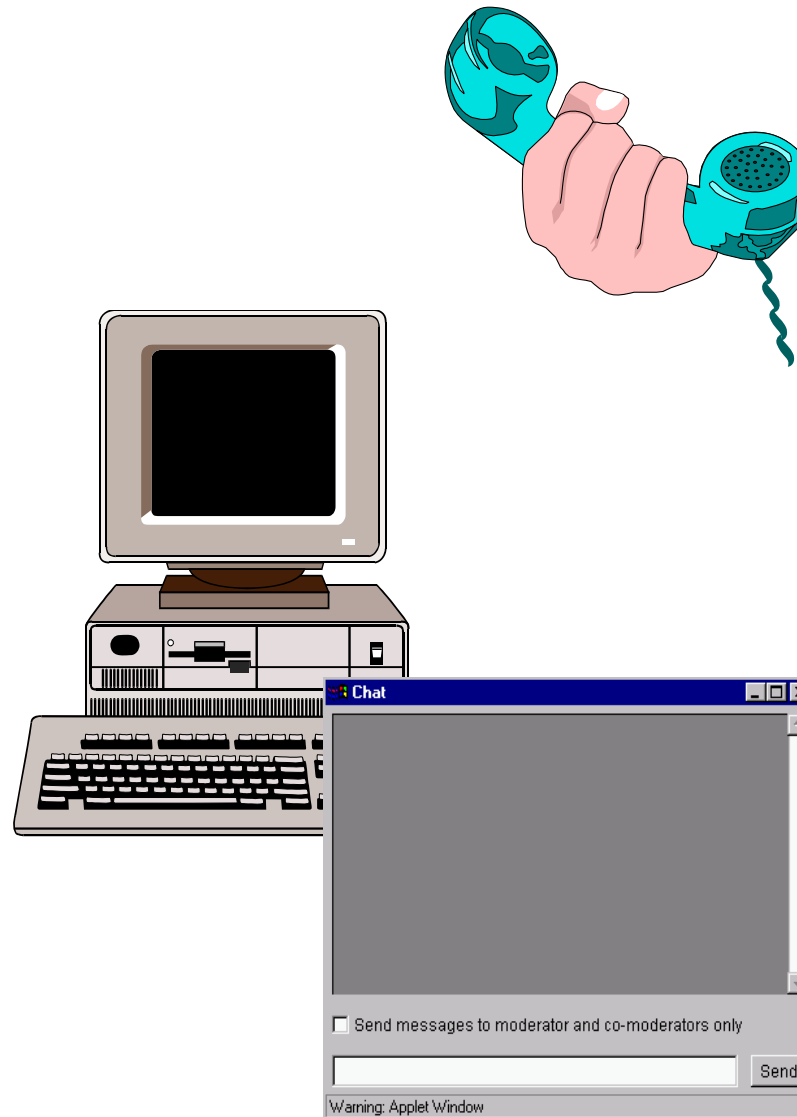
- Customizable to meet YOUR needs
- Easy to use but POWERFUL



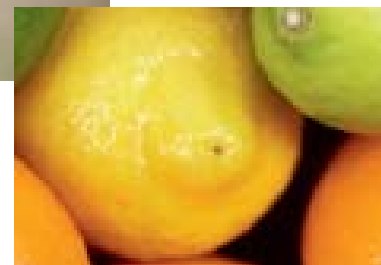
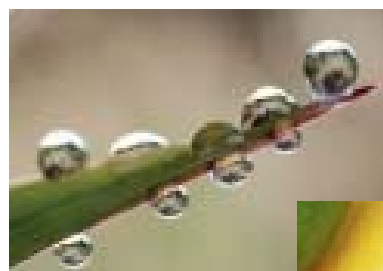
Break for Questions

For questions,

- a) type onto the Q&A box at any time during the presentation.
- b) Dial *1 on your phone and wait for your name to be announced.



Agilent LC/MS Pesticide Application Kits



Agilent Technologies



SampliQ
Extraction and
Dispersive SPE Kits

Agilent 1200SL LC



Agilent 6460 LC/QQQ

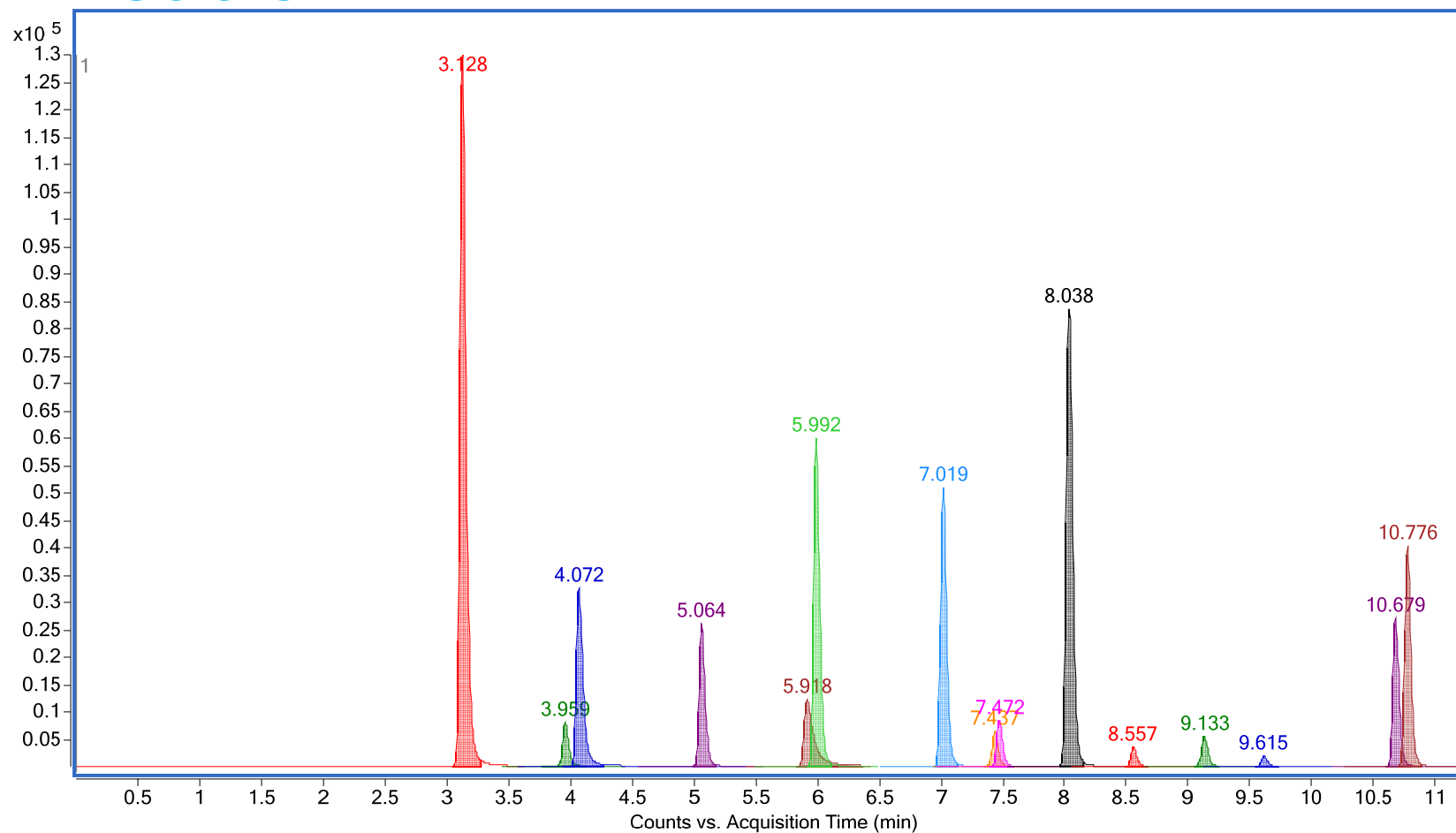
Pesticide Application Kit with Dynamic MRM Database for the

LC/MS/MS TRIPLE QUADRUPOLE

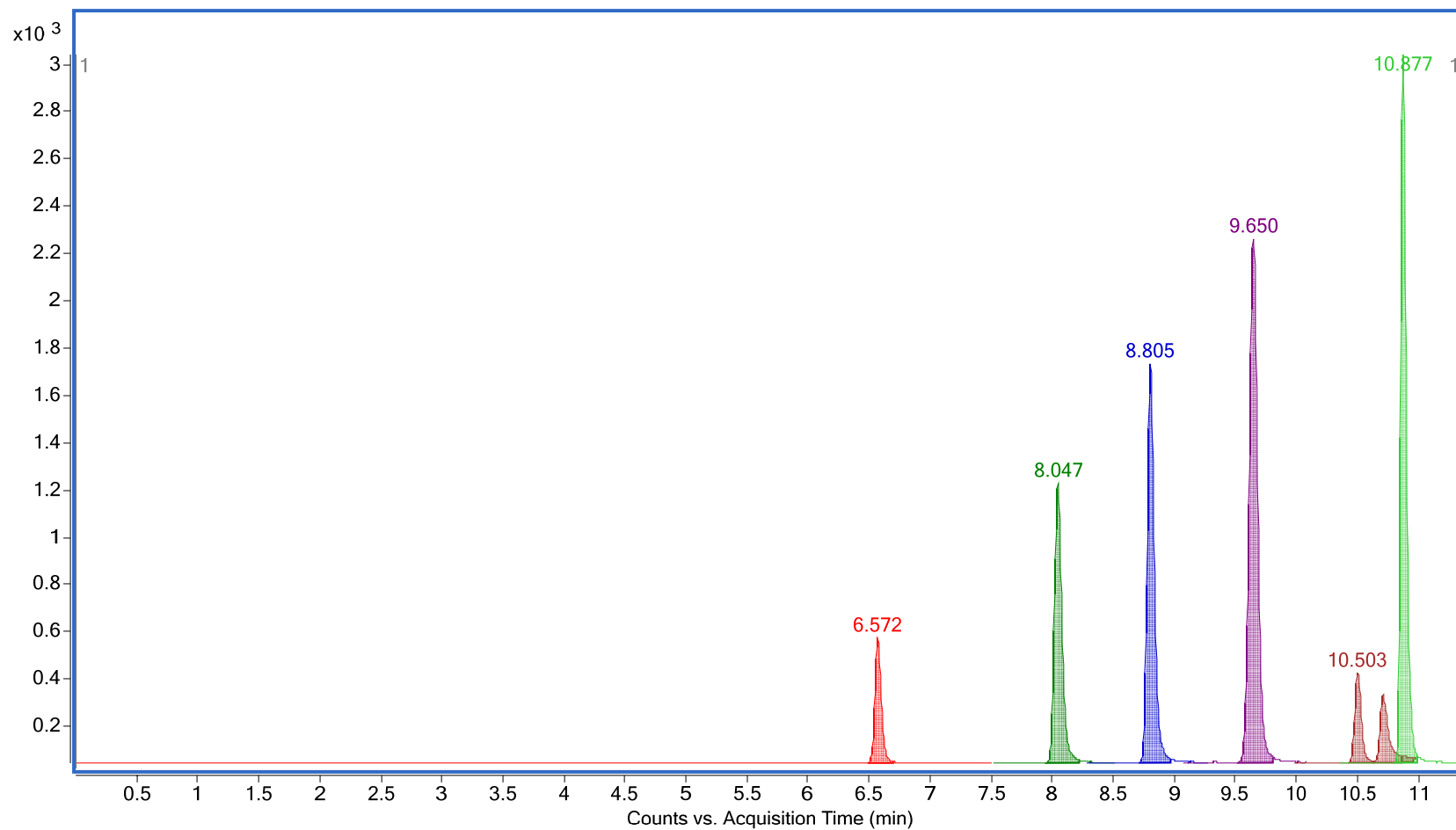


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Test Mix Positive Ion Mode: Quick Start Verification

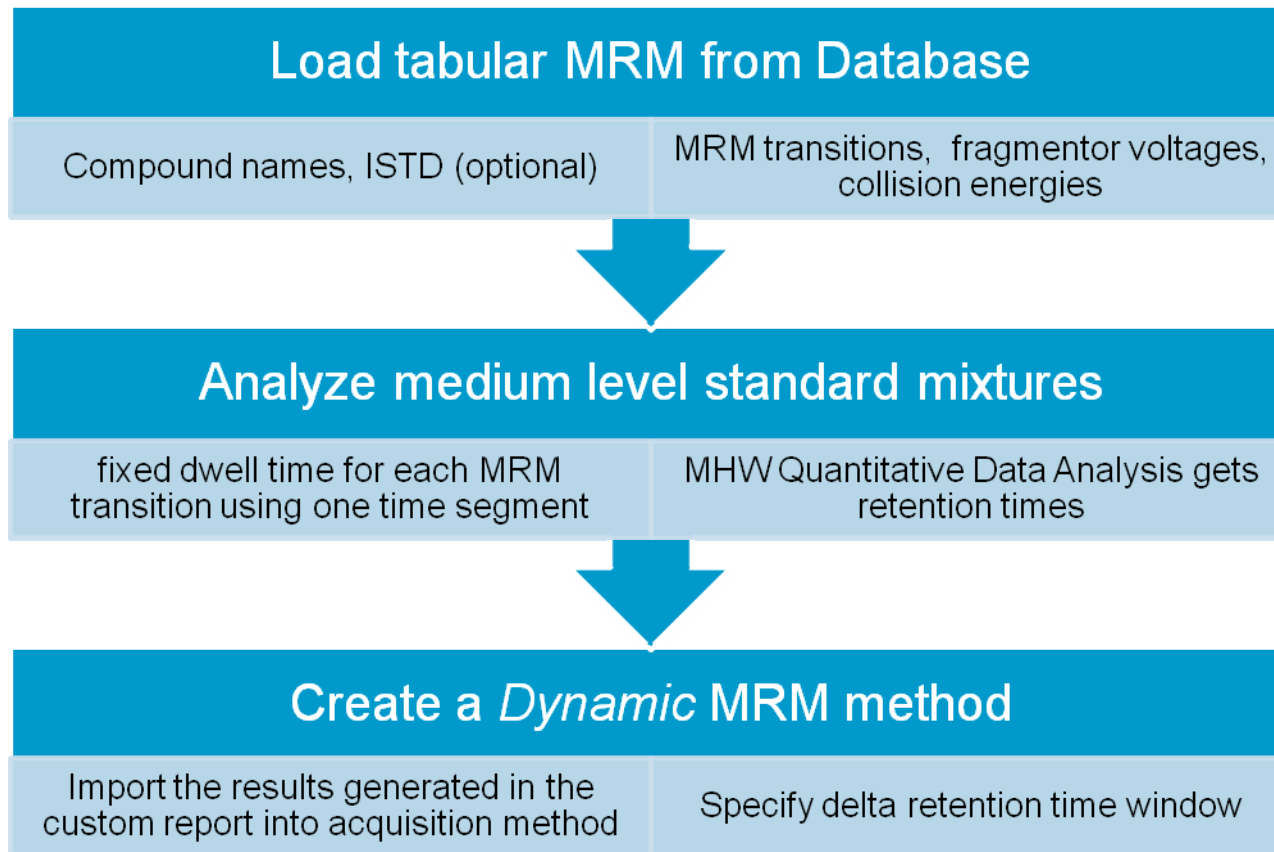


Test Mix Negative Ion Mode



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Building a Dynamic MRM Acquisition Method



Agilent 600 Compound Dynamic MRM Database

Database Browser

Database

Filter Compounds

Optimized Compounds

Date From To

Group Name

Project Name

Polarity

Search Compounds

Compound Name

Formula

Method

Show All Records Show results summary

Compound Information

<input type="checkbox"/>	Compound Name	Group	Formula	Nominal Mass	Vial Number	Project Name
<input type="checkbox"/>	Acetamidid	Insecticide	C10H11N4Cl	222.07	Vial 1	DefaultProject

<input type="checkbox"/>	Project Name	Method	Polarity	Ion Source	Instrument ID	Date Optimized	Flagged	Flag ID
<input type="checkbox"/>	DefaultProject	E:\MassHunter\Metho	Positive	ESI			<input checked="" type="checkbox"/>	

<input type="checkbox"/>	Precursor Ion	Fragmentor	Abundance
<input type="checkbox"/>	223.07	80	

<input type="checkbox"/>	Product Ion	Collision Energy	Abundance
<input type="checkbox"/>	126.01	15	321734
<input type="checkbox"/>	56	15	152499

<input type="checkbox"/>	Compound Name	Group	Formula	Nominal Mass	Vial Number	Project Name
<input type="checkbox"/>	Penconazol	Fungicide	C13H15Cl2N3	283.06	Vial 1	DefaultProject
<input type="checkbox"/>	Quinoxifen	Fungicide	C15H8Cl2FNO	307	Vial 1	DefaultProject
<input type="checkbox"/>	Parathion-methyl	Insecticide	C8H10NO5PS	263	Vial 1	DefaultProject
<input type="checkbox"/>	Indoxacarb	Insecticide	C22H17ClF3N3O	527.07	Vial 1	DefaultProject
<input type="checkbox"/>	Fenfuram	Fungicide	C12H11NO2	201.08	Vial 1	DefaultProject
<input type="checkbox"/>	Dodemorph	Fungicide	C18H35NO	281.27	Vial 1	DefaultProject

Current Database : D:\MassHunter\Databases\MassHunter_Pesticide_DynamicMRM_Database

Refresh Save Import Cancel

Dynamic MRM Acquisition Parameters – *Customized Methods from Database*

Tune file
atunes.tune.xml
Browse ...

Stop time
 No limit/As Pump
 1 min

Ion source
ESI

Time filtering
 Peak width 0.04 min

Time segments

#	Start Time	Scan Type	Polarity	Div Valve	Delta EMV	Stored
1	0	Dynamic MRM	Negative	To MS	300	<input checked="" type="checkbox"/>

Acquisition | Source | Chromatogram | Instrument | Diagnostics

Scan segments

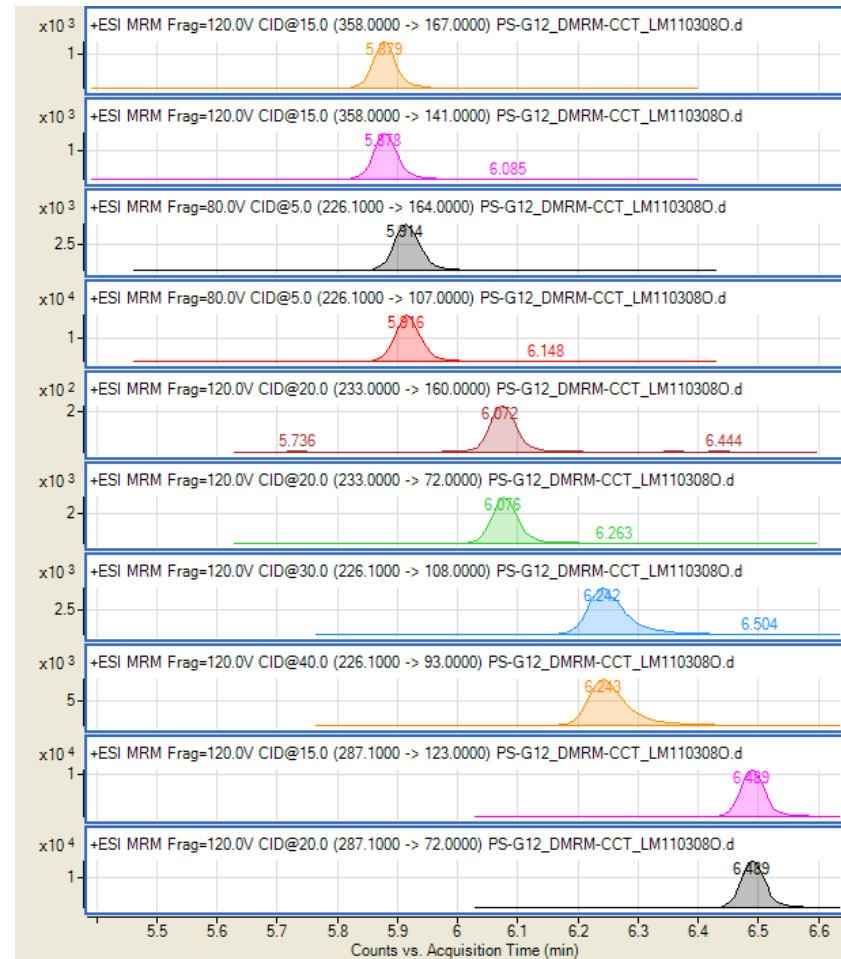
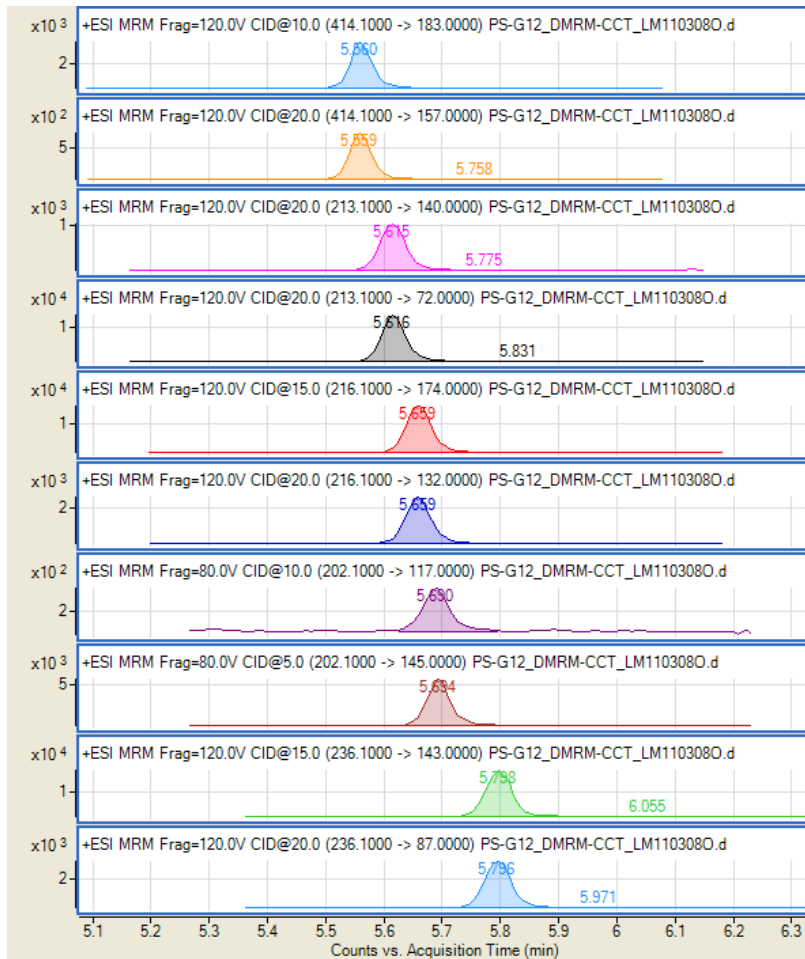
Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Fragmentor	Collision Energy	Ret Time (min)	Delta Ret Time
Bentazon	<input type="checkbox"/>	239.1	Unit	132	Unit	80	32	7.117	1
2,4,5-T	<input type="checkbox"/>	252.9	Unit	194.8	Unit	76	9	8.565	1
Silvex	<input type="checkbox"/>	266.9	Unit	194.9	Unit	90	5	9.325	1
Acifluorfen	<input type="checkbox"/>	360	Unit	315.9	Unit	78	5	10.119	1
Dinoseb	<input type="checkbox"/>	239.1	Unit	207	Unit	154	21	11.226	1
Hexafluoron	<input type="checkbox"/>	459	Unit	438.9	Unit	102	5	11.423	1

Dynamic MRM Parameters

- Add Row
- Delete Row
- Sort
- Import from optimizer...**
- Cut
- Copy
- Paste
- Paste from Clipboard
- Fill Down
- Fill Column

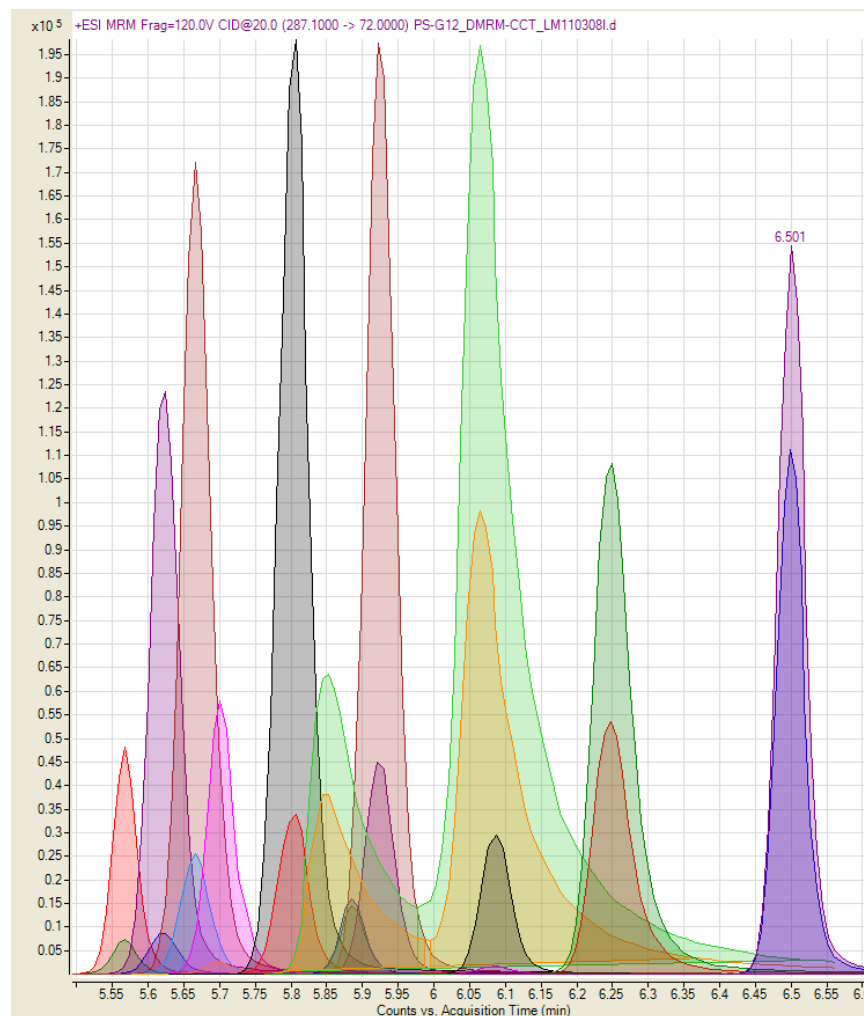
Dynamic MRM at the 10 pg level for 100 pesticides

1 min $\Delta R.T.$ - based acquisition window for each MRM transition



Dynamic MRM 11 Compounds (22 MRMs) eluting in about 1 min window

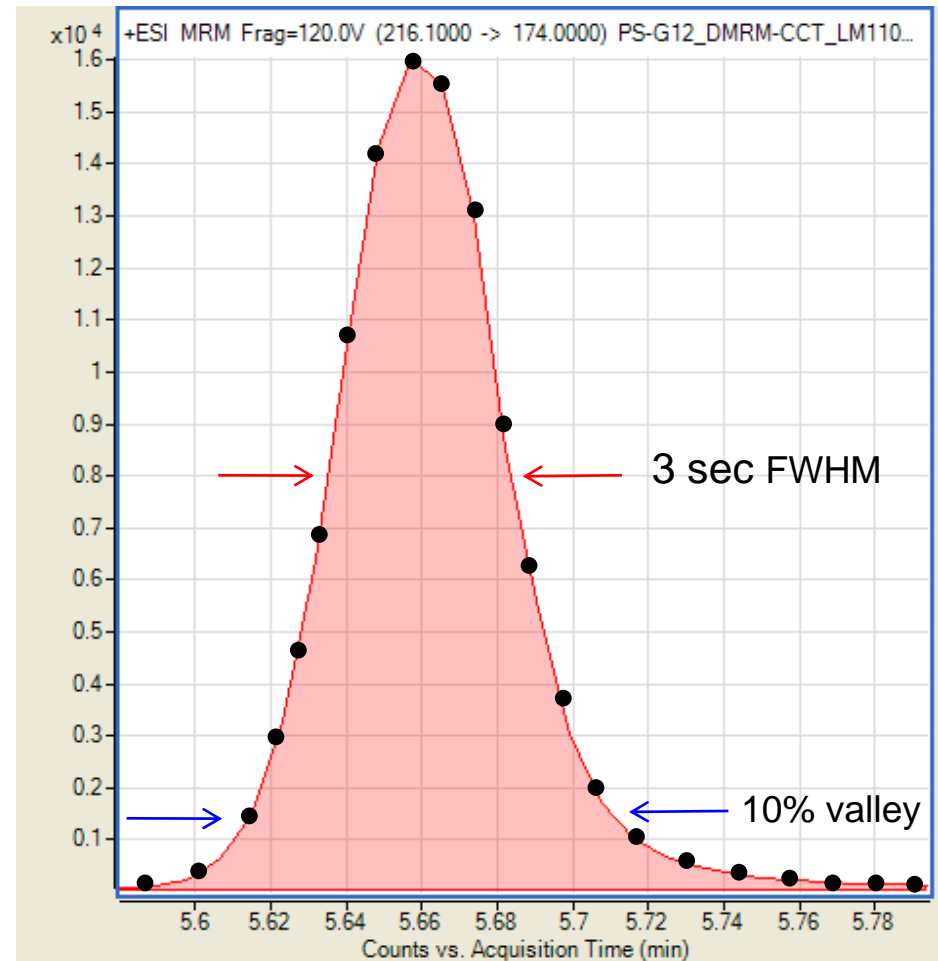
Compound Name	Precursor Ion	Product Ion	Retention Time
Cinosulfuron	414.1	183	5.579
Cinosulfuron (Q)	414.1	157	5.579
Chlorotoluron	213.1	72	5.642
Chlorotoluron (Q)	213.1	140	5.642
Atrazine	216.1	174	5.682
Atrazine (Q)	216.1	132	5.682
Carbaryl	202.1	145	5.736
Carbaryl (Q)	202.1	117	5.734
Carboxin	236.1	143	5.836
Carboxin (Q)	236.1	87	5.836
Chlorsulfuron	358.0	167	5.896
Chlorsulfuron (Q)	358.0	141	5.896
Ethiofencarb	226.1	107	5.937
Ethiofencarb (Q)	226.1	164	5.936
Dodemorph	282.3	116	6.073
Dodemorph (Q)	282.3	98	6.074
Diuron	233.0	72	6.101
Diuron (Q)	233.0	160	6.101
Cyprodinil	226.1	108	6.245
Cyprodinil (Q)	226.1	93	6.246
Difenoxurone	287.1	123	6.509
Difenoxurone (Q)	287.1	72	6.509



Typical results: 10 pg Atrazine on-column using Dynamic MRM 6460A QQQ with Jet Stream Technology

- **Avg. Signal Height: 15,650**
- **Avg. Signal Area: 50,966**
- **RSD: 3.2 %**
- **Estimated LOQ: 100 fg or less**

- **6-7 data points above FWHM**
- **3 sec FWHM, 6 sec @10% valley**
- **20 data points baseline-to-baseline**



Pesticides LC/MS method

1200 LC parameters

Column
Column temperature
Injection volume
Autosampler temp
Needle wash
Mobile phase

Eclipse Plus-C18, 2.1 x 100mm, 1.8 μ m
35 °C
5.0 μ L
6 °C
flushport (MeOH:H₂O 75:25), 5 secs
A = 0.01% formic acid in water
B = 5 mM ammonium formate 0.01% formic acid in 95:5 acetonitrile:water

Flow rate
Gradient

0.3 mL/min
0 min 6% B
15 min 95% B
20 min 6% B
1 min

Stop time
Post time

Drying gas temperature
Drying gas flow (nitrogen)
Nebulizer gas pressure (nitrogen)
Capillary voltage
Sheath gas temperature
Sheath gas flow
Nozzle voltage

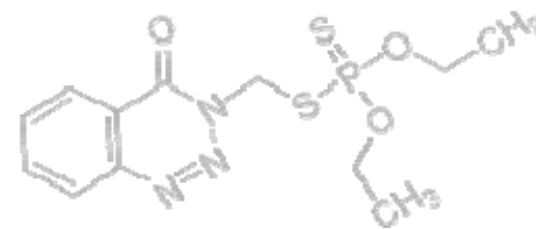
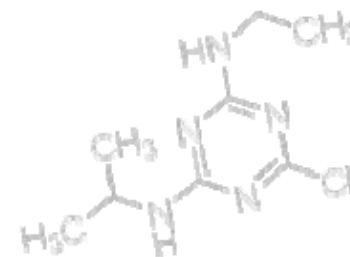
Jet stream conditions

275 °C
6 L/min
35 psig
4000 V
325 °C
12 L/min
Off

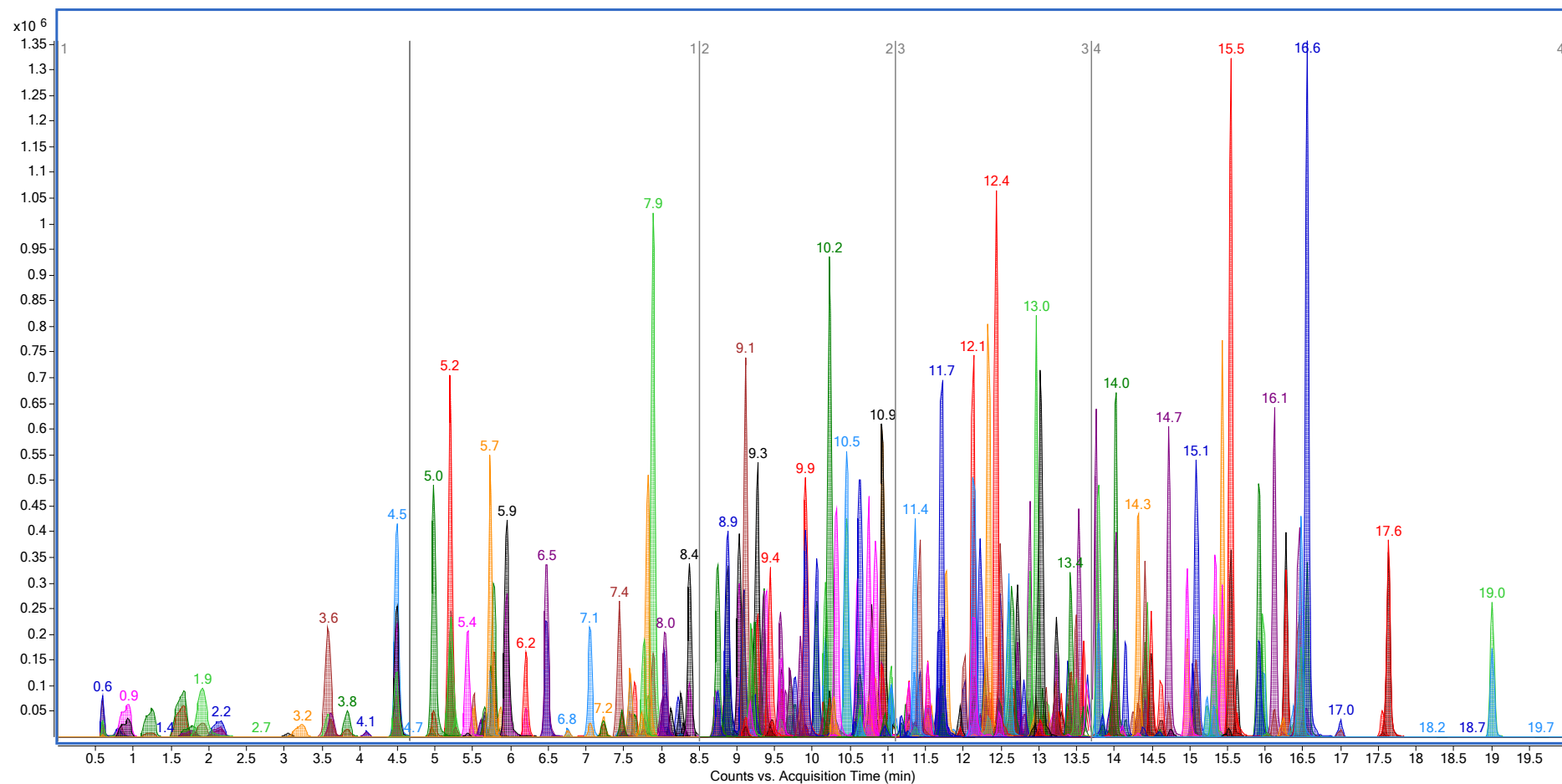
MS1 and MS2 resolution
Time Filtering
Dynamic MRM transitions
Constant cycle time
Delta EMV

6460A QQQ settings

Unit
peak width = 0.03 min
up to 4000
373 ms
400 V

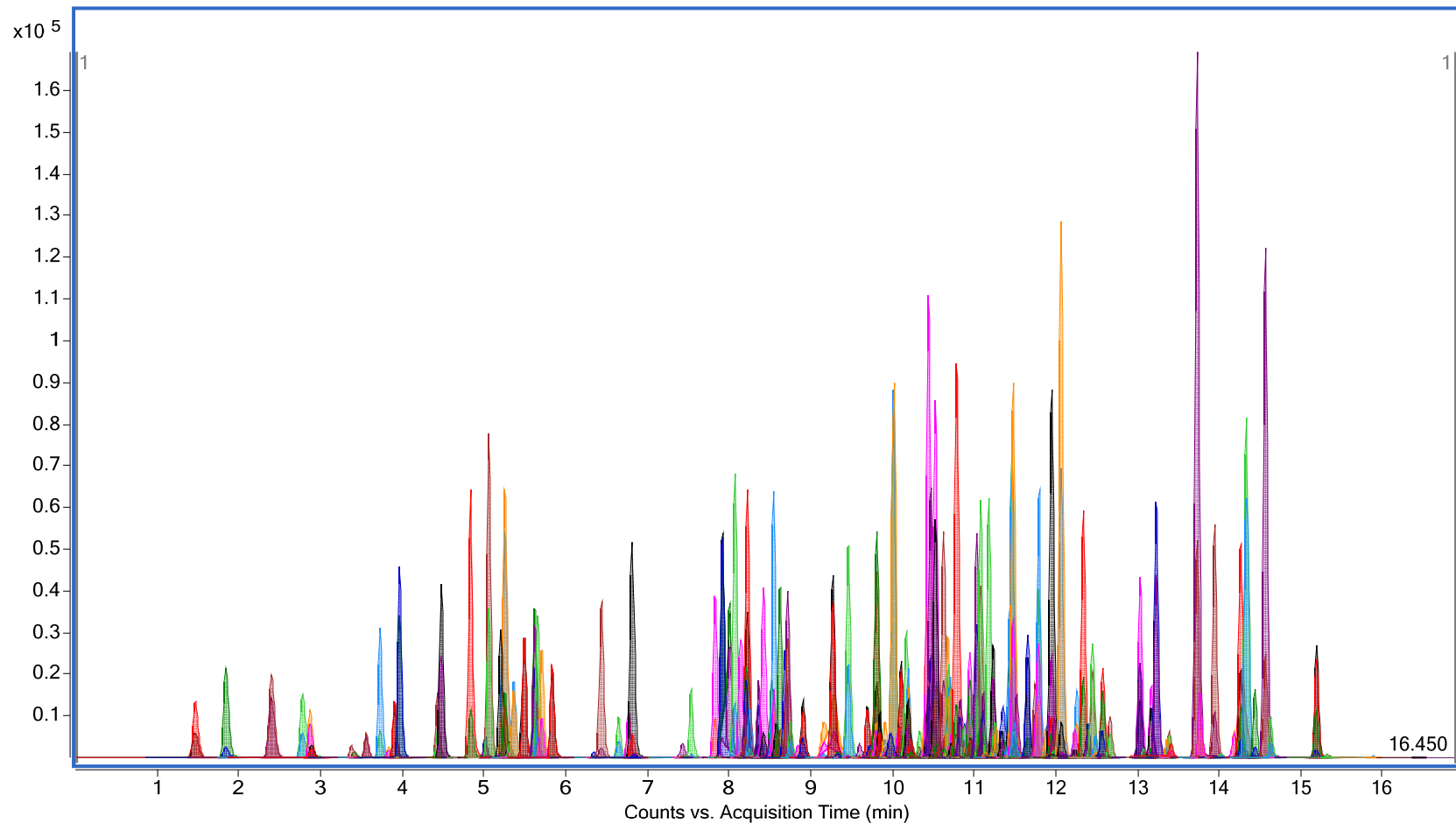


Dynamic MRM of 300 Pesticides two Transitions Each



Run with 1200-SL LC 2.1 x 100 C18 Eclipse PLUS 1.8 u

Pesticide Mix run with Agilent 1290 Infinity 1200 Bar LC: Benefit of *HIGHER PEAK CAPACITY*

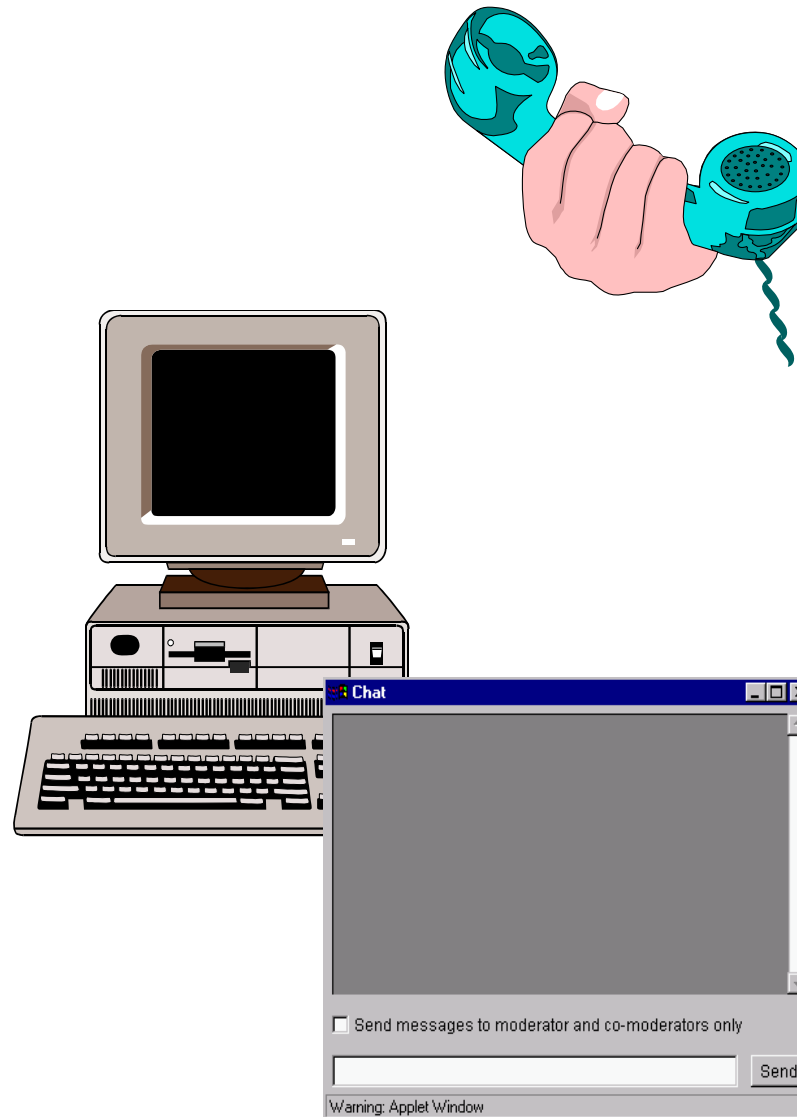


LC 2.1 x 150 C18 Eclipse PLUS HD 1.8 μ , 0.6 mL/min, 800 bar

Break for Questions

For questions,

- a) type onto the Q&A box at any time during the presentation.
- b) Dial *1 on your phone and wait for your name to be announced.



6230 TOF



6530 QTOF



6540 QTOF



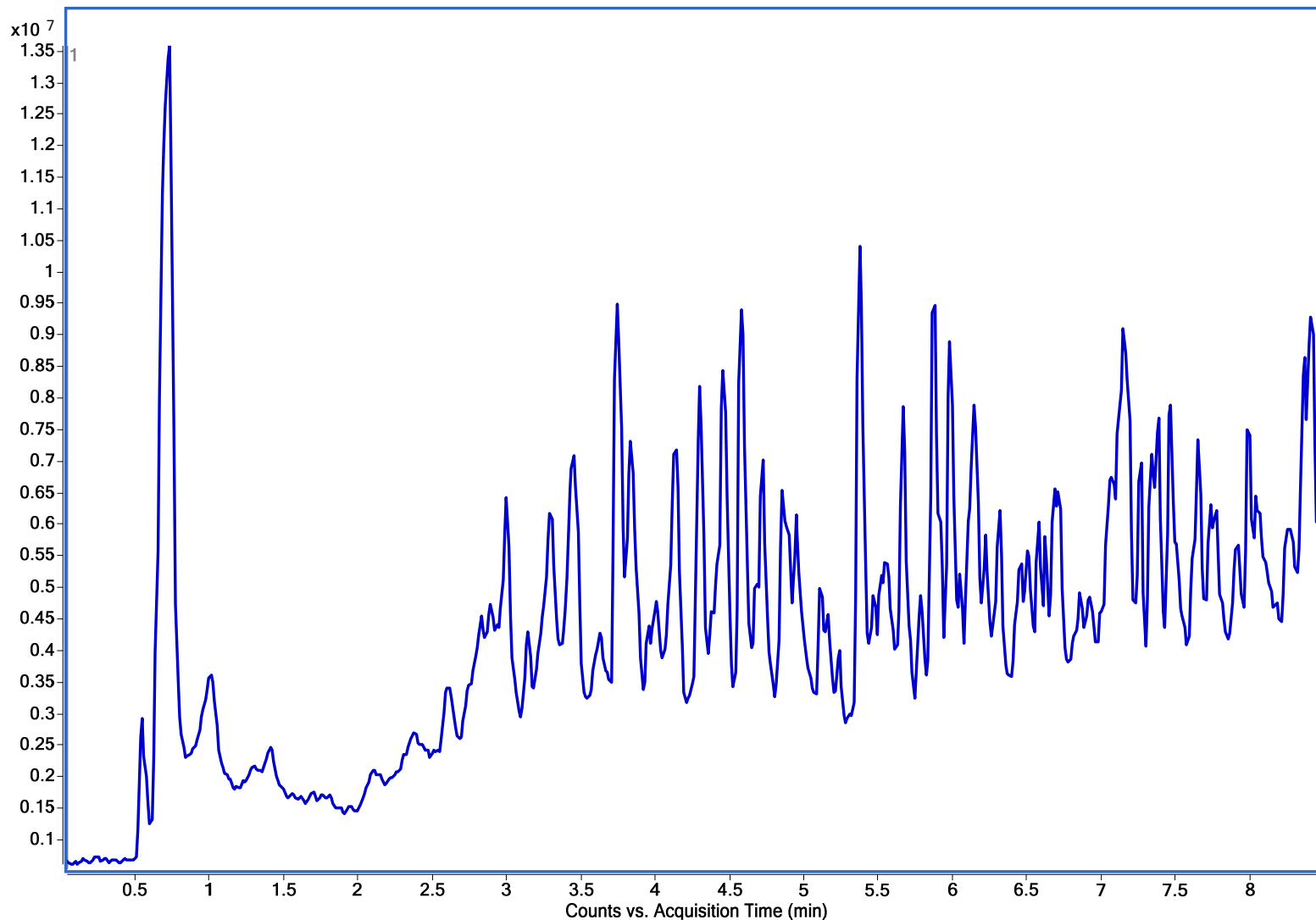
**Pesticide Application Kit with Accurate Mass
Retention Time Personal Compound Database
for the**

LC/MS TOF AND QTOF

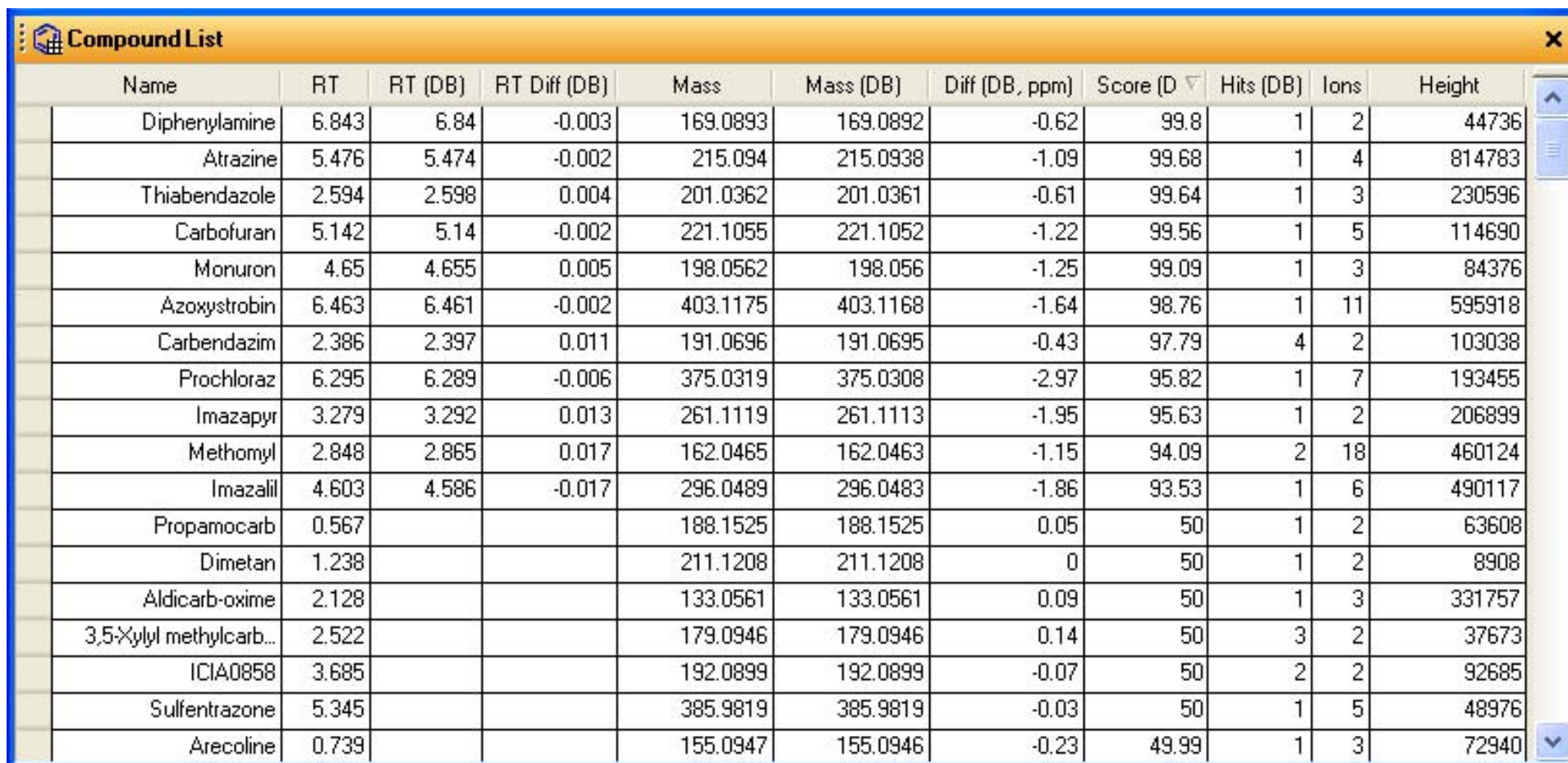


Agilent Technologies

Complex Pepper Extract: How do you Identify Pesticides in this Full Spectrum Accurate Mass Chromatogram?



Answer: Automated Exact Mass Database Search



Name	RT	RT (DB)	RT Diff (DB)	Mass	Mass (DB)	Diff (DB, ppm)	Score (D)	Hits (DB)	Ions	Height
Diphenylamine	6.843	6.84	-0.003	169.0893	169.0892	-0.62	99.8	1	2	44736
Atrazine	5.476	5.474	-0.002	215.094	215.0938	-1.09	99.68	1	4	814783
Thiabendazole	2.594	2.598	0.004	201.0362	201.0361	-0.61	99.64	1	3	230596
Carbofuran	5.142	5.14	-0.002	221.1055	221.1052	-1.22	99.56	1	5	114690
Monuron	4.65	4.655	0.005	198.0562	198.056	-1.25	99.09	1	3	84376
Azoxystrobin	6.463	6.461	-0.002	403.1175	403.1168	-1.64	98.76	1	11	595918
Carbendazim	2.386	2.397	0.011	191.0696	191.0695	-0.43	97.79	4	2	103038
Prochloraz	6.295	6.289	-0.006	375.0319	375.0308	-2.97	95.82	1	7	193455
Imazapyr	3.279	3.292	0.013	261.1119	261.1113	-1.95	95.63	1	2	206899
Methomyl	2.848	2.865	0.017	162.0465	162.0463	-1.15	94.09	2	18	460124
Imazalil	4.603	4.586	-0.017	296.0489	296.0483	-1.86	93.53	1	6	490117
Propamocarb	0.567			188.1525	188.1525	0.05	50	1	2	63608
Dimetan	1.238			211.1208	211.1208	0	50	1	2	8908
Aldicarb-oxime	2.128			133.0561	133.0561	0.09	50	1	3	331757
3,5-Xylyl methylcarb...	2.522			179.0946	179.0946	0.14	50	3	2	37673
ICIA0858	3.685			192.0899	192.0899	-0.07	50	2	2	92685
Sulfentrazone	5.345			385.9819	385.9819	-0.03	50	1	5	48976
Arecoline	0.739			155.0947	155.0946	-0.23	49.99	1	3	72940

But how do you get from the previous slide to here?

The Pesticide Personal Compound Database: 1600 Pesticides and Related compounds

MassHunter Personal Compound Database - C:\MassHunter\databases\Pesticides.mtl

File Edit View Database Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds


Mass: [M+H]⁺ Neutral [M-H]⁻
Mass tolerance: ppm mDa

Retention time: RT tolerance: min
 Require

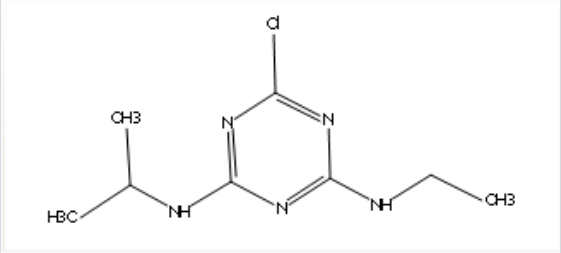
Formula:
Name:
Notes:

CAS:

Radical ion search mode
 Include neutrals
 Include anions
 Include cations

Molecule: 

Structure MDL Text

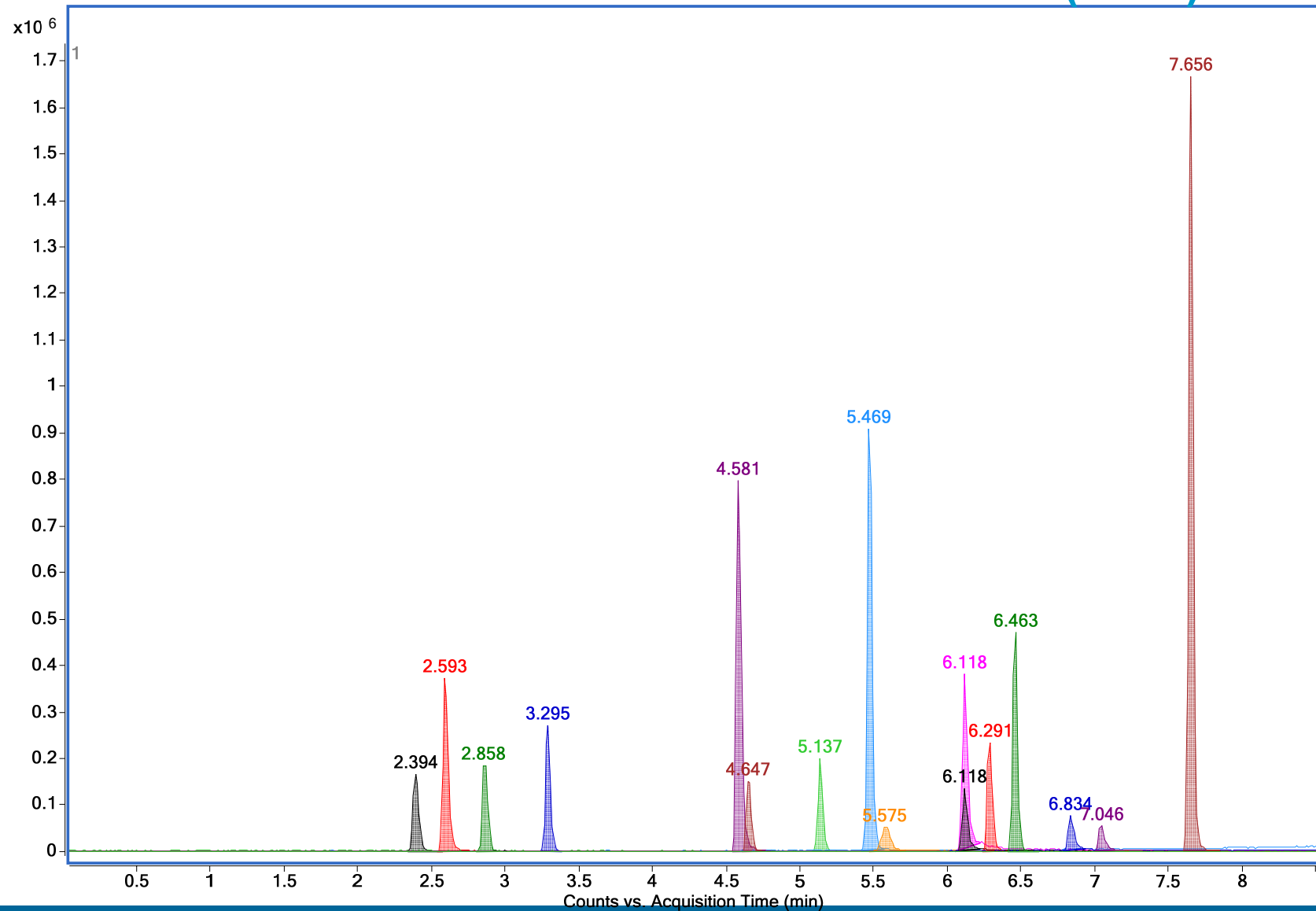


Notes:

Single Search Results: 11 hits

Name	Formula	Mass	RT (min)	CAS
Hydroxyatrazine	C8H15N5O	197.12766		2163-68-0
▶ Atrazine	C8H14ClN5	215.09377	5.475	1912-24-9
Atrazine-D5	C8H9D5ClN5	220.12516		
Atrazine-2-ethylamino	C10H20N6	224.17494		30360-19-1

Run a Set or Sets of Pesticide Standards: Process with Masshunter's Molecular Feature Extractor (MFE)



Run “Find Compounds” and Resolve Conflicts

MassHunter Personal Compound Database - C:\MassHunter\databases\Pesticides.mtl

File Edit View Database Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds

Masses:

Mass	RT	Hits
225.1593	3.773	4
193.1106	5.729	4
179.0946	2.522	3
187.0632	2.094	2
151.0631	4.948	2
151.0641	2.598	2
255.15	4.237	2
254.152	5.807	2
269.117	6.865	2
151.0634	3.685	2

File ...
Clear

Masses:
 [M+H]⁺ Neutral [M-H]⁻
Mass tolerance: 10 ppm mDa

Retention times:
 Ignore Optional Required
RT tolerance: 0.1 min

Radical ion search mode:
 Include neutrals
 Include anions
 Include cations

Molecule: Structure MDL Text

Notes:

Batch Search Results: 2 hits for Mass: RT:

Best	Name	Formula	Mass	Delta Mass (ppm)	RT (min)	Delta RT	CAS
<input checked="" type="checkbox"/>	Ferimzone[E]	C15H18N4	254.15315	4.52			89269-64-7
<input type="checkbox"/>	Ferimzone[Z]	C15H18N4	254.15315	4.52			89269-64-7

Paste or Import Masslist from MassHunter Qual MFE Results

MassHunter Personal Compound Database - C:\MassHunter\databases\P...

File Edit View Database Links Help

Find Compounds

Single Search Batch Search Batch Summary Edit Compounds

Masses: File ... Clear

Mass	RT	Hits
269.1187	7.018	2
403.1176	6.46	2
162.0462	2.866	2
191.0695	2.396	1
173.0467	2.996	1
261.1117	3.292	1
215.0941	5.474	1
375.0316	6.289	1
198.0561	4.655	1
169.0892	6.84	1

Masses: [M+H]⁺ Neutral [M-H]⁻
Mass tolerance: 10 ppm mDa

Retention times: Ignore Optional Required
RT tolerance: 0.1 min

Radical ion search mode: Include neutrals Include anions Include cations

Molecule: Structure MOL Text

Notes:

Batch Search Results: 2 hits for Mass: 269.1187 RT: 7.018

Best	Name	Formula	Mass	Delta Mass (ppm)	RT (min)
<input checked="" type="checkbox"/>	Acetochlor	C ₁₄ H ₂₀ ClNO ₂	269.11826	-1.63	
<input type="checkbox"/>	Alachlor	C ₁₄ H ₂₀ ClNO ₂	269.11826	-1.63	

Batch Summary: Update Retention Times for “Targeted” Analysis

MassHunter Personal Compound Database - C:\MassHunter\databases\custom pesticides.mtl

File Edit View Database Links Help

Find Compounds

Single Search Batch Search **Batch Summary** Edit Compounds

Report comments:

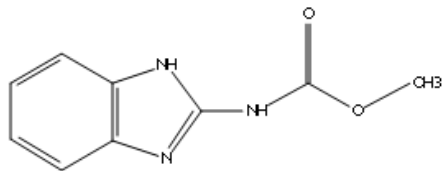
Mass list search parameters
 Mass list file:
 Masses: +/- 10 ppm Neutral Search: Neutrals

Retention time parameters
 RT's: +/- 0.1 min (Optional)

Best mass match results
 Total hits: 12 / 17 (70.6%)
 Conflicting hits: 0 / 12 (0%)
 Single matches: 10 / 17 (58.8%)

Apply Retention Times

Molecule: Structure MOL Text



Notes:

Batch Summary Results: 12 hits (12 total hits, 10 single matches, 17 submitted)

Name	Formula	Mass Submitted	Mass	Delta Mass (ppm)	RT Submitted	RT (min)	Delta RT	CAS
Carbendazim	C9H9N3O2	191.06950	191.06948	-0.10	2.397	2.397	0.000	10605-21-7
Methomyl	C5H10N2O2S	162.04620	162.04630	0.62	2.865	2.865	0.000	16752-77-5
Prochloraz	C15H16Cl3N3O2	375.03160	375.03081	-2.11	6.289	6.289	0.000	67747-09-5
Imazapyr	C13H15N3O3	261.11170	261.11134	-1.38	3.292	3.292	0.000	81334-34-1
Imazalil	C14H14Cl2N2O	296.04870	296.04832	-1.28	4.586	4.586	0.000	35554-44-0
Diazinon	C12H21N2O3PS	304.10180	304.10105	-2.47	7.653	7.653	0.000	333-41-5
Azoxystrobin	C22H17N3O5	403.11760	403.11682	-1.93	6.461	6.461	0.000	131860-33-8
Carbofuran	C12H15NO3	221.10550	221.10519	-1.40	5.140	5.140	0.000	1563-66-2
Atrazine	C8H14ClN5	215.09410	215.09377	-1.53	5.474	5.474	0.000	1912-24-9
Diphenylamine	C12H11N	169.08920	169.08915	-0.30	6.840	6.840	0.000	122-39-4
Monuron	C9H11ClN2O	198.05610	198.05599	-0.56	4.655	4.655	0.000	150-68-5

Repeat Process for Real Sample: Targeted and Non-Targeted

MassHunter Personal Compound Database - C:\MassHunter\databases\Pesticides_RT_Seiko...

File Edit View Database Links Help

Find Compounds

Single Search Batch Search **Batch Summary** Edit Compounds

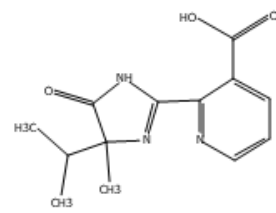
Report comments:

Mass list search parameters
 Mass list file:
 Masses: +/- 10 ppm Neutral Search: Neutrals

Retention time parameters
 RT's: +/- 0.1 min (Optional)

Best mass match results
 Total hits: 12 / 16 (75.0%)
 Conflicting hits: 0 / 12 (0%)
 Single matches: 11 / 16 (68.8%)

Molecule: Structure MDL Text



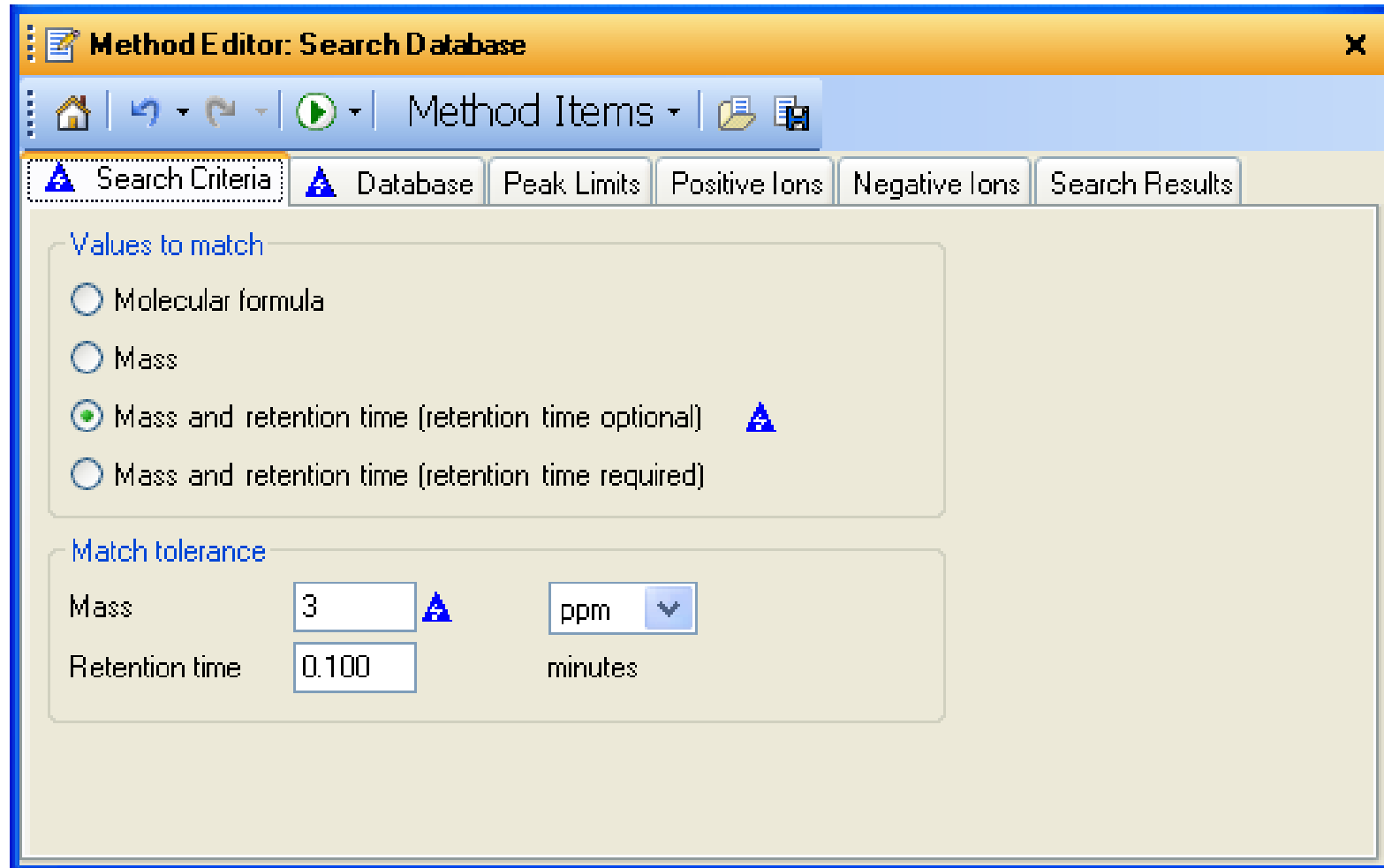
Notes:

Batch Summary Results: 12 hits (12 total hits, 11 single matches, 16 submitted)

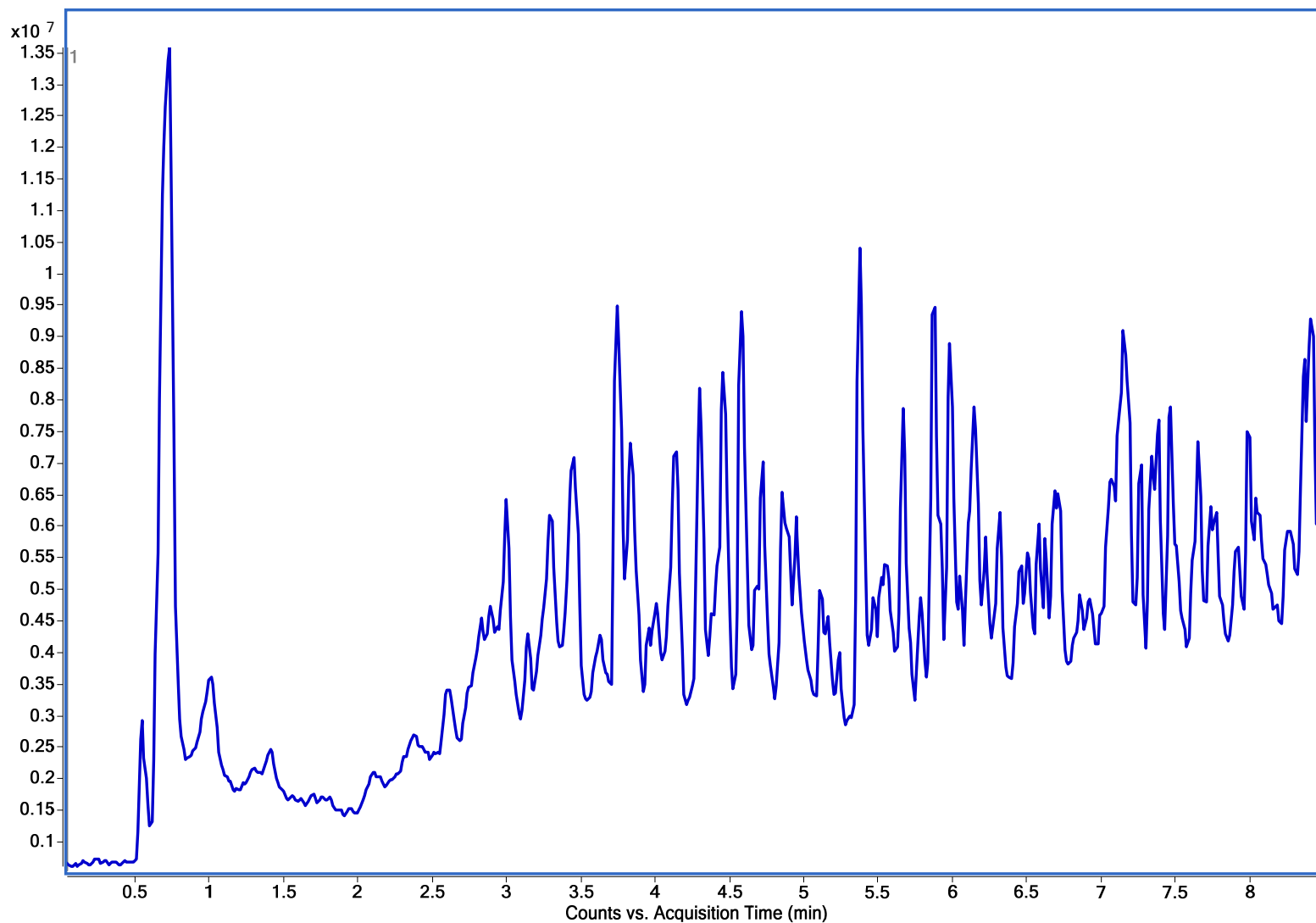
	Name	Formula	Mass Submitted	Mass	Delta Mass (ppm)	RT Submitted	RT (min)	Delta RT	CAS
	Methomyl	C5H10N2O2S	162.04600	162.04630	1.85	2.251			16752-77-5
▶	Imazapyr	C13H15N3O3	261.11140	261.11134	-0.23	2.759	2.767	0.008	81334-34-1
	Imazalil	C14H14Cl2N2O	296.04850	296.04832	-0.61	4.236	4.236	0.000	35554-44-0
	Diazinon	C12H21N2O3PS	304.10150	304.10105	-1.48	7.453	7.453	0.000	333-41-5
	Prochloraz	C15H16Cl3N3O2	375.03090	375.03081	-0.24	5.988	5.988	0.000	67747-09-5
	Azoxystrobin	C22H17N3O5	403.11690	403.11682	-0.20	6.201	6.201	0.000	131860-33-8
	Carbofuran	C12H15NO3	221.10510	221.10519	0.41	4.788	4.791	0.003	1563-66-2
	Atrazine	C8H14ClN5	215.09360	215.09377	0.79	5.139	5.140	0.001	1912-24-9
	Thiabendazole	C10H7N3S	201.03610	201.03607	-0.15	1.769	1.769	0.000	148-79-8



Automate Search with MassHunter Qualitative Analysis



Pepper Extract Run on LC/TOF MS



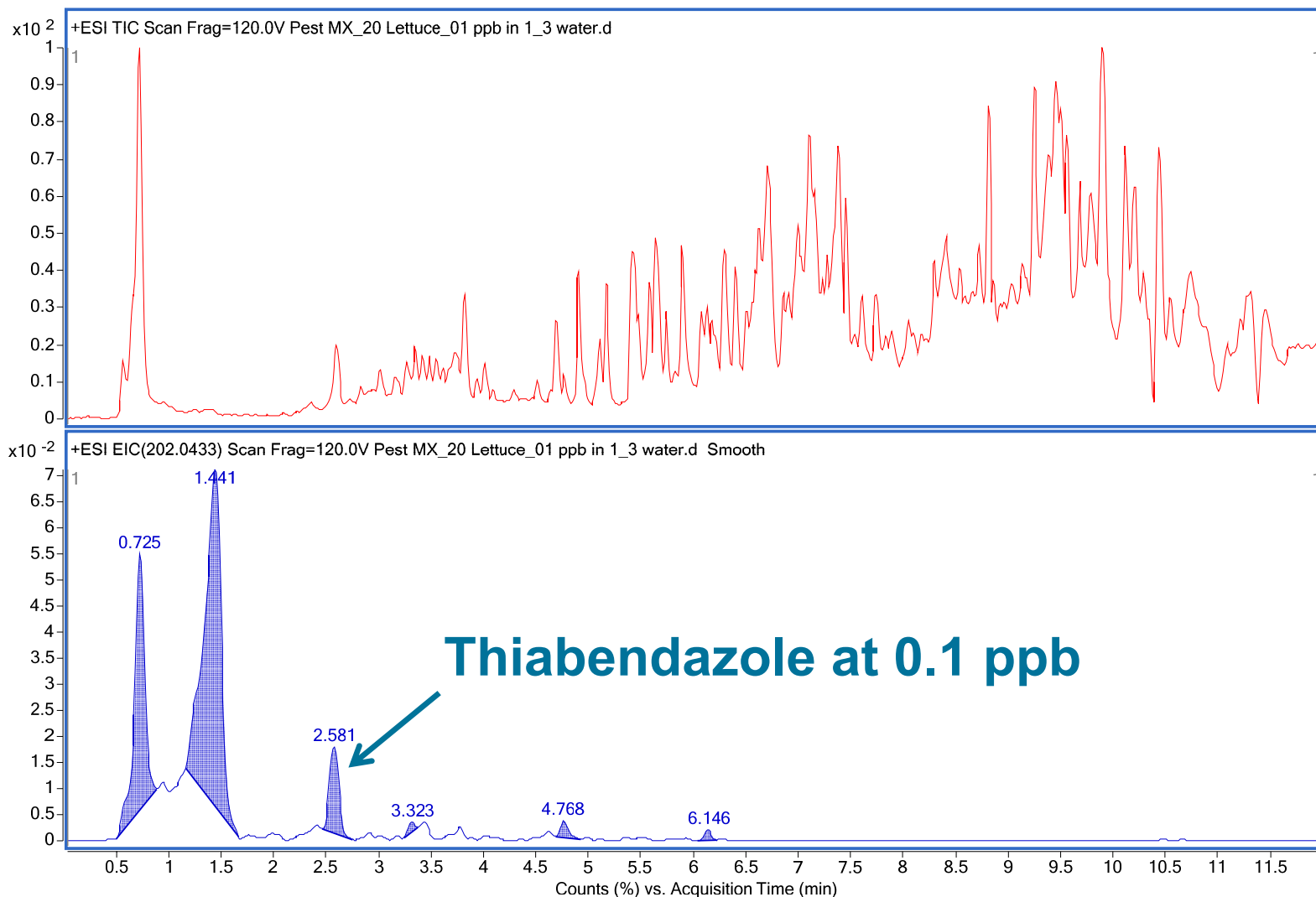
Agilent Technologies

Screening Result of Pepper Extract using MFE and the Pesticide Personal Compound Database

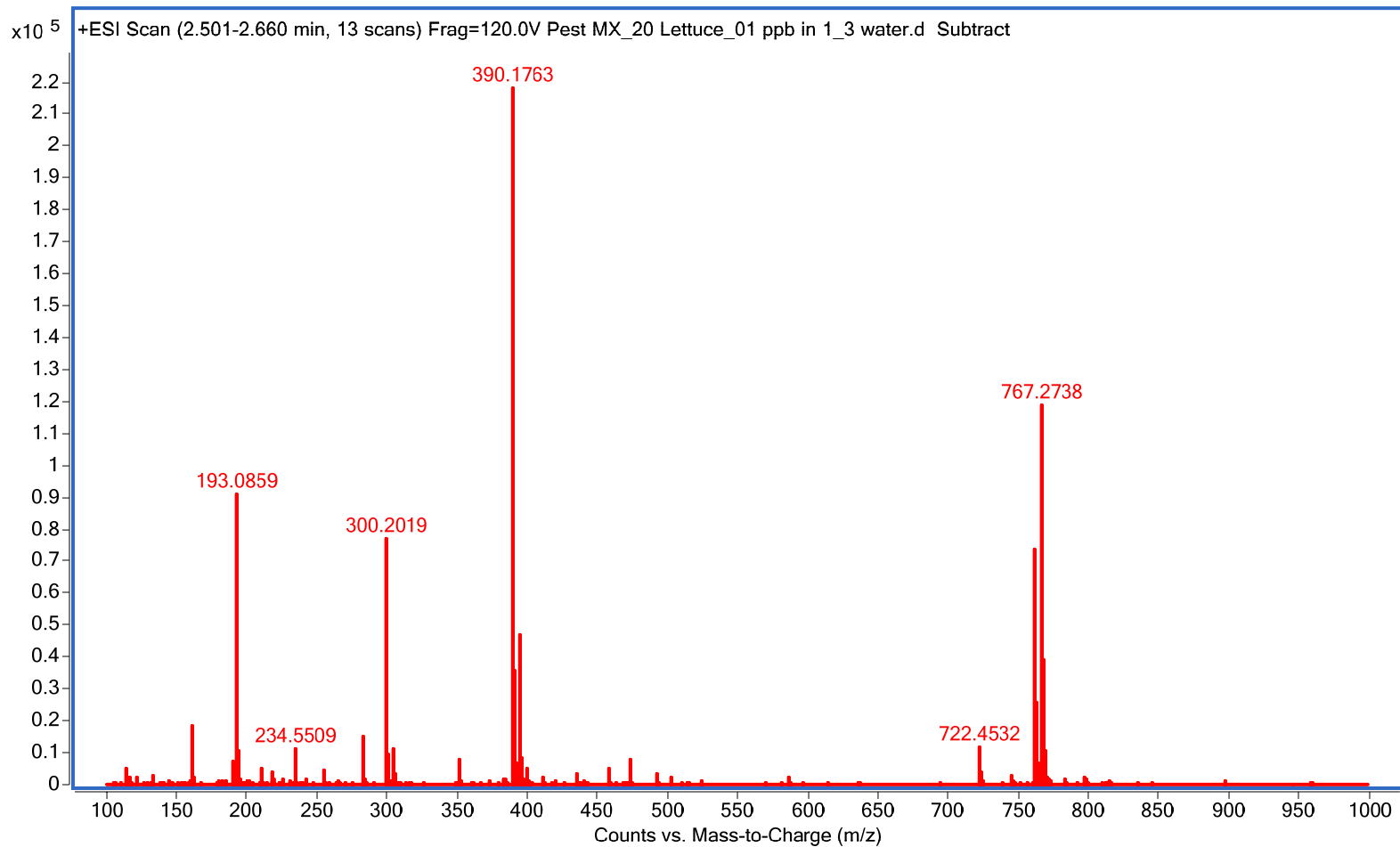
Name	RT	RT (DB)	RT Diff (DB)	Mass	Mass (DB)	Diff (DB, ppm)	Score (D ▾)	Hits (DB)	Ions	Height
Diphenylamine	6.843	6.84	-0.003	169.0893	169.0892	-0.62	99.8	1	2	44736
Atrazine	5.476	5.474	-0.002	215.094	215.0938	-1.09	99.68	1	4	814783
Thiabendazole	2.594	2.598	0.004	201.0362	201.0361	-0.61	99.64	1	3	230596
Carbofuran	5.142	5.14	-0.002	221.1055	221.1052	-1.22	99.56	1	5	114690
Monuron	4.65	4.655	0.005	198.0562	198.056	-1.25	99.09	1	3	84376
Azoxystrobin	6.463	6.461	-0.002	403.1175	403.1168	-1.64	98.76	1	11	595918
Carbendazim	2.386	2.397	0.011	191.0696	191.0695	-0.43	97.79	4	2	103038
Prochloraz	6.295	6.289	-0.006	375.0319	375.0308	-2.97	95.82	1	7	193455
Imazapyr	3.279	3.292	0.013	261.1119	261.1113	-1.95	95.63	1	2	206899
Methomyl	2.848	2.865	0.017	162.0465	162.0463	-1.15	94.09	2	18	460124
Imazalil	4.603	4.586	-0.017	296.0489	296.0483	-1.86	93.53	1	6	490117
Propamocarb	0.567			188.1525	188.1525	0.05	50	1	2	63608
Dimetan	1.238			211.1208	211.1208	0	50	1	2	8908
Aldicarb-oxime	2.128			133.0561	133.0561	0.09	50	1	3	331757
3,5-Xylyl methylcarb...	2.522			179.0946	179.0946	0.14	50	3	2	37673
ICIA0858	3.685			192.0899	192.0899	-0.07	50	2	2	92685
Sulfentrazone	5.345			385.9819	385.9819	-0.03	50	1	5	48976
Arecoline	0.739			155.0947	155.0946	-0.23	49.99	1	3	72940

And that is how you get from a complex dataset to results

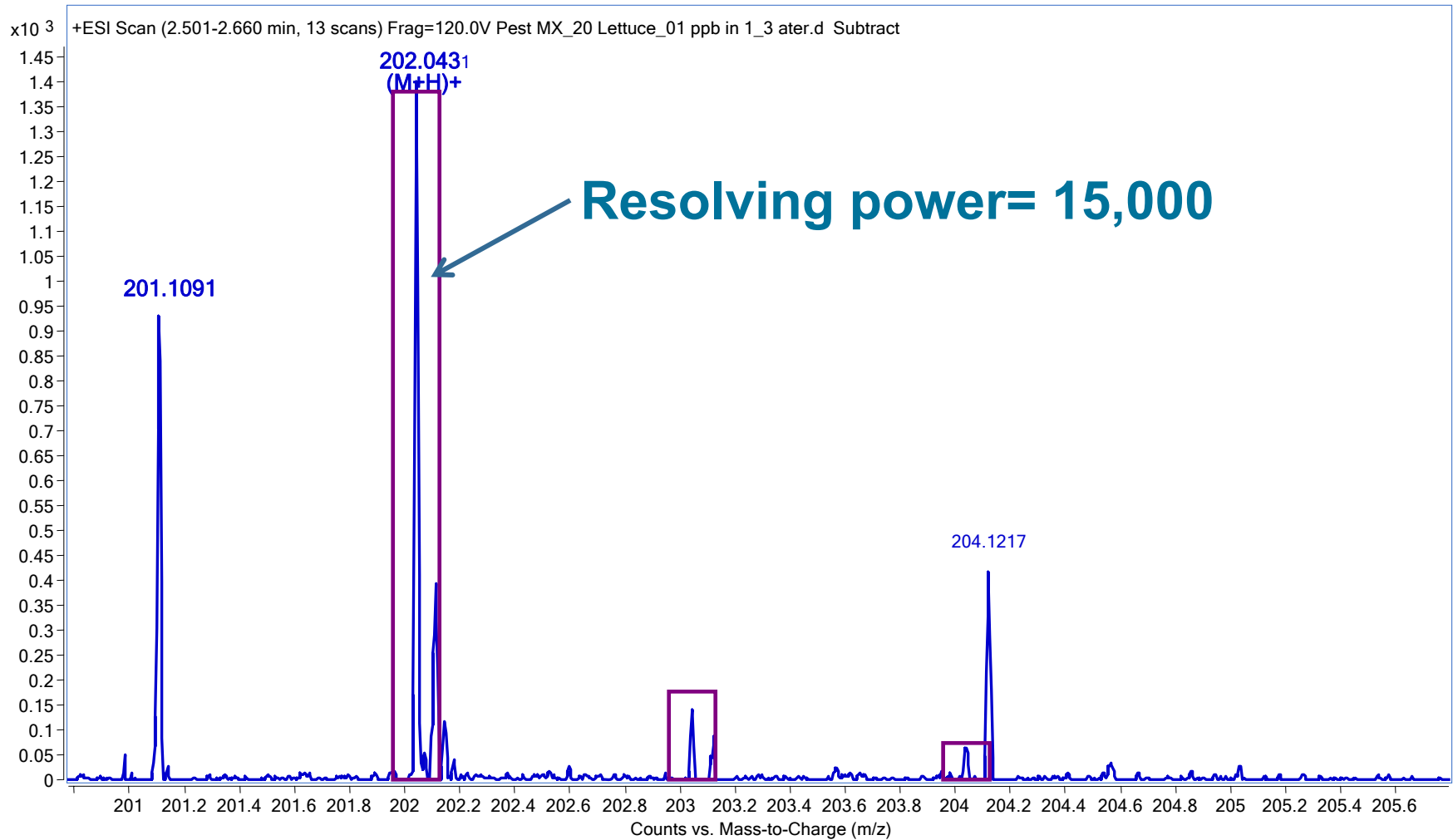
Extracted Ion Chromatogram m/z 202.0433±0.002 of Lettuce Extract



Mass Spectrum of Chromatographic Peak for Thiabendazole



Spectrum of Thiabendazole at 0.1 ppb in Extracted Pepper



Calculated Formula of Thiabendazole at 0.1 ppb in Extracted Pepper

MS Formula Results: + Scan (2.501-2.660 min) Sub

m/z	Ion	Formula	Abundance
202.0431	(M+H) ⁺	C ₁₀ H ₈ N ₃ S	1415.4

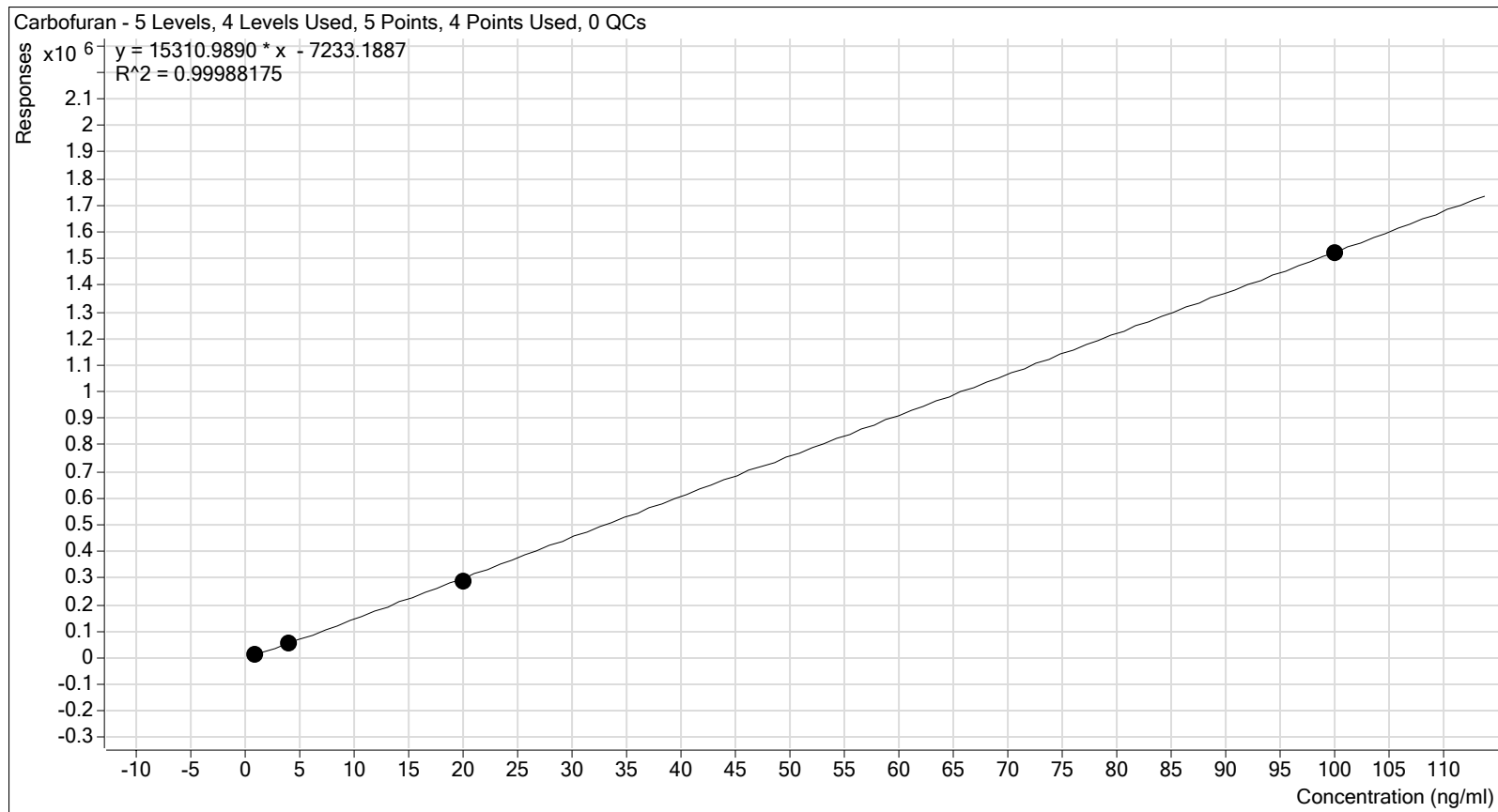
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
<input checked="" type="checkbox"/>	C ₁₀ H ₇ N ₃ S	C ₁₀ H ₈ N ₃ S	95.86		202.0433	1.3	99.31	94.72	90.32

Isotope	Abund Sum%	Calc Abund Sum%	m/z	Calc m/z	Diff (ppm)
1	86.84	84.73	202.0431	202.0433	1.28
2	9.16	10.84	203.0447	203.0459	5.87
3	4.01	4.43	204.0382	204.0405	11.11

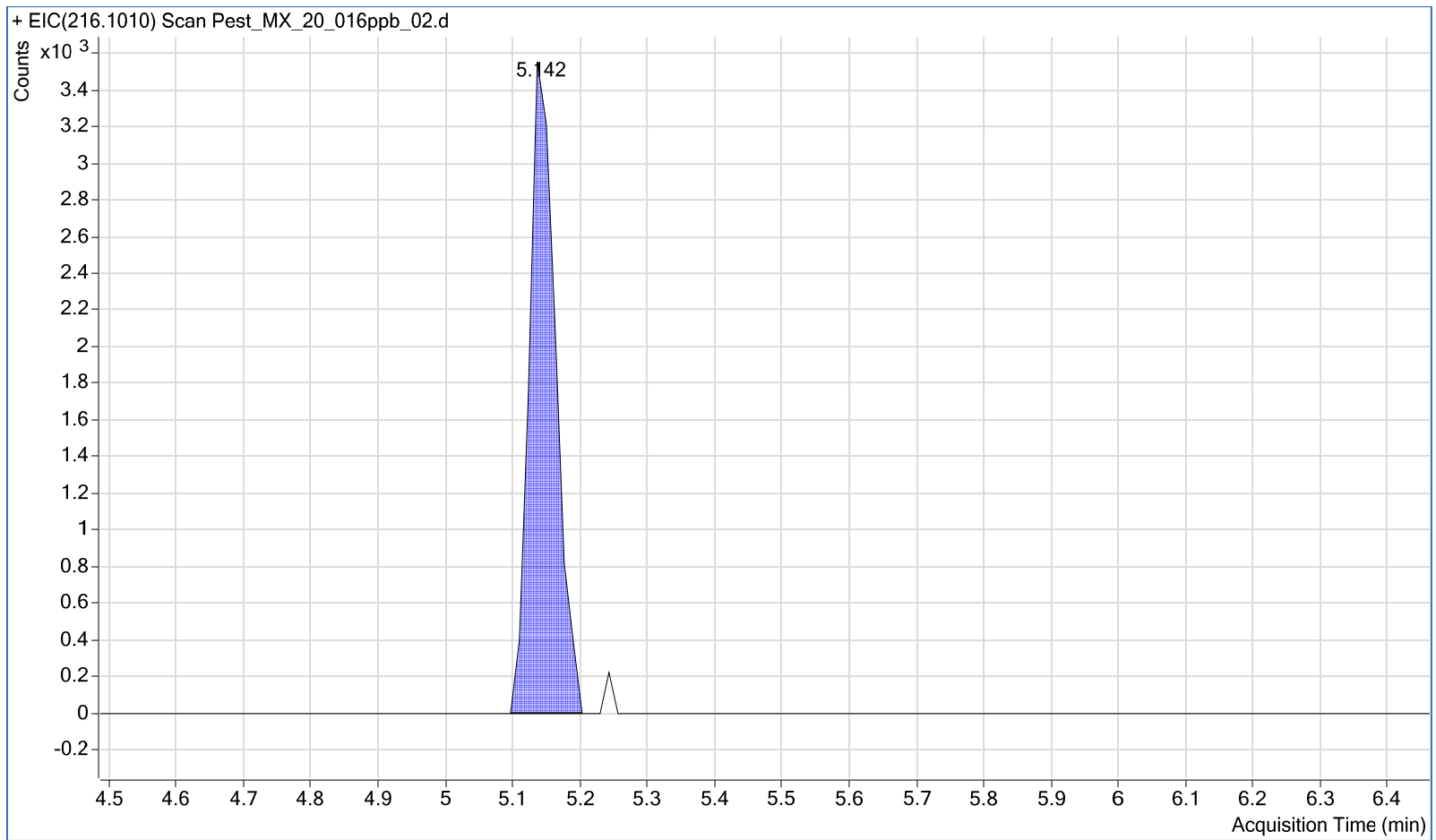
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Mass Match	Abund Match	Spacing Match
<input type="checkbox"/>	C ₆ H ₇ N ₃ O ₅	C ₆ H ₈ N ₃ O ₅	59.68		202.0458	13.75	45.89	81.12	61.54
<input type="checkbox"/>	C ₁₂ H ₈ ClN	C ₁₂ H ₉ ClN	59.62		202.0418	-6.36	84.62	0.31	80.79
<input type="checkbox"/>	C ₄ H ₁₂ ClN ₃ O...	C ₄ H ₁₃ ClN ₃ O ₂ S	55.62		202.0412	-9.62	68.31	0.02	96.94
<input type="checkbox"/>	C ₉ H ₁₂ ClN ₃ S	C ₉ H ₁₃ ClN ₃ S	51.04		202.0452	10.4	64.03	0.05	86.24
<input type="checkbox"/>	C ₁₃ H ₃ N ₃	C ₁₃ H ₄ N ₃	48.82		202.04	-15.46	37.32	64.34	53.17

Chromatogram Results | MS Formula Results: + Scan (2.501-2.660 min) Sub

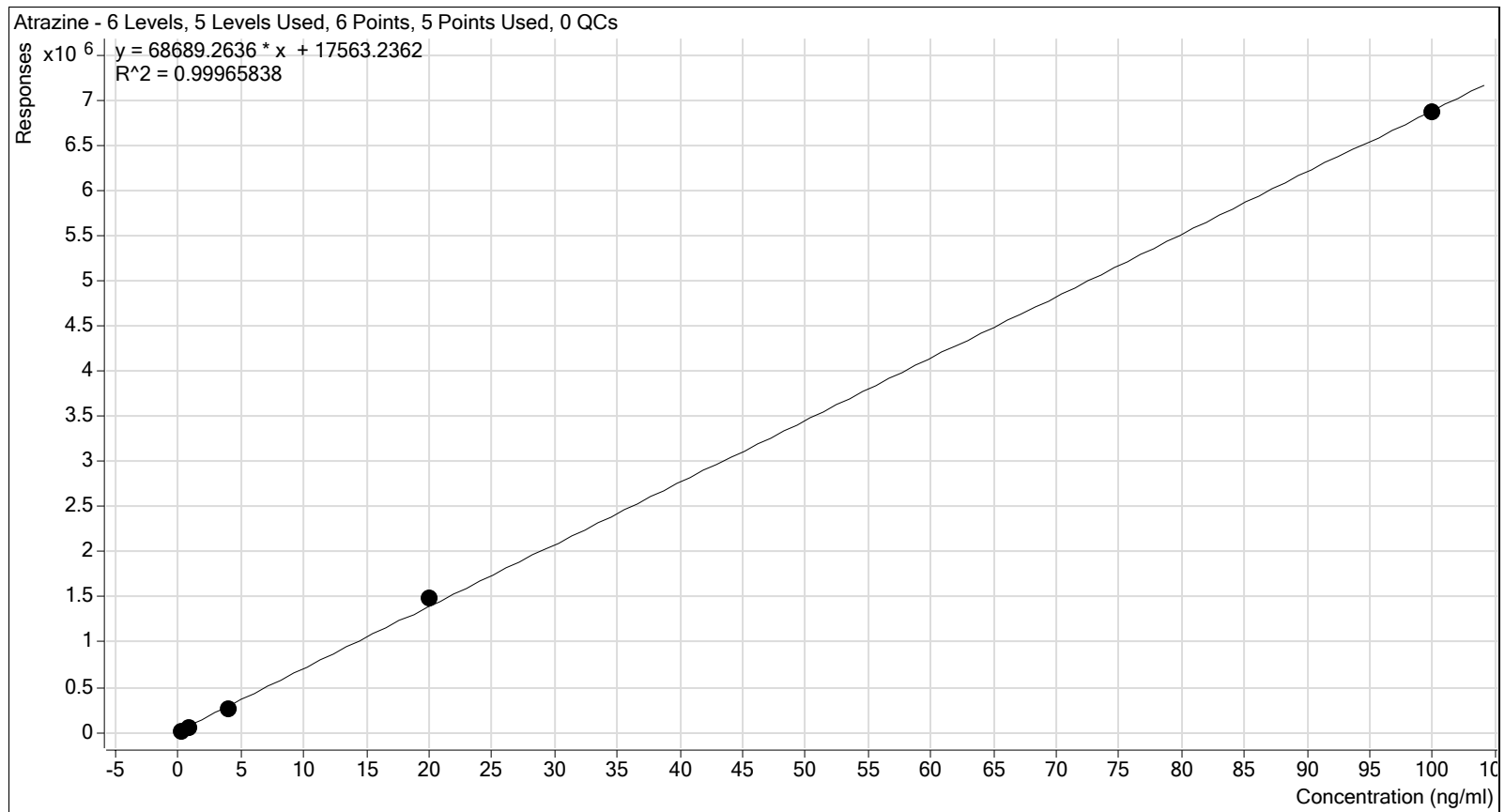
Calibration of Carbofuran



Atrazine at 0.16 ppb (0.8 pg on-column)



Atrazine 0.16 ppb to 100



Summary

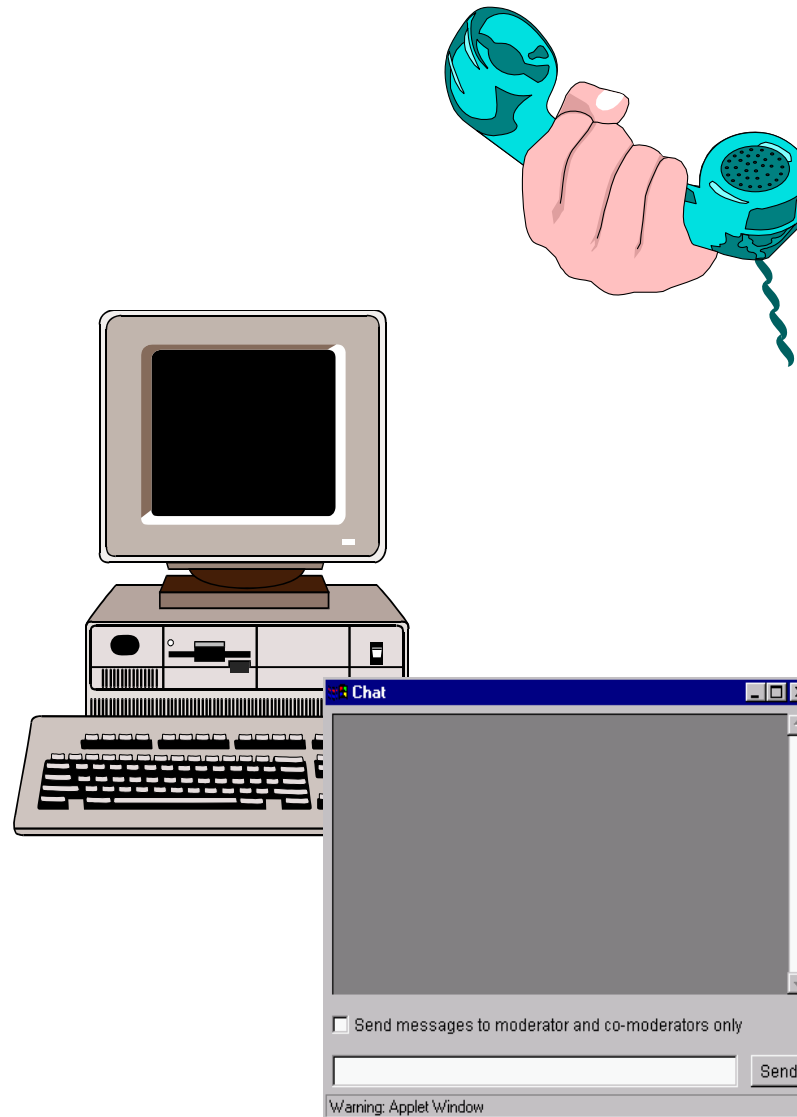
- **Designed for high sensitivity**
- **High MS resolution**
- **Mass Accuracy better than 2 ppm**
- **High dynamic range (in spectrum)**
- **Excellent for Screening**
 - **New Personal Compound Database**
 - **First offering 1600 pesticides**
 - **Customizable**



Break for Questions

For questions,

- a) type onto the Q&A box at any time during the presentation.
- b) Dial *1 on your phone and wait for your name to be announced.

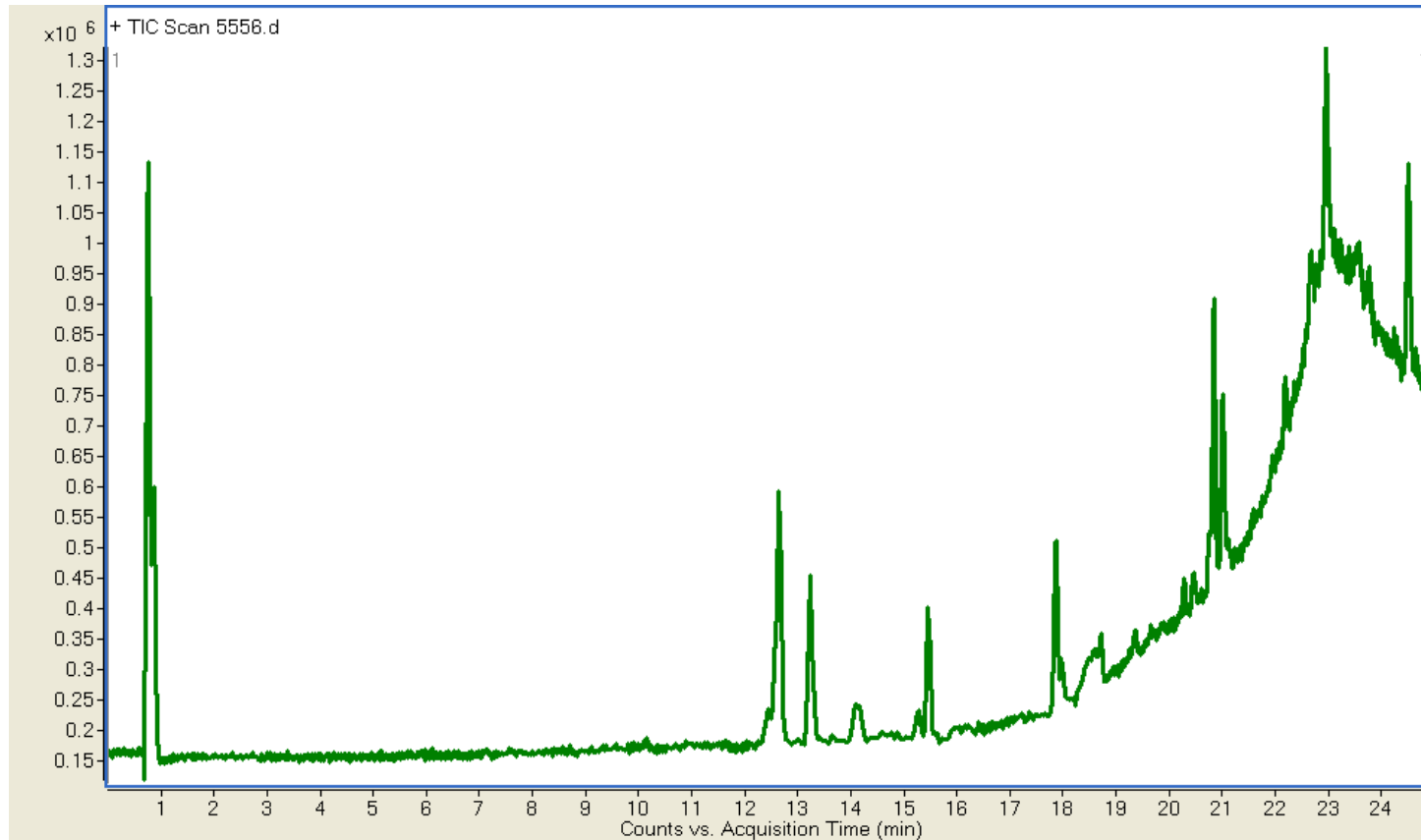


Workflow for QTOF Pesticide Analysis

- **Extract sample**
- **Run in Single MS Mode**
- **Database Search for compound ID**
- **Targeted MS/MS for found Compounds**
- **Confirm and Quantify**



Screen with QTOF – Single MS of Fruit Extract



DataBase Search of 1600 Pesticides

Compound Table

Name	RT	Mass	Abund.	Formula	Tgt Mass	Diff (ppm)	DB Formula	DB Diff (ppm)	Hits (DB)
Cpd 527: Famoxadone	0.9	374.12628	2696	C22H18N2O4	374.12666	-1.01	C22H18N2O4	1.01	1
Cpd 335: SPIROXAMINE	11	297.26687	2710	C18H35NO2	297.26678	0.31	C18H35NO2	-0.31	1
Cpd 375: Tebuconazole	14	307.14498	28381	C16H22ClN3O	307.14514	-0.54	C16H22ClN3O	0.54	1
Cpd 491: TEBUFENOZIDE	15	352.21569	4345	C22H28N2O2	352.21508	1.74	C22H28N2O2	-1.74	1

Identification by Accurate Mass Formula Generation

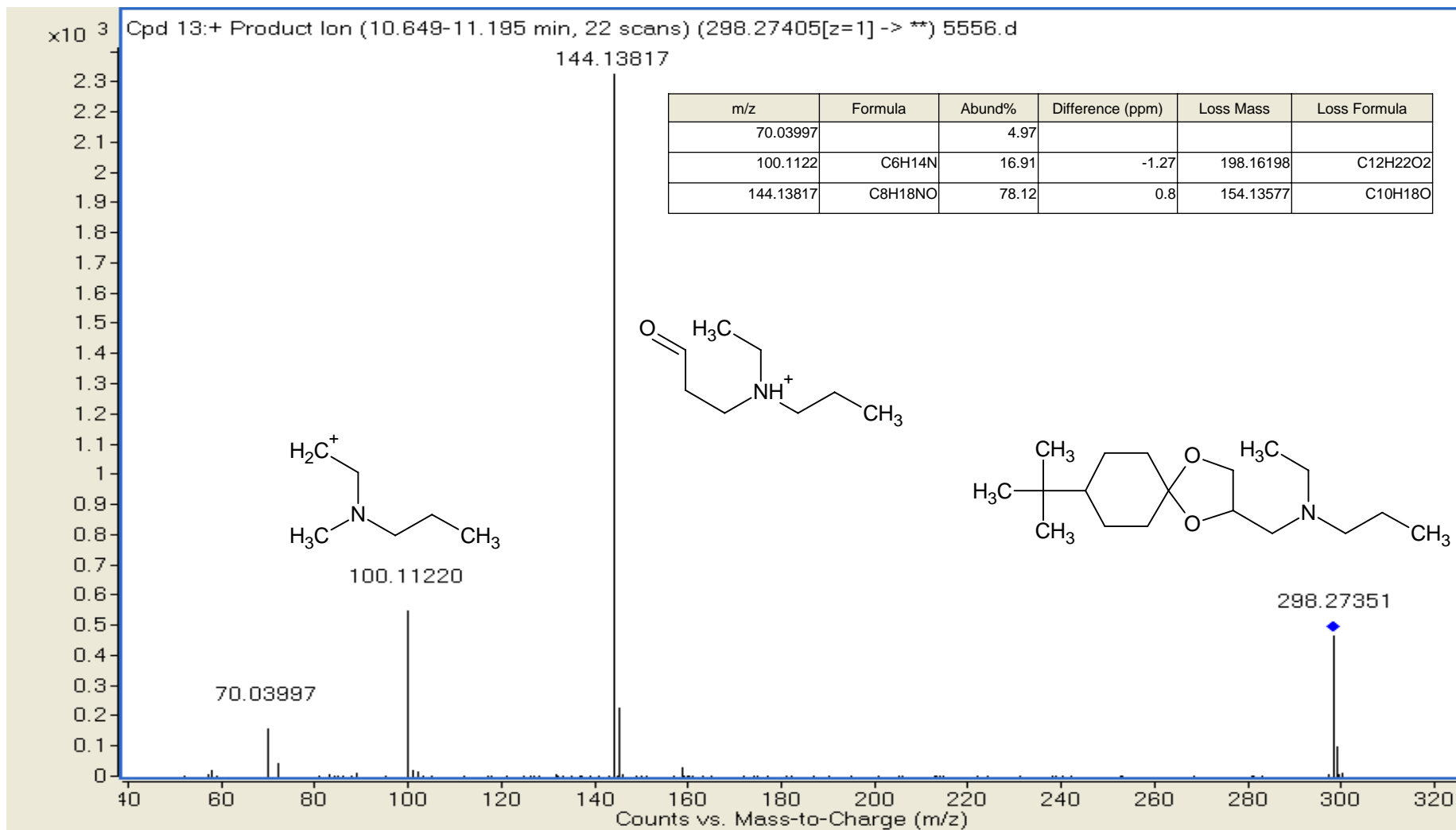
MS Formula Results: Cpd 13: SPIROXAMINE (5556.d)

m/z	Ion	Formula	Abundance
298.27416	(M+H) ⁺	C ₁₈ H ₃₆ NO ₂	2076.7

Best	Formula (M)	Score	Cross Score	Mass	Calc Mass	Difference (ppm)	Abs Diff (ppm)	DBE
<input checked="" type="checkbox"/>	C ₁₈ H ₃₅ NO ₂	100		297.26688	297.26678	-0.34	0.34	2

Isotope	Abund%	Calc Abund%	m/z	Calc m/z	Difference (ppm)
1	100	100	298.27416	298.27406	-0.34
2	19.03	20.32	299.27815	299.27736	-2.65
3	1.34	2.37	300.28432	300.28025	-13.54

Accurate Mass MS/MS for Confirmation

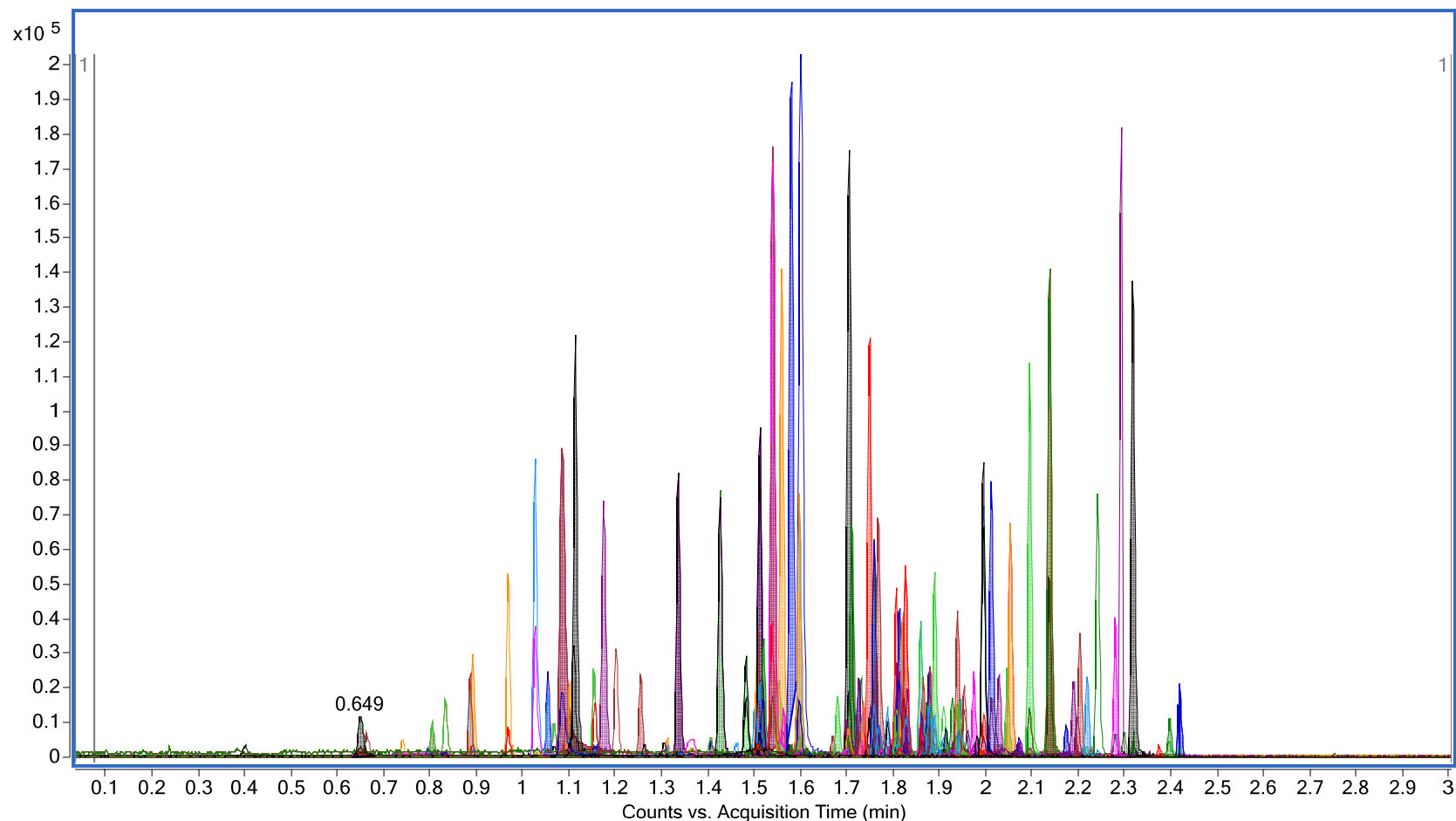


New 1290 Infinity LC with 6540 QTOF LC/MS



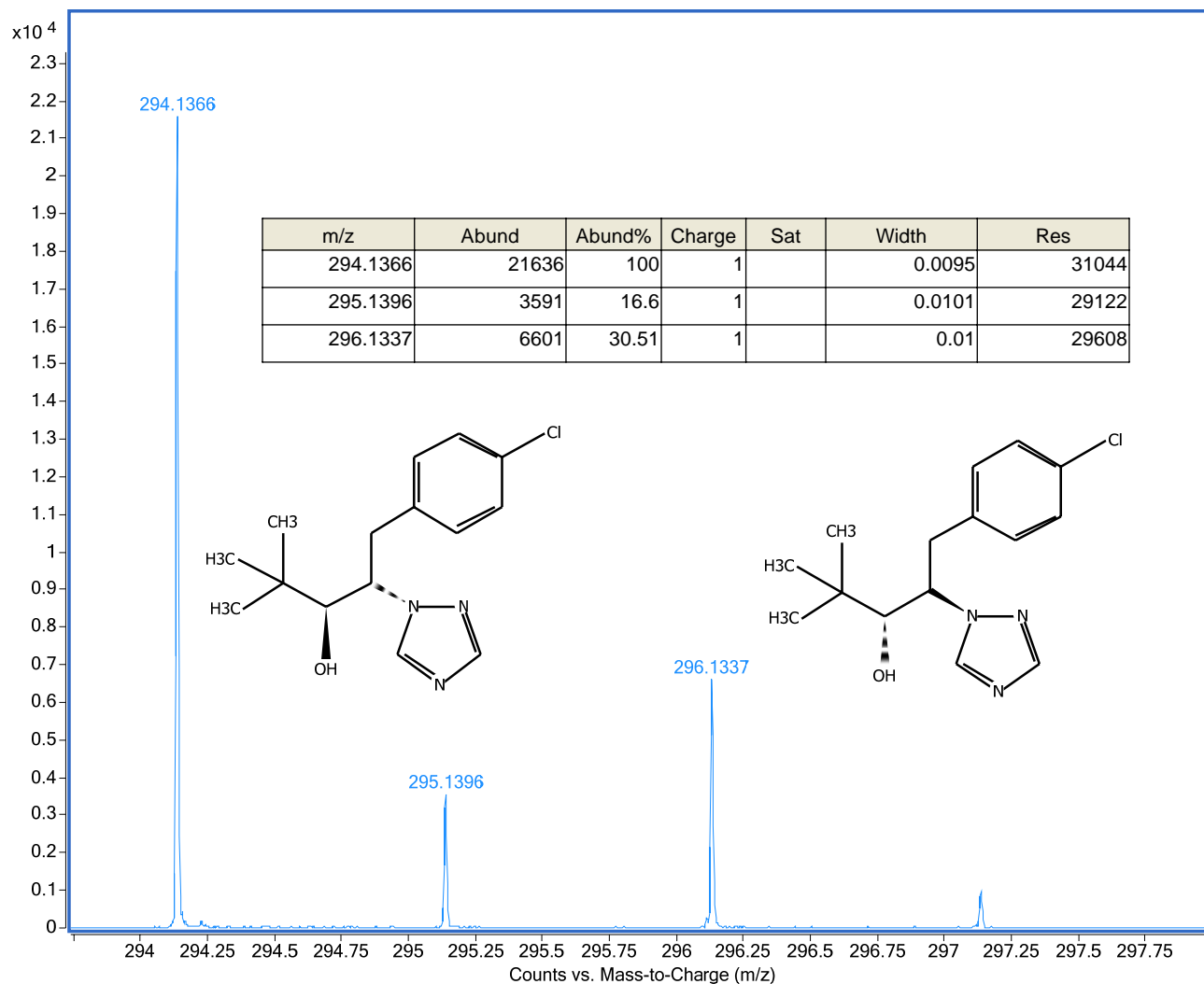
Agilent Technologies

ECC of 100 Pesticides in 3 min using new *Agilent 1290 Infinity LC* with the new *Agilent 6540 QTOF*



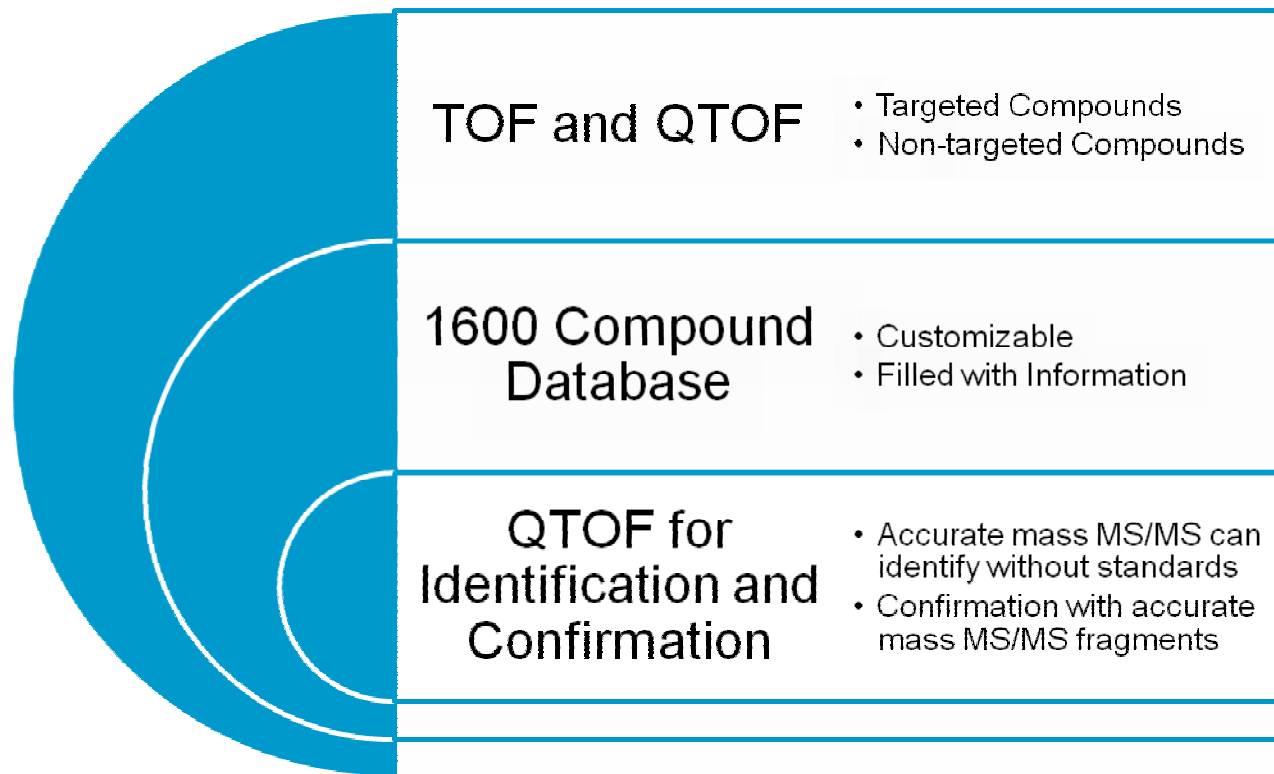
With FULL SPECTRA Benefit from FAST RUN TIMES

Example mass spectrum from data on 3 min run with 1290 Infinity LC and 6540 QTOF.



Note the mass resolution at 10 spectra per second

Summary



Agilent LC/MS Pesticide Application Kits

Fast Start-up

- **Latest Technology for Multi-residue Analysis**

Easy Customization

- **Solutions for YOUR Needs**



Agilent's 35+ Years in Mass Spectrometry

Nearly 40,000 systems – Applied to Chromatographic Analysis



5930A
1971



5992A
1976



5970B MSD
1986



5971 - 5975
1988 - present



LC/MSD Series
1997-2005



Ion Trap Series
2000-2009



ESI-TOF Series
2003-Present



6100 Single Quad
2006, 2007



6000 Series
2006-Present



6410 Triple Quad
2006, 2007



6510, 6520 Q-TOF
2006, 2007



Agilent 7700 Series

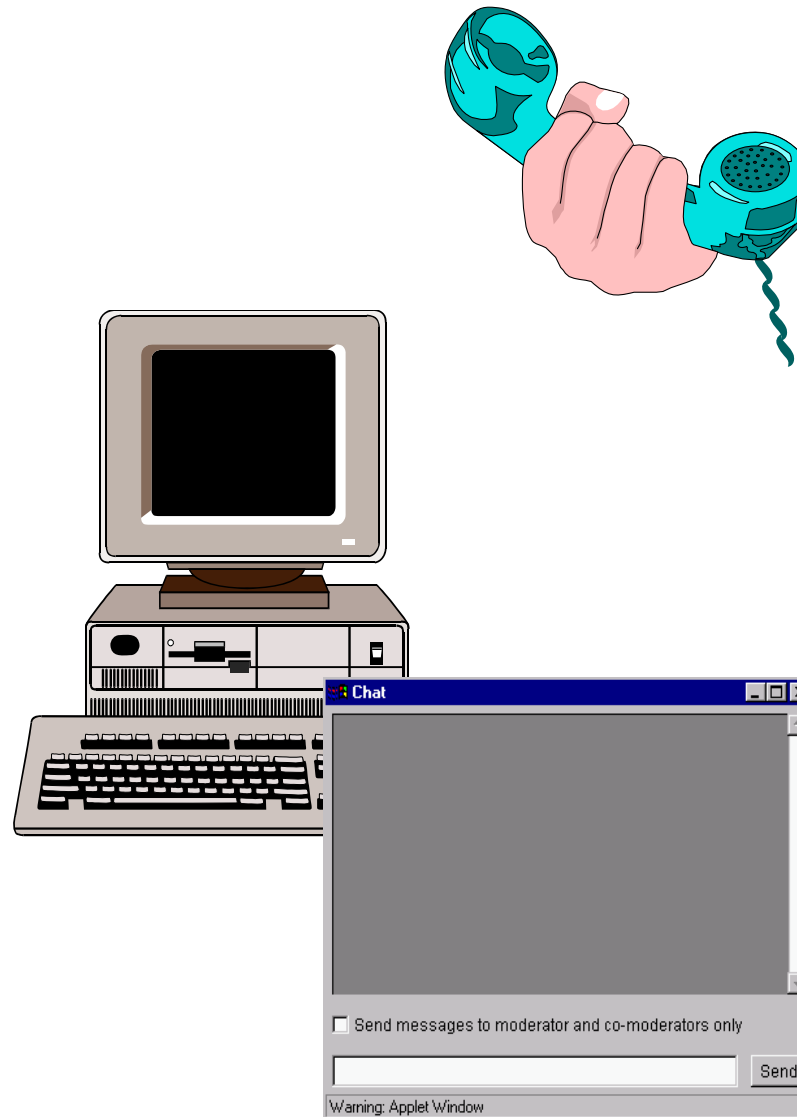


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Agilent E-seminar on Emerging Contaminants

9 to 12 March @ 11am Singapore time

- **9 March** - What is the future of environmental testing? An overview of the state of emerging contaminants including the implications of RoHS2, REACH legislation
- **10 March** - PFOS/PFOA, PBDE and PPCP (Pharmaceutical and Personal Care Products), Measuring New Contaminants of Environmental Interest
- **11 March** - Choosing the Best LC/MS Solution for your Environmental Laboratory
- **12 March** - Identifying inorganic contaminants in water sources using ICP-MS