

# Using High Resolution, Accurate Mass Instruments for the Simultaneous Quantitative and Qualitative Analysis of Banned and Hazardous Compounds in Food and Environmental Analysis

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*Agilent Technologies*

*EMEA & Nordic Team*





”Accurate and sensitive qualitative and quantitative analysis of any compound in food and environmental samples is probably one of the biggest challenges for an analytical chemist”





Trace amounts (low ppt)

Difficult matrices

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Identification/Confirmation issues

Multimethods





# BACKGROUND

Triple quadrupole type of instruments dominates

- Why QQQ?
- "MS/MS is required to get sufficient **selectivity**"
- "MS/MS is required to get sufficient **sensitivity**"
- "The only instrument type **robust** enough to work in routine
- "Minimum user dependant results"
- "Superior sensitivity"
- "Superior linearity"

# BACKGROUND

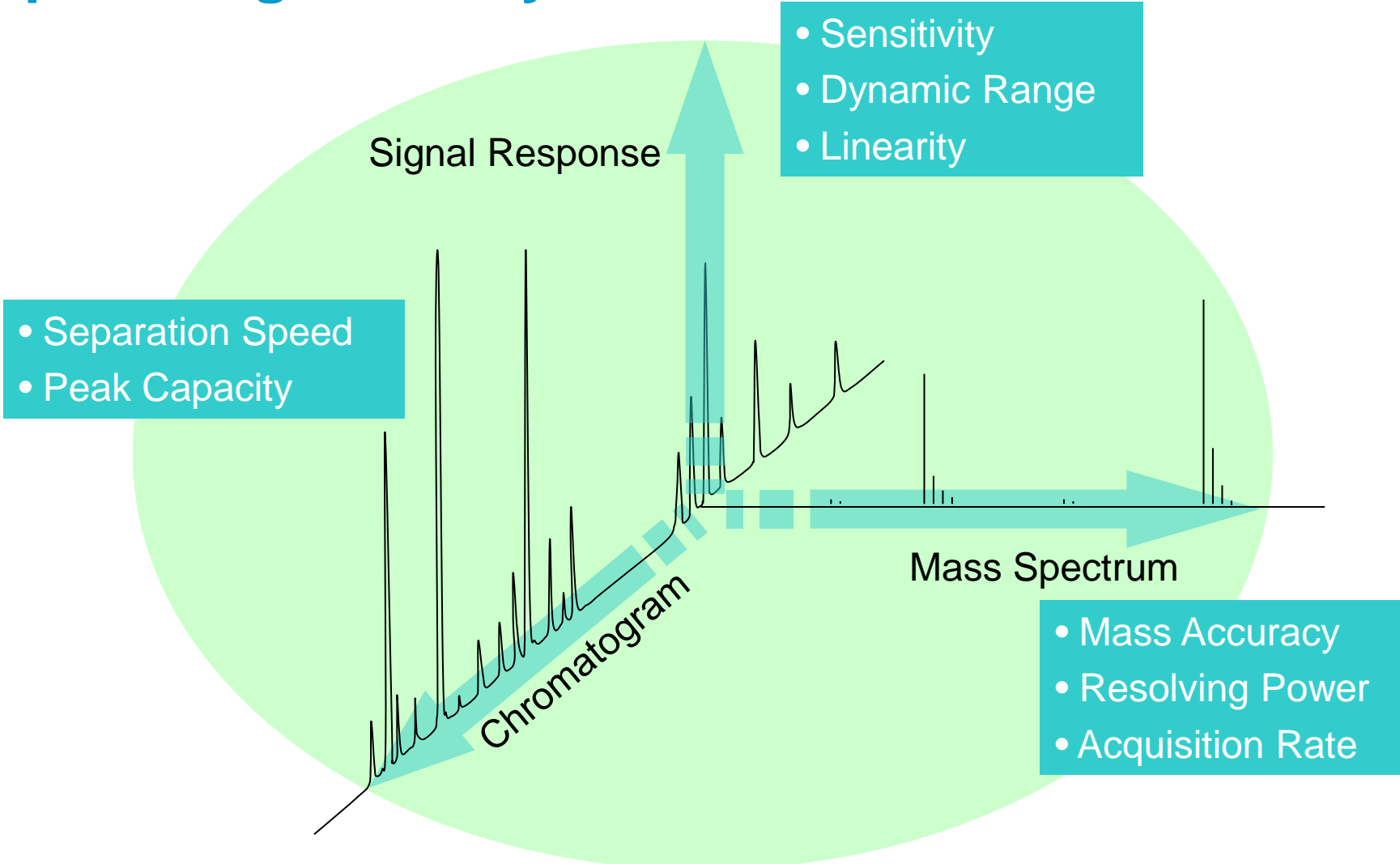
..but why not high resolution instruments like TOF?

- High **resolving power** and **accurate mass** for selective and sensitive quantification
- No need to setup **MRM** transitions
- No need to decide upfront **what to detect**
- **"All the ions all the time"**. Speed and sensitivity (**Ferrer et.al.**)
- Possibility to build **accurate mass MS/MS libraries**
- Modern ToF/Q-ToF's are **easy to operate**
- Modern ToF/Q-ToF's are **stable and reliable**



# Ultra High Definition

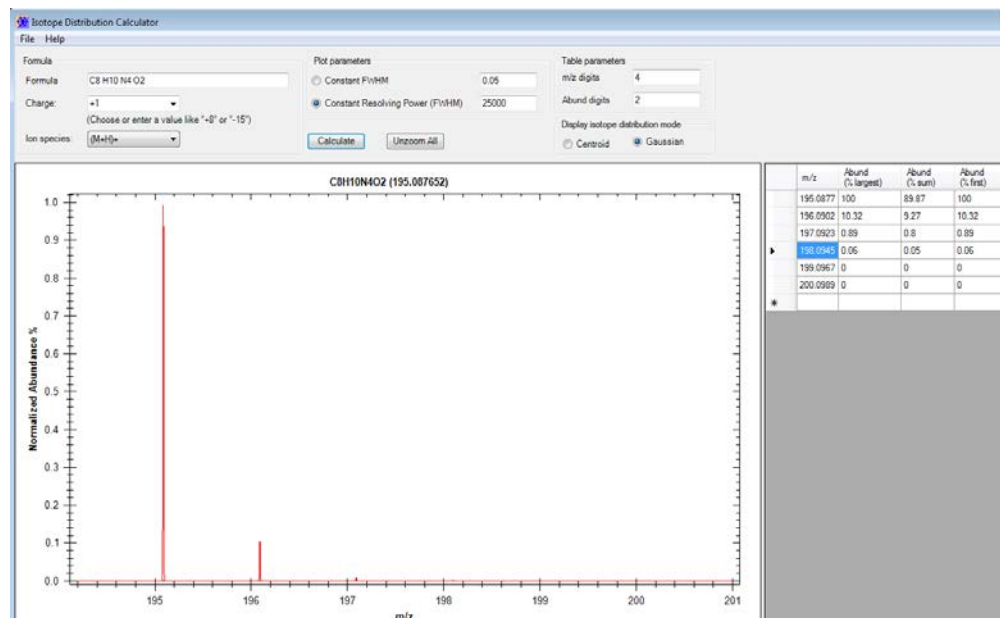
## Optimizing all Analytical Dimensions



e.g. **Caffeine, C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>O<sub>2</sub>**

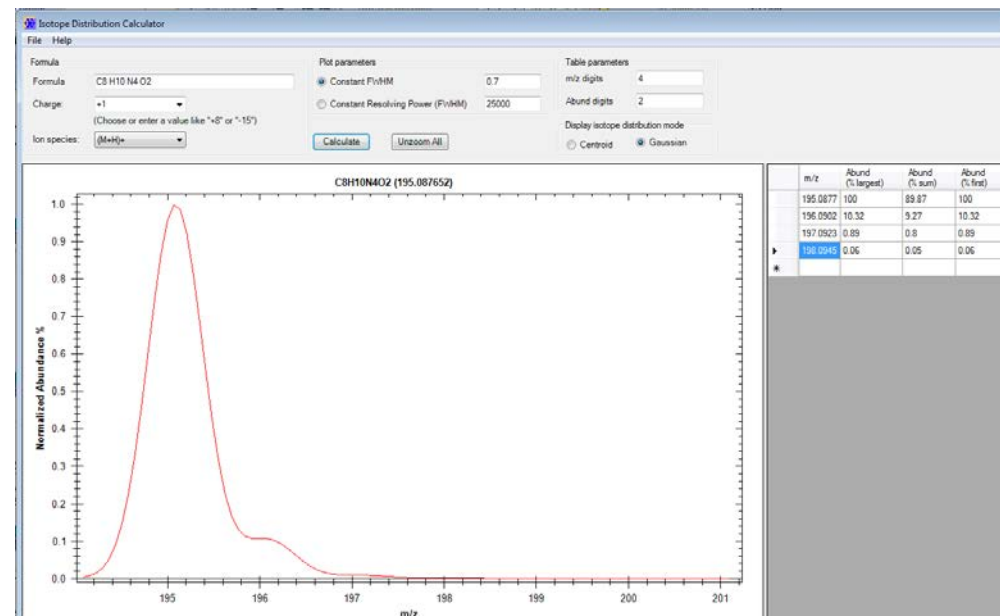
**Tof/Q-Tof:**

Resolution: 25.000



**Quadrupole:**

Resolution: 280





## Mass accuracy:

e.g. Caffeine

Tof/Q-Tof:

$195.0877 \pm 1 \text{ ppm}$

$195.0875 - 195.0879 \text{ m/z}$

Quadrupole:

$195.1 \pm 0.1 \text{ Da}$

$195.0 - 195.2 \text{ m/z}$

or  $\sim \pm 500 \text{ ppm}$



**Mass accuracy:**

e.g. Caffeine

Number of hits searching the  
METLIN DB.....~**45.000 cpd's**

Tof/Q-Tof:

195.0877±1ppm

195.0875 - 195.0879m/z

**1 (one)**

Quadrupole:

195.1±0.1Da

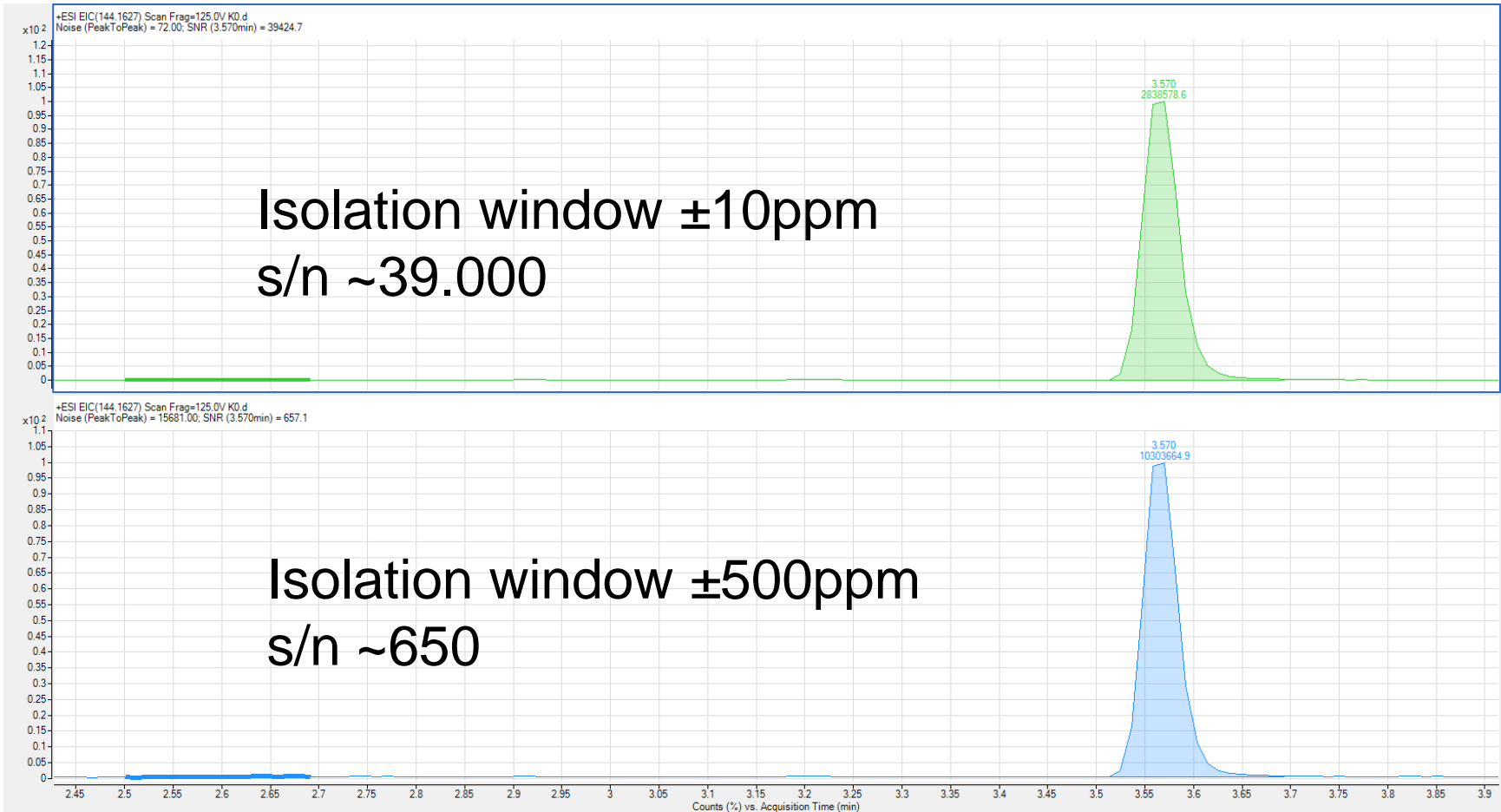
195.0 - 195.2m/z

or ~ **±500ppm**

**24 (twenty four)**

# Effect of resolution and mass accuracy

## EIC of m/z 144.1627



## Statement 1 and 2:

- "MS/MS is required to get sufficient selectivity"
- "MS/MS is required to get sufficient sensitivity"

## Statement 1 and 2:

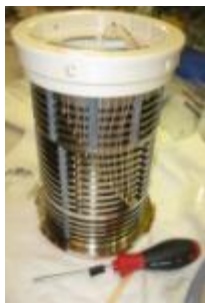
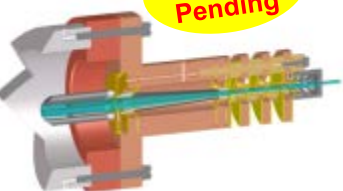
- "MS/MS is required to get sufficient selectivity"
- "MS/MS is required to get sufficient sensitivity"
- Low resolving power instruments e.g. Quadrupole based, **requires MS/MS** to achieve sufficient **selectivity** and **sensitivity**

# 6540 UHD Accurate Mass Q-TOF LC/MS

The Highest Performing Benchtop Q-TOF



Patent Pending



Ultra High Definition  
Quadrupole Time of Flight Mass Spectrometer

## Exceptional Ultra High Definition Performance... With No Trade-Offs

- 40,000 resolution
- Excellent isotopic fidelity
- Mass accuracy < 1 ppm
- 5 orders of linear dynamic range
- Femtogram-level sensitivity with Agilent Jet Stream
- Fast acquisition for UHPLC – up to 20 spectra/second

## Made Possible by Continuing Technology Breakthroughs

- Ion Beam Compression (IBC) cools & focuses ion beam
- Extended Flight Tube with Enhanced Mirror Technology (EMT)
- New Photonis Fast Bipolar Detector

## The Ultimate Qualitative Analysis System

- Proteomics/Metabolomics
- Non-targeted food/environmental screening
- Impurity analysis
- Metabolite ID



# Technology Innovation

Dual-stage ion mirror (resolution)

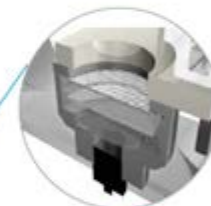


Ion Beam Compression Technology (resolution + mass accuracy)



INVAR flight tube (mass accuracy)

ADC (dynamic range)



4 GHz electronics (resolution, mass accuracy, sensitivity, dynamic range)

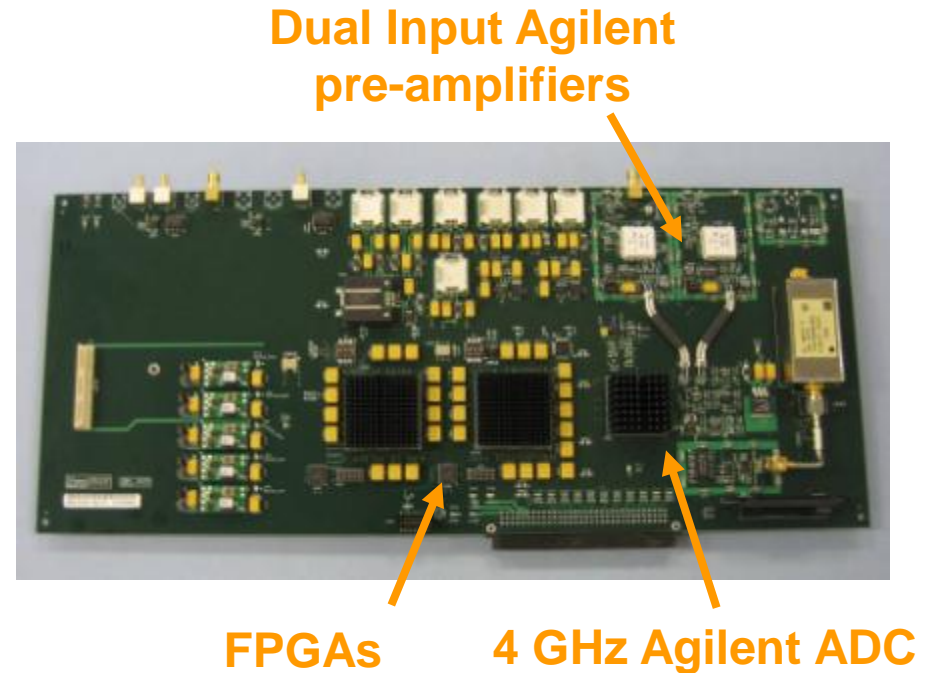
Ion acceleration in hexapole collision cell (faster MS/MS spectra)



# Ultra High Speed Acquisition

*From Agilent's Leadership in GHz Speed Electronics*

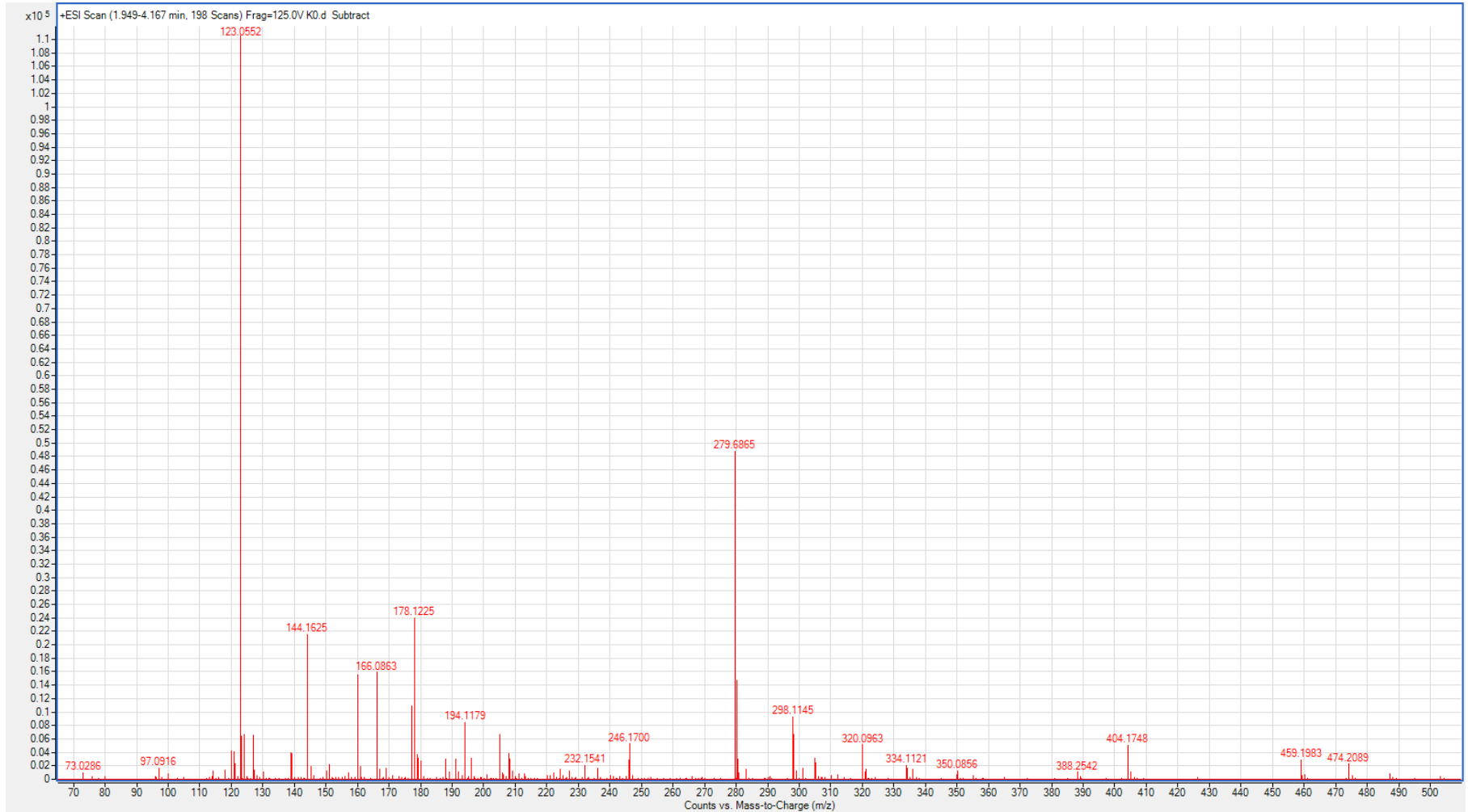
- **4 GHz Acquisition for Maximum Resolving Power and <1ppm Mass Accuracy**
- **5 Decades of in-Spectrum Dynamic Range from 2-Channel x 2 GHz Dual Gain Mode**
- **4 GHz (8 bit) Analog-Digital-Converter Adapted from Agilent's High Speed Oscilloscope Systems**
- **Ultra High Speed FPGAs process and store transients in real time**



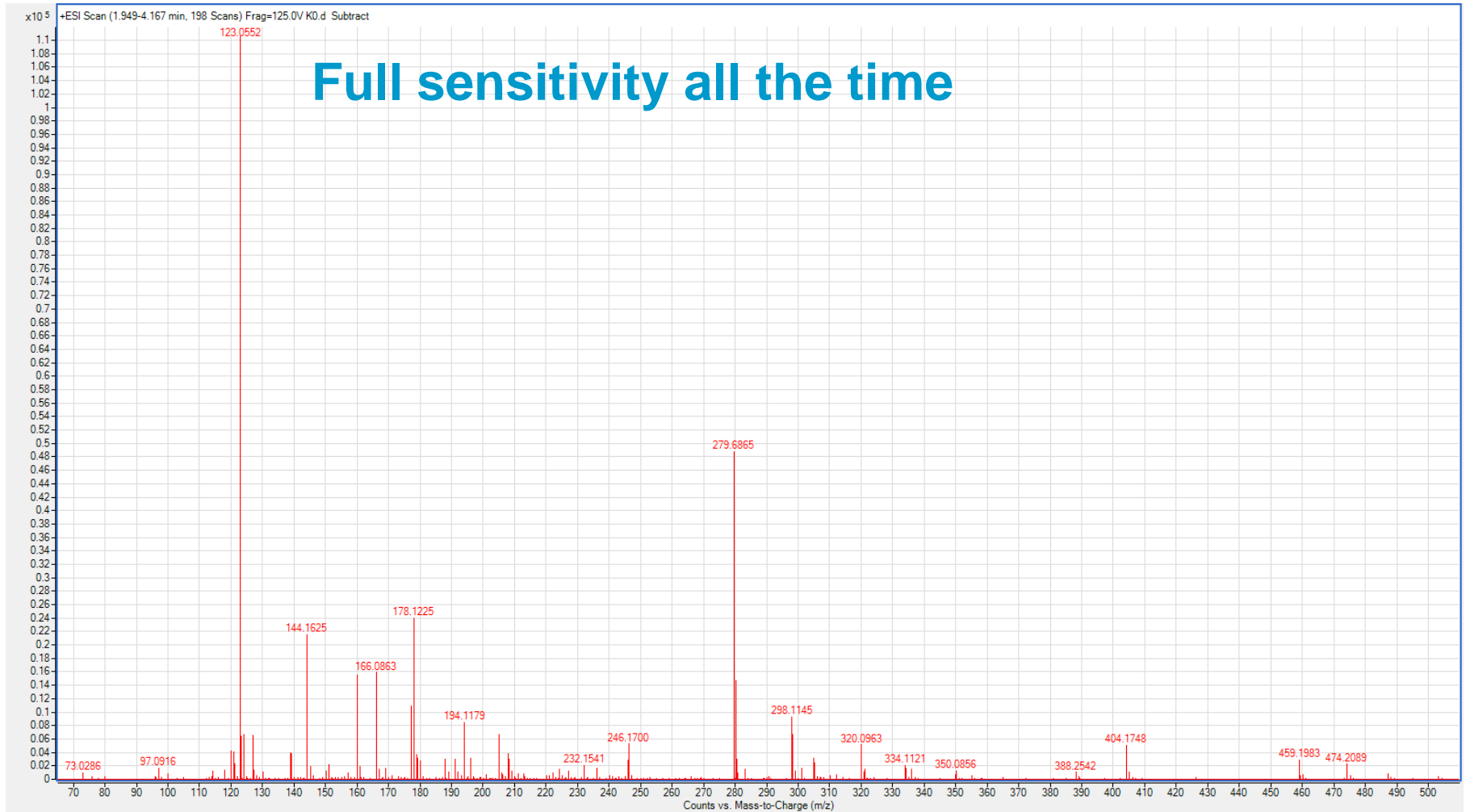
**Making Research Grade Performance possible in a Benchtop Format**



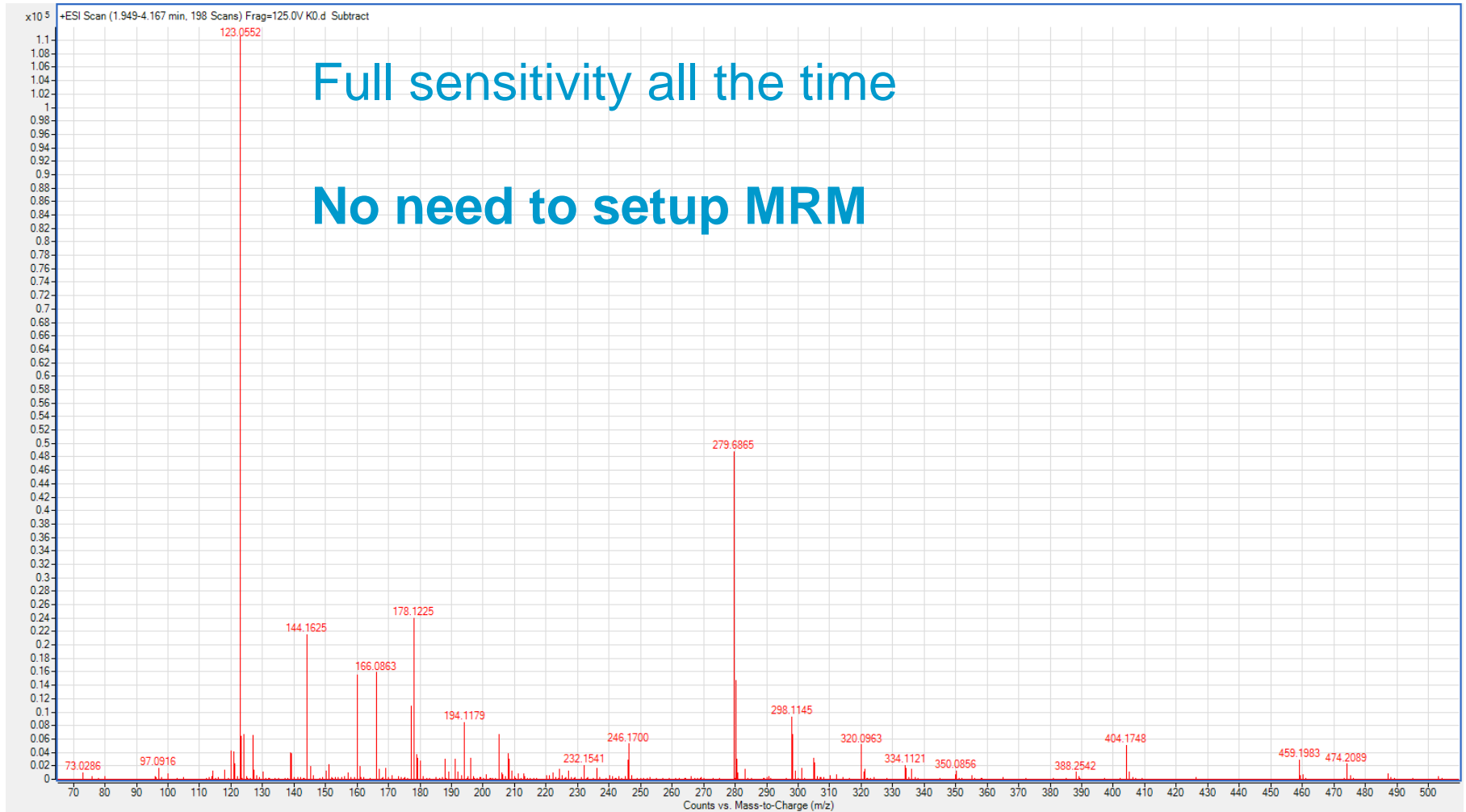
# "All the ions all the time"



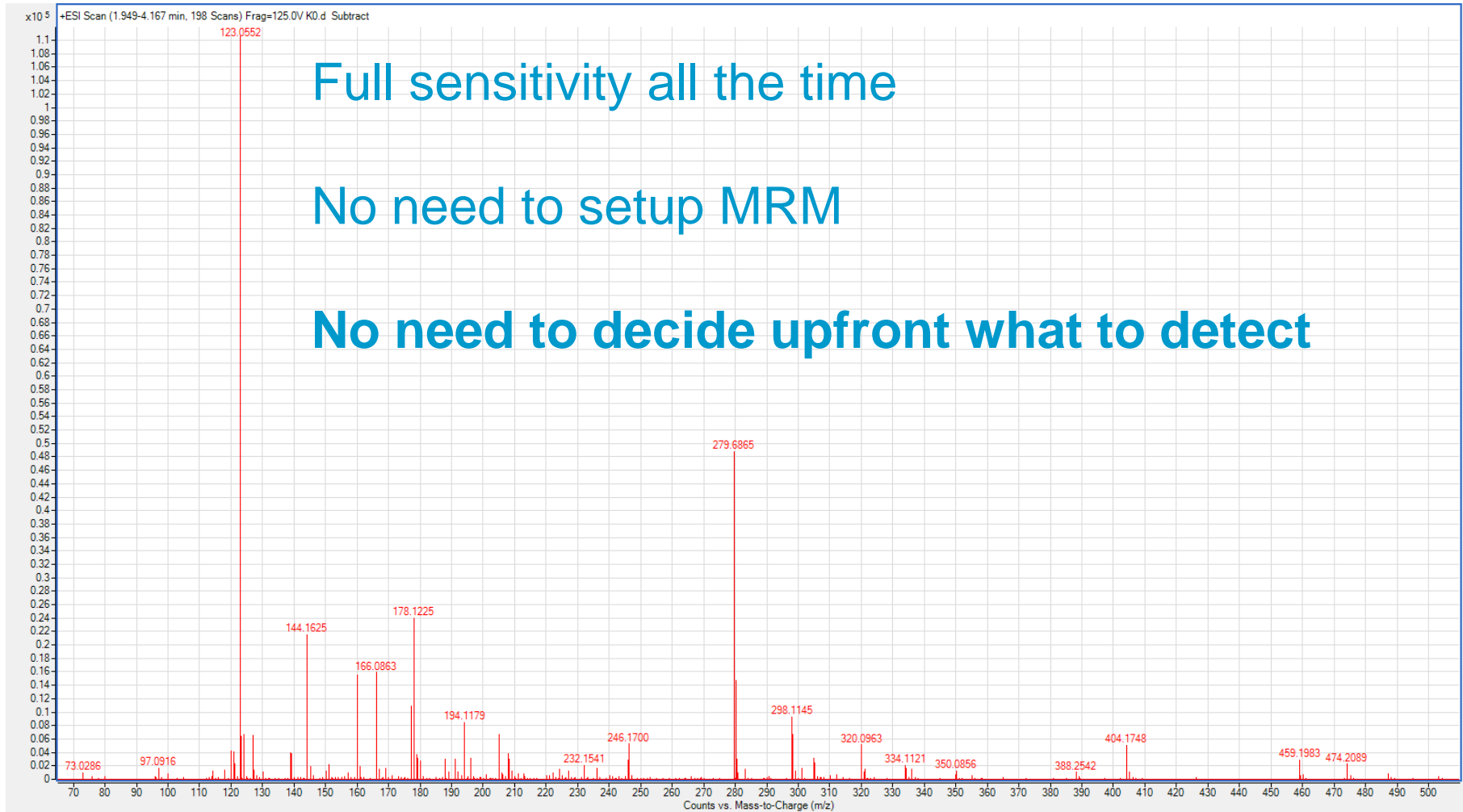
# ”All the ions all the time”



# ”All the ions all the time”



# ”All the ions all the time”

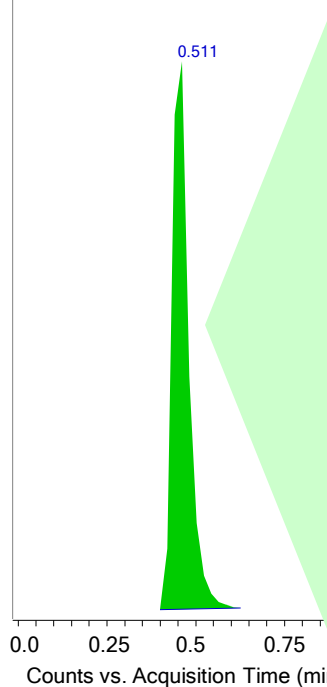


# 6540 Ultra High Definition Q-TOF

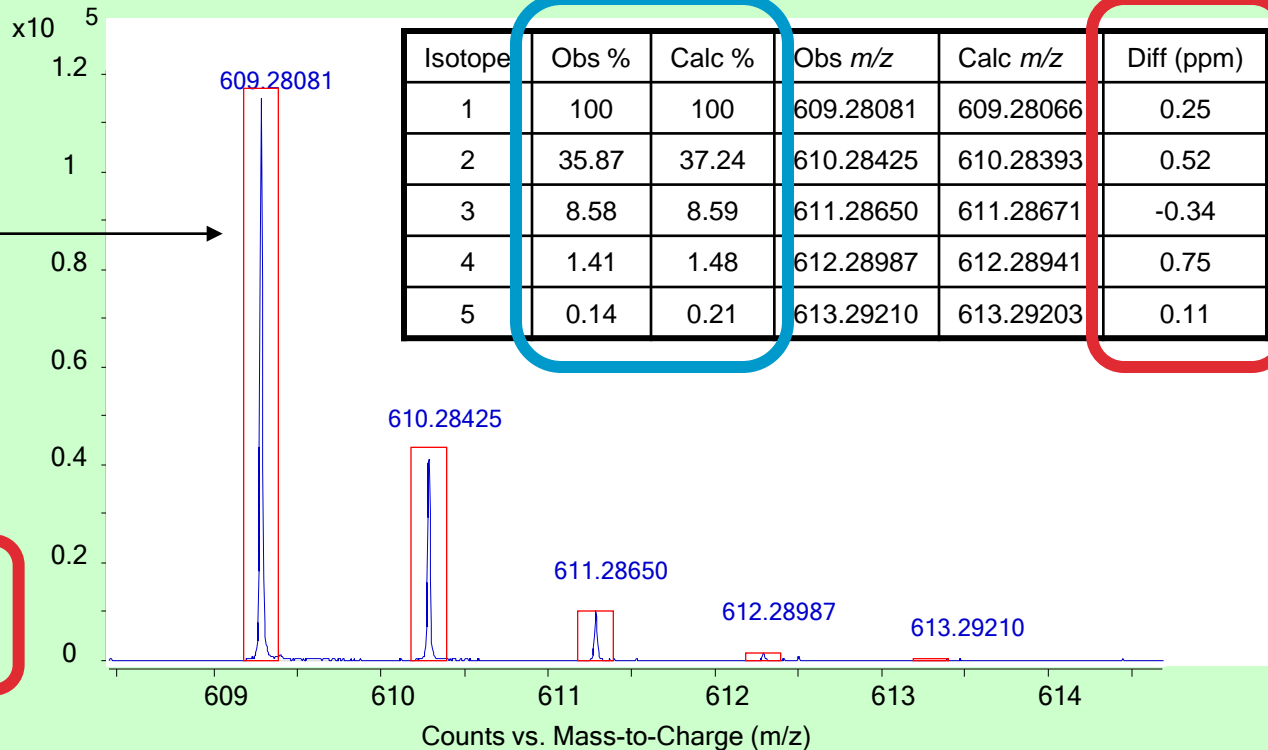
## Mass Accuracy – Repetitive Injections

40 pg reserpine on-column, 10 injections

+ESI EIC(609.28066)  
Scan Frag=240.0V Reserpine\_40pgms3.d



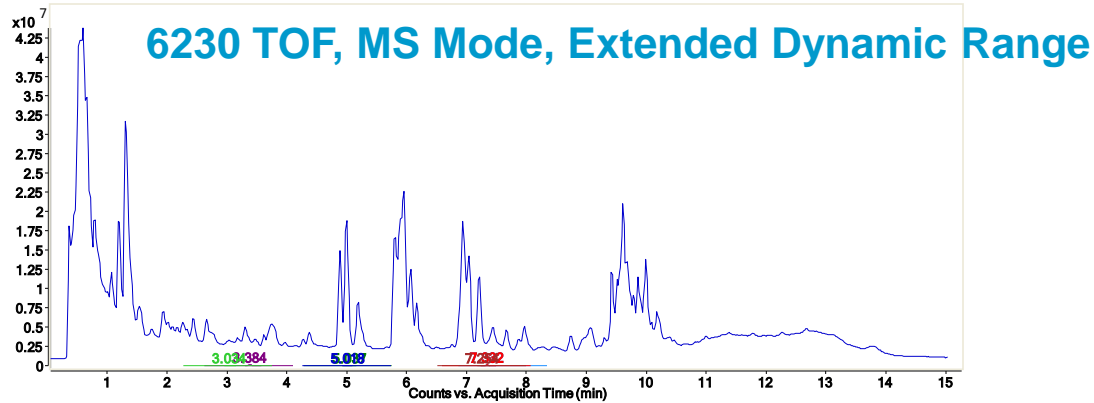
Run	Error (ppm)
1	0.96
2	-0.17
3	0.25
4	0.02
5	0.39
6	0.13
7	0.01
8	0.52
9	0.04
10	0.30
<b>Mean</b>	<b>0.25</b>
<b>Std Dev</b>	<b>0.32</b>



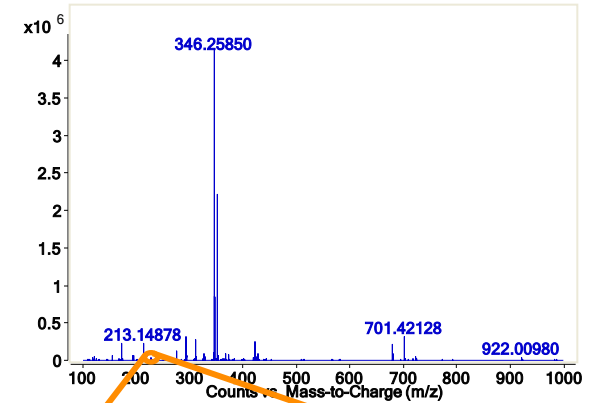
250 ppb mass accuracy calibration and very accurate isotopic ratios

# Food Safety Screening for Triazines in Tomato Matrix

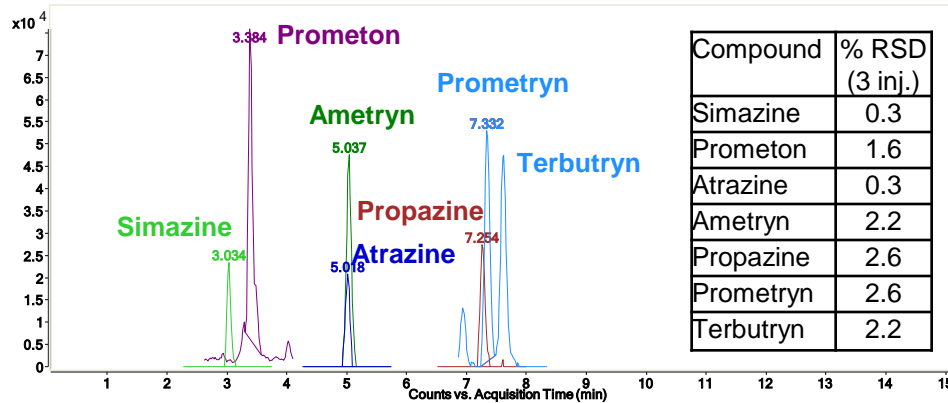
TIC



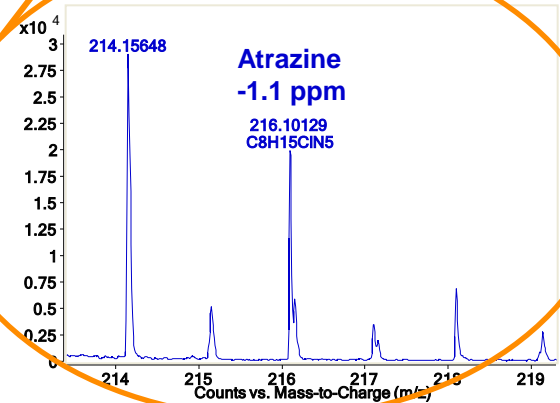
Spectrum at 5.018 min



EICs



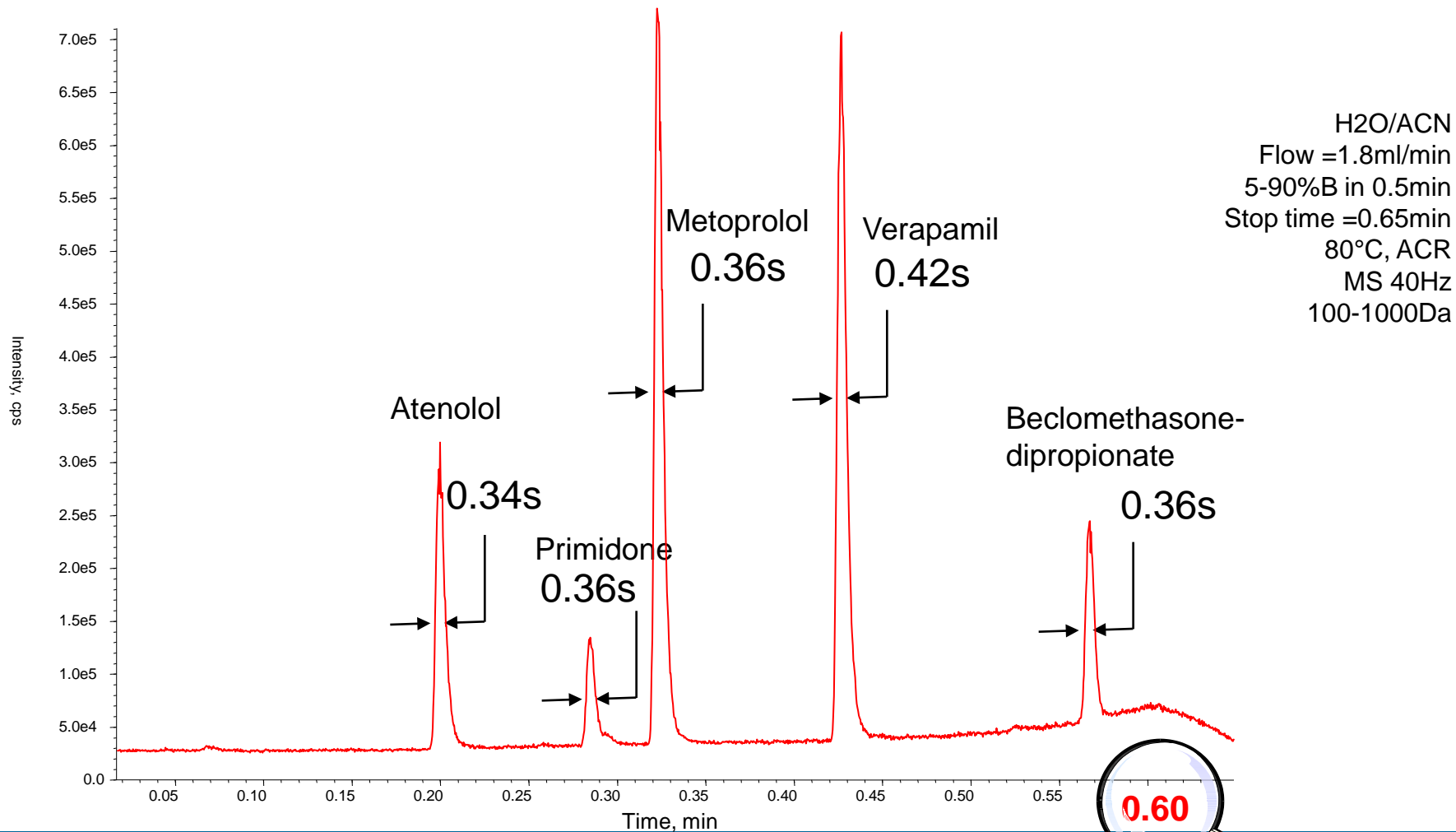
Zoom view



Note: on-column amount is 5 pg (10  $\mu$ L x 500 ppt).  
 Identification done by database searching

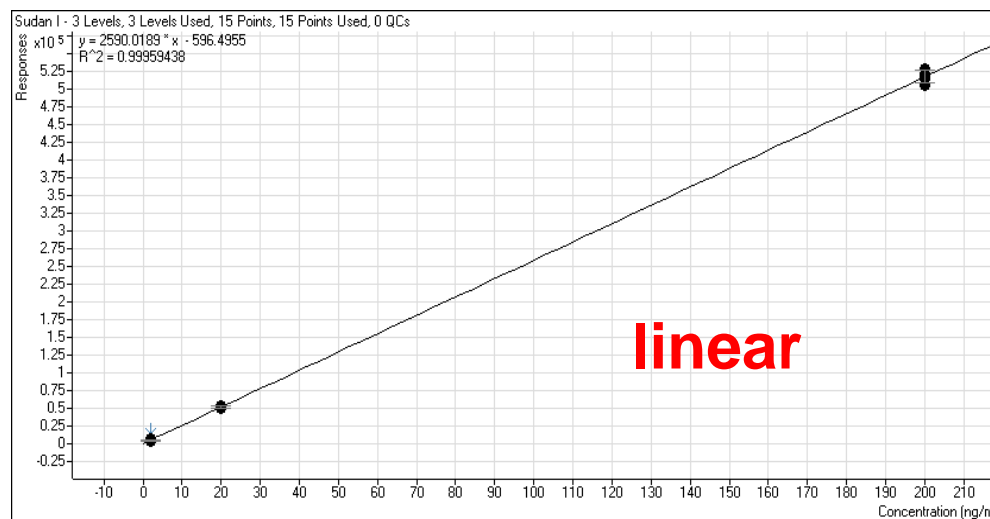
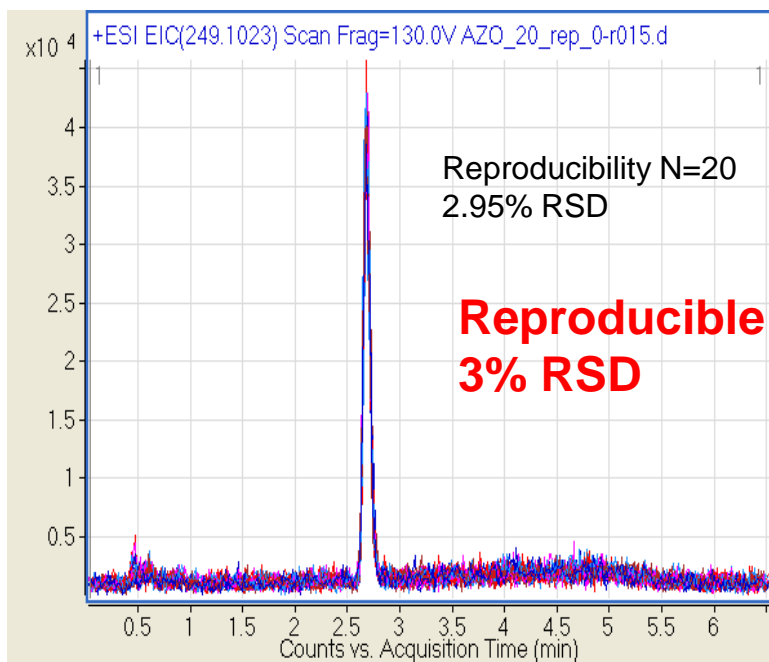
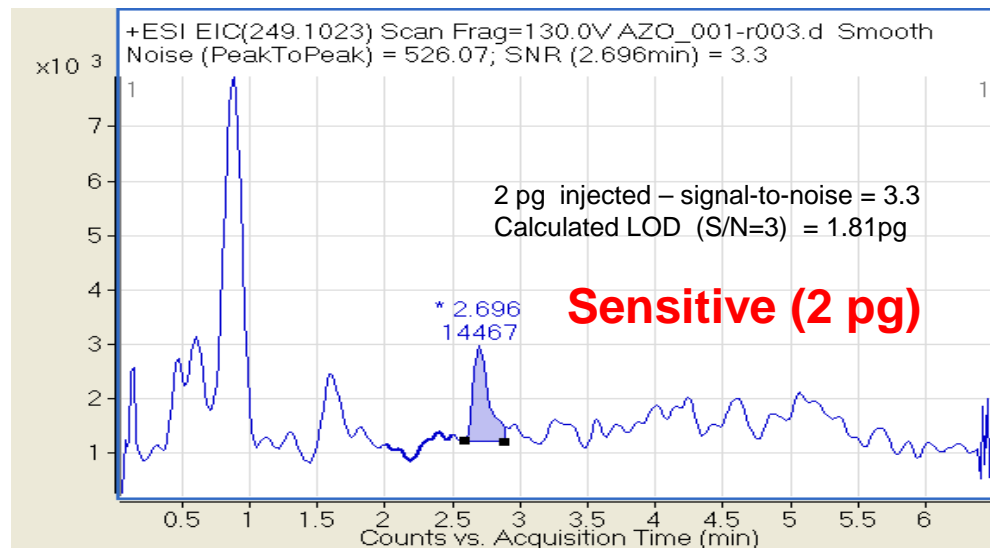
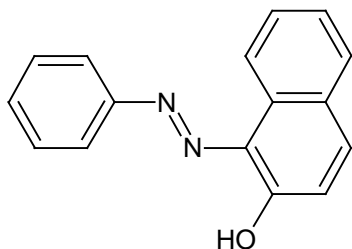
# Rapid Analysis of Pharmaceutical Compounds

TOF - MS with 40 Hz acquisition rate over 39-second run time



# Analysis of Sudan I: Reproducibility, Sensitivity, Quantitation

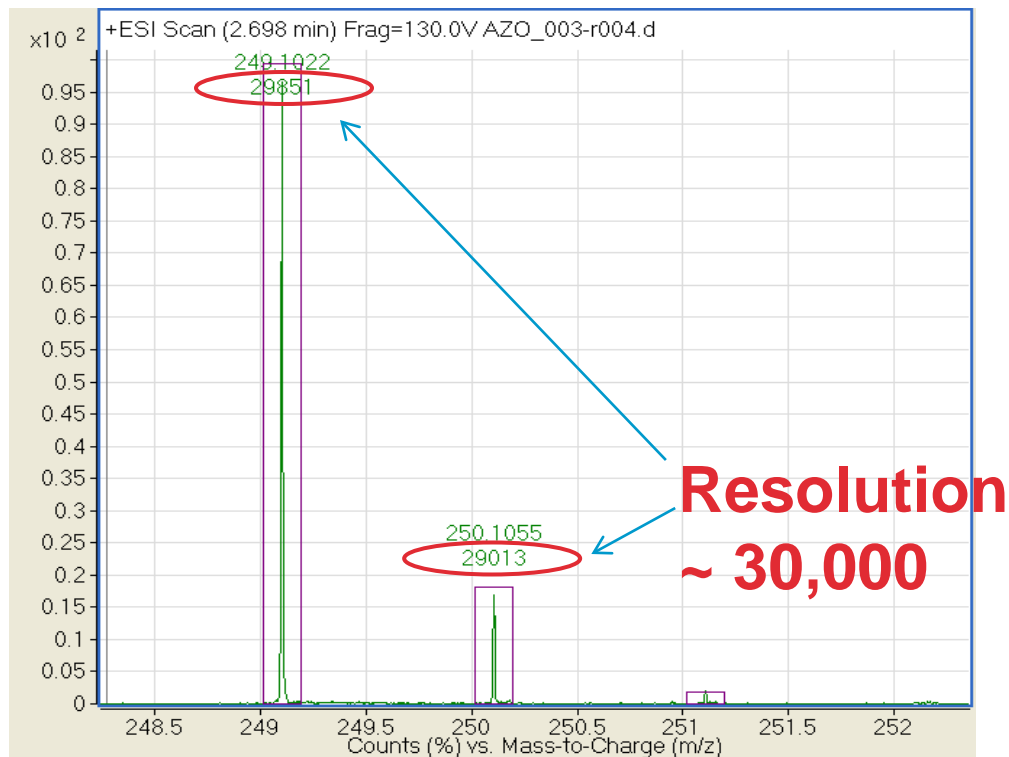
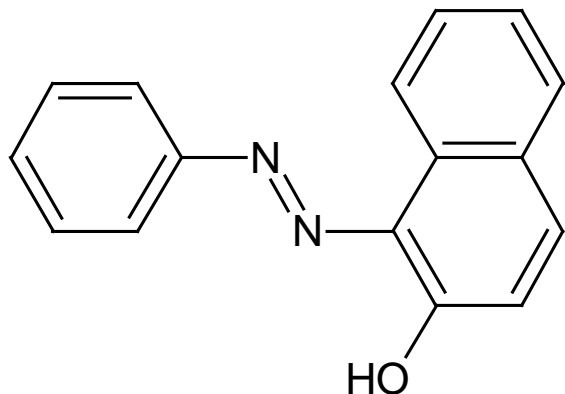
- Sudan I - 249.1023 m/z





# Analysis of Sudan I: Mass Accuracy, Resolution

Sudan I - 249.1023 m/z



MS Formula Results: + Scan (2.698 min) - AZO\_003-r004.d

m/z	Ion	Formula	Abundance							
249.1022	(M+H) <sup>+</sup>	C <sub>16</sub> H <sub>13</sub> N <sub>2</sub> O	101311.2							
Best	Formula (M)	Ion Formula	Score	Cross Score	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match
<input checked="" type="checkbox"/>	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O	C <sub>16</sub> H <sub>13</sub> N <sub>2</sub> O	99.42		249.1022	0.29	0.29	99.86	98.96	99.12

Mass accuracy 0.29 ppm

# Sudan Dyes: Outstanding Mass Accuracy and Resolution Enable Quantitation

Name	<i>m/z</i>	Mass error (ppm)	Resolution	Signal/noise (2 pg)	Calc. LOD at 3x RMS noise (pg)
Dimethyl (Butter) Yellow	226.1339	-0.11	28884	43.5	0.14
Sudan I	249.1023	0.29	29851	3.3	1.8
Sudan II	277.1336	-0.59	31267	6.9	0.87
Para Red	294.0873	0.64	31413	13.5 (20 pg)	4.4
Sudan III	353.1397	-0.34	32653	3.9	3.0
Sudan Red 7B	380.1870	0.31	32526	11.3	0.50
Sudan IV	381.1710	0.32	33515	8.9 (20 pg)	6.7
Sudan Red B	381.1710	0.56	34131	18.7	3.2
Rhodamine B	443.2330	-0.14	35607	58.4	0.10
Average:		0.37 ppm	<b>&lt; 0.5 ppm mass error</b>	<b>2.3</b>	
Standard deviation:		0.19 ppm			

# Vitamin B Analysis in Food

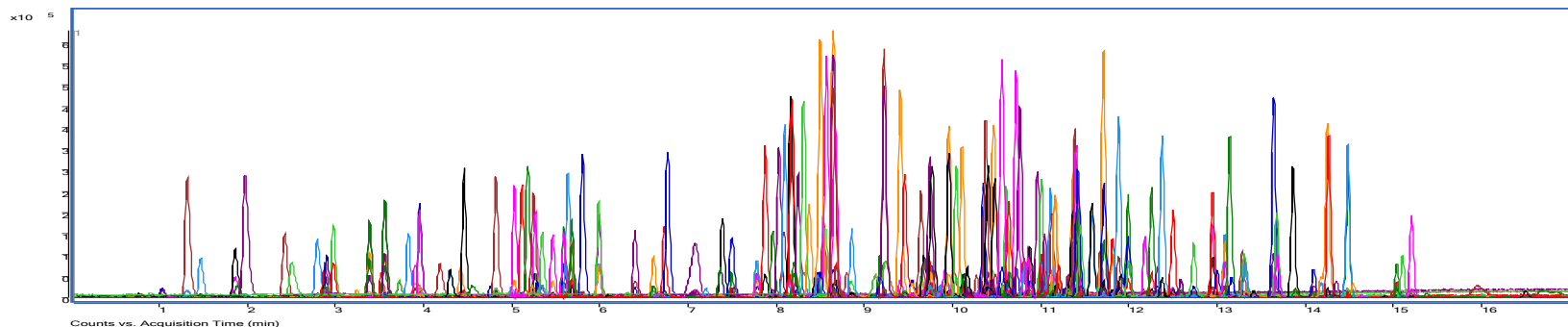
**By courtesy to Q&Q Laboratories, Sweden**

R Wahlström, E. Hermansson, G. Hägglund

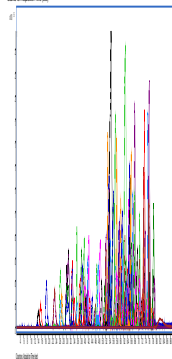
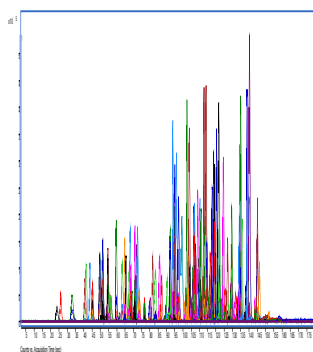
# TOF Pesticide Screening

## 250 pesticides, 50 pg on column

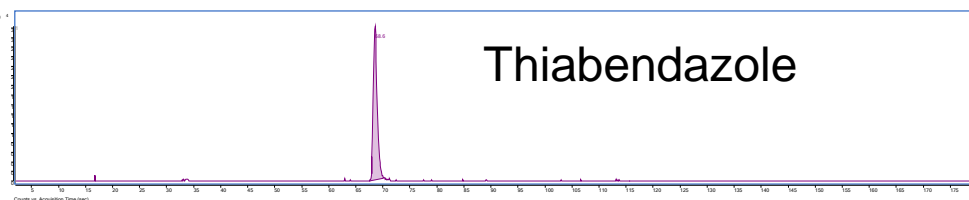
17 min.



3 min.

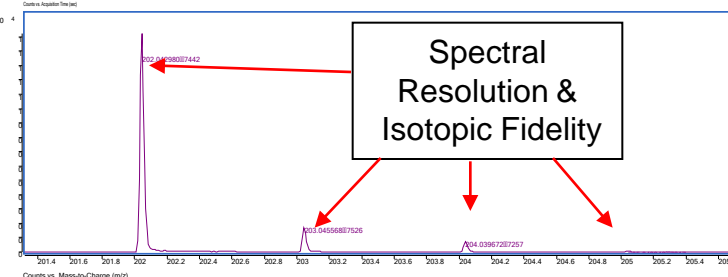
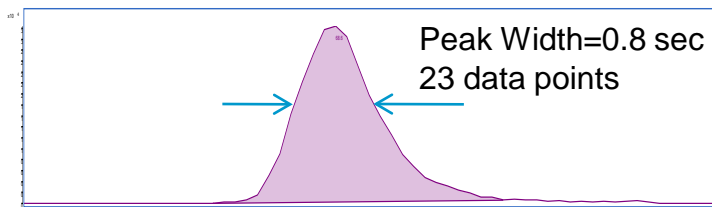


1.5 min.



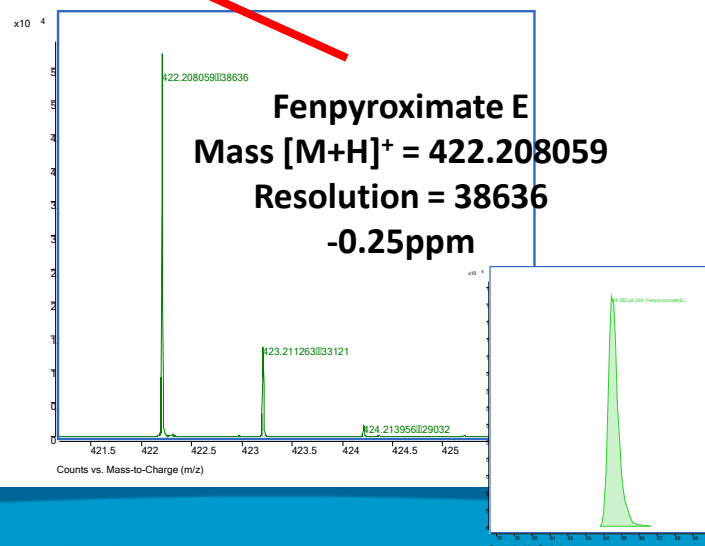
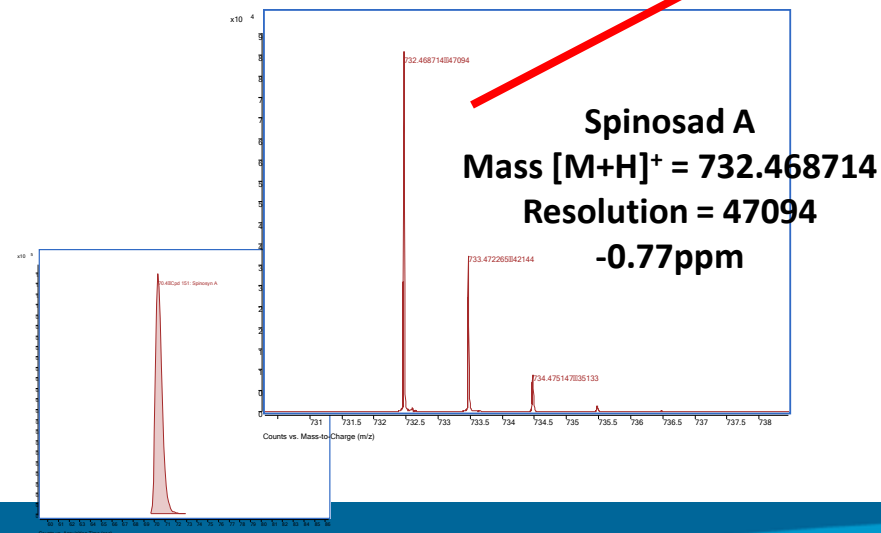
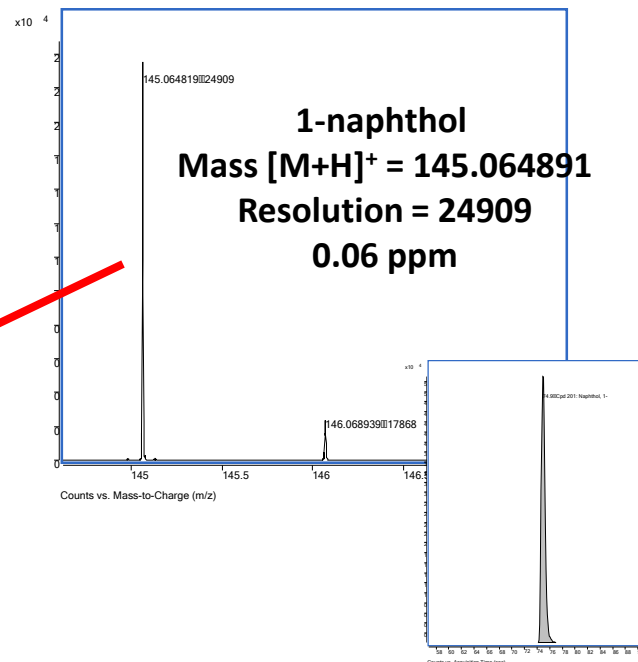
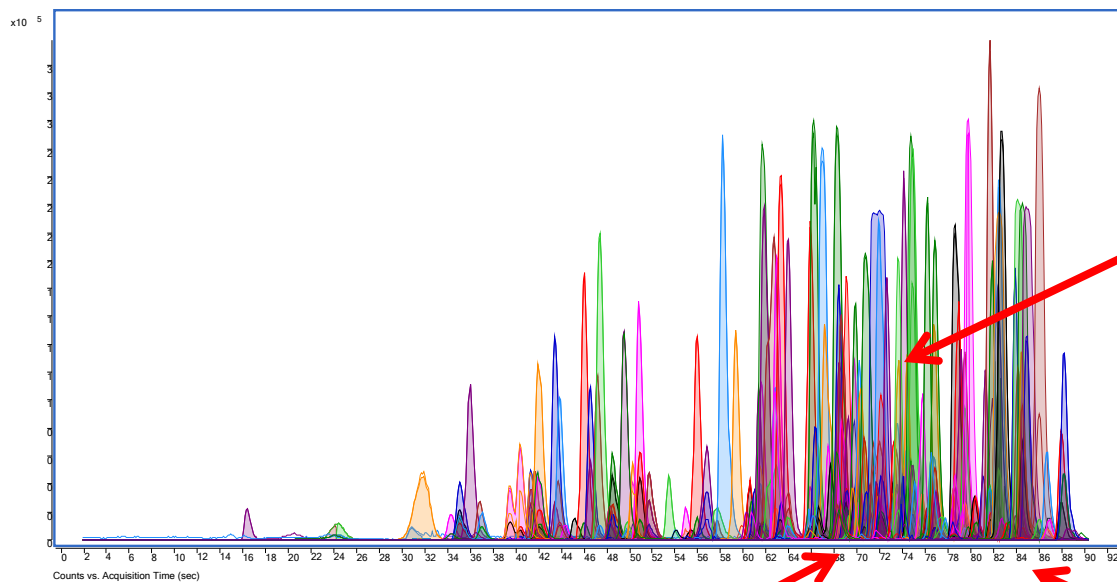
Cpd	Name	RT	Mass	Diff (Tgt. ppm)	Diff (Tgt. mDa)
191	Tebufenpyrad	123	333.1613	1.43	0.48
174	Tebupirimfos	138	318.1172	1.65	0.52
145	Tebupirimfos oxone	107.1	302.1397	0.36	0.11
77	Tebuthiuron	81.7	228.1044	-0.21	-0.05
115	Terbufos	120	288.0437	-1.59	-0.46
74	Terbumeton	97.7	225.1589	-0.05	-0.01
28	Terbutylazine-desethyl	54.7	201.0788	3.46	0.7
91	Terbutyn	112.8	241.1362	0.5	0.12
215	Tetraconazol	110.8	371.0216	0.24	0.09
25	Thiabendazole	68.6	201.0357	-1.81	-0.36
94	Thiacloprid	77	252.0233	-1.38	-0.35
118				0.08	
127				-11.66	
167				-0.16	
169	Tribufos	146.3	314.0964	0.76	0.24
161	Trifluraldo	77	189.0994	-0.97	-0.18

**-1.8 ppm**



# 1290 UHPLC with 6540 UHD Q-TOF

## 250 pesticides in 90 seconds





# Successful Identification of Isobaric Co-eluting Species by 1290/ 6540 UHD QTOF System

Formula	m/z		Compound	ppm difference	Identify by
C9H7N3S	190.0433	1a	tricyclazole		
C9H16ClN5	190.0667	1b	propazine F1 Cl-37	123	RT difference
C14H21NO4	226.1074	2a	diethofencarb F1		
C14H15N3	226.1339	2b	cyprodinil	117	MS difference
C15H18ClN3O	294.1181	3a	cyproconazole Cl-37		
C15H20ClN3O	294.1368	3b	paclobutrazol	63	MS difference
C13H11Cl2F4N3O	372.0288	4a	tetraconazole		
C21H13N3O4	372.0979	4b	Azoxystrobin-F1	186	MS difference

**Complex sample challenge:**

**Insufficient chromatographic or mass spectrometry resolution for these isobaric coeluting species (ICS)**

# SUMMARY

Modern ToF and Q-ToF instruments offers...

- High **resolving power** and **accurate mass** for selective and sensitive quantification
- No need to setup **MRM** transitions
- No need to decide upfront **what to detect**
- **Excellent linearity** over 3-3.5 orders of magnitude
- Possibility to build **accurate mass MS/MS libraries**
- Modern ToF/Q-ToF's are **easy to operate**
- Modern ToF/Q-ToF's are **stable and reliable**
- **Still sensitivity gap to QQQ systems (10-20 times)**



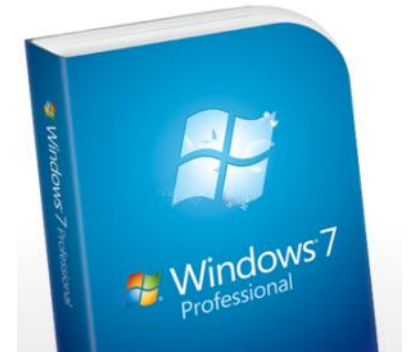
# MassHunter Software

# MassHunter Workstation

*Future proof with support of Windows 7 (64-bit)*

- **New and updated components (Feb-2011)**

- MassHunter Acquisition for QQQ B.04.01
- MassHunter Acquisition for TOF/Q-TOF B.04.00
- MassHunter Qualitative Analysis B.04.00
- MassHunter BioConfirm B.04.00
- MassHunter PCDL Manager B.04.00
- MassHunter Forensics/Tox PCD B.04.00
- MassHunter Forensics/Tox PCDL B.04.00 (Broecker, Herre & Pragst)
- MassHunter METLIN AMRT PCD B.04.00 - **NEW**
- MassHunter METLIN PCDL B.04.00 - **NEW**
- MassHunter Pesticide PCD B.04.00



- **All run on Win 7 64-bit (in 32-bit mode), supports Excel 2010**

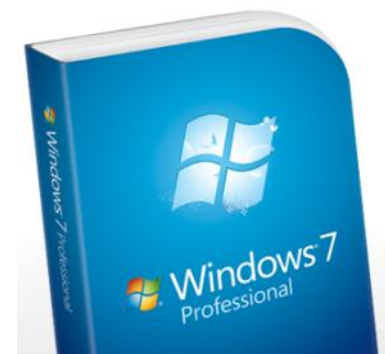
- Future proof your analytical instrument software NOW
- Prepare for future native 64-bit versions of MassHunter Qual and Quant

# MassHunter Workstation

*Future proof with support of Windows 7 (64-bit)*

- **New and updated components (Feb-2011)**

- MassHunter Acquisition for QQQ B.04.01
- MassHunter Acquisition for TOF/Q-TOF B.04.00
- MassHunter Qualitative Analysis B.04.00
- MassHunter BioConfirm B.04.00
- ➔ MassHunter PCDL Manager B.04.00
- MassHunter Forensics/Tox PCD B.04.00
- ➔ MassHunter Forensics/Tox PCDL B.04.00 (Broecker, Herre & Pragst)
- ➔ MassHunter METLIN AMRT PCD B.04.00 - **NEW**
- MassHunter METLIN PCDL B.04.00 - **NEW**
- ➔ MassHunter Pesticide PCD B.04.00

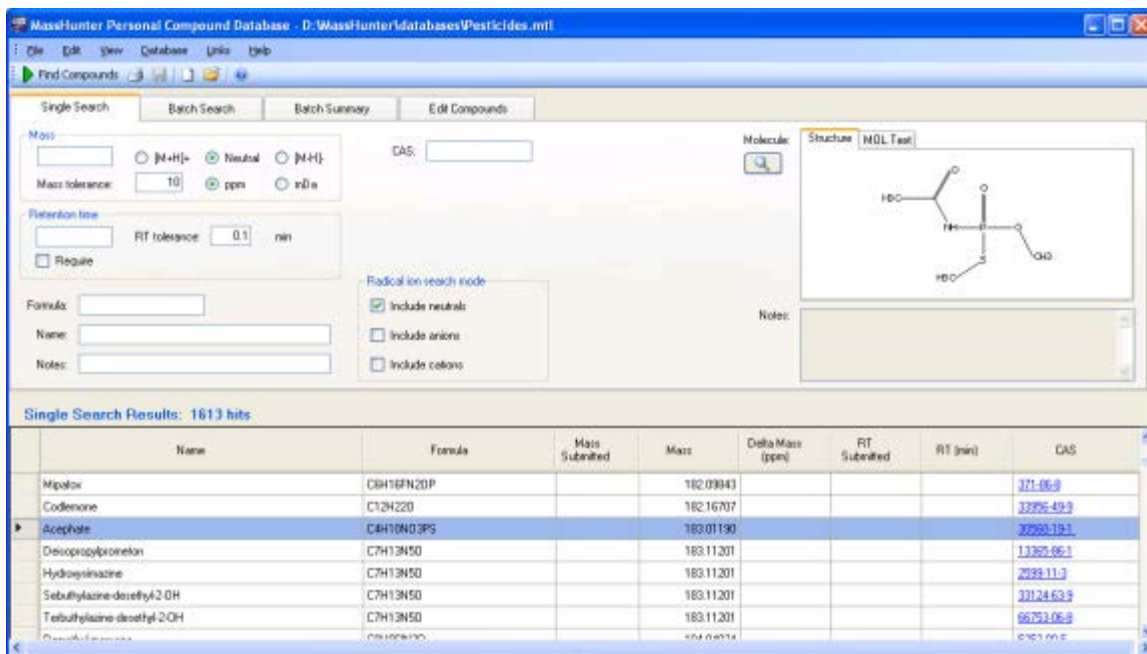


- **All run on Win 7 64-bit (in 32-bit mode), supports Excel 2010**

- Future proof your analytical instrument software NOW
- Prepare for future native 64-bit versions of MassHunter Qual and Quant

# Agilent Personal Compound Database

## Food Safety Screening, Metabolomics, Forensics

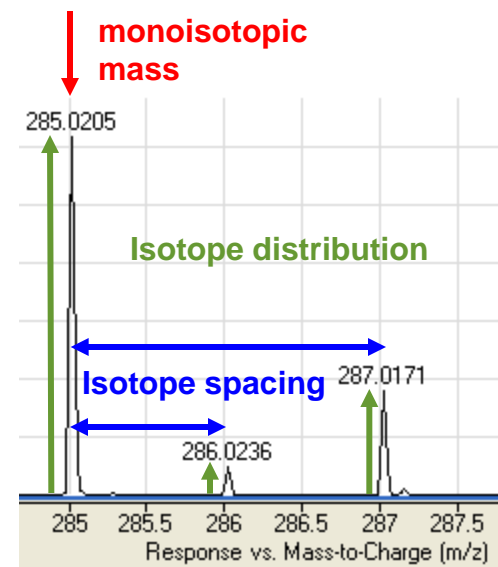


MassHunter Personal Compound Database - D:\MassHunter\databases\Pesticides.mtl

Single Search Results: 1613 hits

Name	Formula	Mass Submitted	Mass	Delta Mass (ppm)	RT Submitted	RT (min)	CAS
Mipox	C8H16FN2OP		182.09843				371-86-9
Codlone	C12H22O		182.16707				33396-49-9
Acephate	C8H10NO3PS		183.01190				30960-19-1
Desopropylproton	C7H13N5O		183.11201				13367-65-1
Hydroxynazine	C7H13N5O		183.11201				2989-11-3
Sebutylazine desethyl-2-OH	C7H13N5O		183.11201				33124-63-9
Terbutylazine desethyl-2-OH	C7H13N5O		183.11201				66753-06-8

Scoring based on



### Accurate mass and optional RT databases (AMRT)

- Endogenous metabolite database (METLIN) ~45,000 compounds including lipids
- Pesticide database (1600 pesticides)
- Forensic, toxicology, pharmaceutical database (7000 compounds)
- Create your own compound database

Public Metlin: [www.metlin.scripps.edu](http://www.metlin.scripps.edu)

# MassHunter PCDL Manager B.04.00

## Create/edit customized local PCDs and PCDLs

The screenshot displays the MassHunter PCDL Manager interface. The top menu includes File, Edit, View, Database/Library, Links, and Help. Below the menu are tabs for Single Search, Batch Search, Batch Summary, Edit Compounds, Spectral Search, Browse Spectra, and Edit Spectra. The main area is divided into search criteria on the left and a results pane on the right. The search criteria include Mass (with [M+H]<sup>+</sup>, Neutral, and [M-H]<sup>-</sup> options), Mass tolerance (10.0 ppm), Retention time (Require checkbox), RT tolerance (0.1 min), and Ion search mode (Include neutrals, anions, cations). The results pane shows a table of search results with columns for Compound Name, Formula, Mass, RT (min), CAS, ChemSpider, IUPAC Name, and Spectra #. The Cocaine entry is highlighted.

Compound Name	Formula	Mass	RT (min)	CAS	ChemSpider	IUPAC Name	Spectra #
Cocacetylen-D3	C18H20D...	320.18154					3
Cocacetylene	C18H23N...	317.16271		529-38-4	559082	Ethyl (1R,2R,3S,5S)-3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate	3
Cocain-D3	C17H18D...	306.16589					3
Cocaine	C17H21N...	303.14706		50-36-2	10194104	Methyl (1R,2R,3S,5S)-3-(benzoyloxy)-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate	3
Codein-D3	C18H18D...	302.17097					3
Codeine	C18H21N...	299.15214		76-57-3	4447447	(5 $\alpha$ ,6 $\alpha$ )-3-Methoxy-17-methyl-7,8-didehydro-4,5-epoxymorphinan-6-ol	3
Codeine glucuronide	C24H29N...	475.18423		20736-11-2			6
Codoxime	C20H24N...	372.16852		7125-76-0	7844721	([(5 $\alpha$ ,6E)-3-Methoxy-17-methyl-4,5-epoxymorphinan-6-ylidene]amino)oxy)acetic acid	0
Coenzyme A	C21H36N...	767.11521		85-61-0	6557		0
Cofosin	C68H79N...	1,085.565...		54063-34-2	16736899	(2-Oxo-2,3-dihydro-1H-indole-3,3-diyldi-3,1-phenylene (5beta,5beta)bis(3,7,12-trioxocholan-24-o...	0
Cogazocine	C21H31NO	313.24056		57653-29-9	171872	10-(Cyclobutylmethyl)-1-ethyl-13,13-dimethyl-10-azatricyclo[7.3.1.0 <sup>2,7</sup> ]trideca-2,4,6-trien-4-ol	0
Colchicine	C21H23N...	385.15254		477-27-0	204164	N-[7S]-10-Hydroxy-1,2,3,4-tetrahydro-9-oxo-5,6,7,9-tetrahydrobenzo[ <i>a</i> ]theoptalen-7-yl]acetamide	0

### SUPPORTS:

METLIN AMRT PCD B.04.00  
METLIN AMRT PCDL B.04.00  
For/Tox AM PCD B.04.00  
For/Tox AM PCDL B.04.00  
Pesticide AM PCD B.04.00

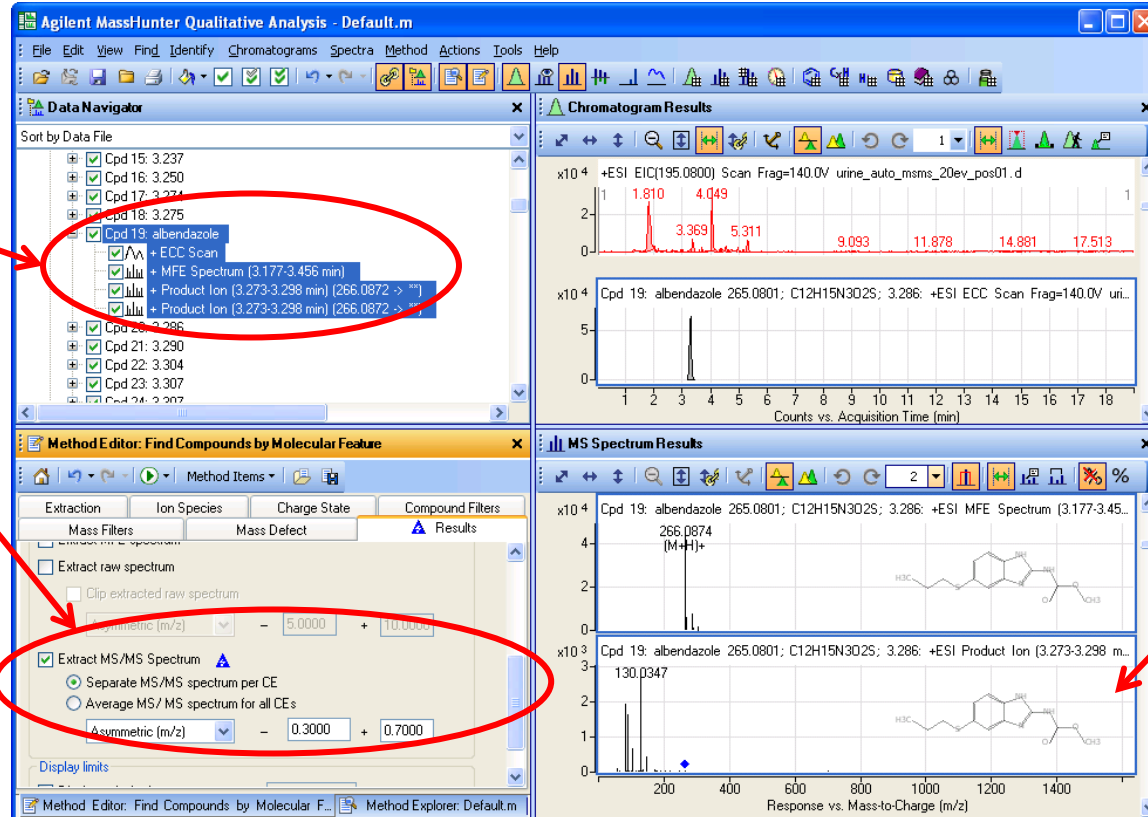
=> The most comprehensive offering of content PCDs and PCDLs

- Personal Compound Database and Libraries (PCDLs) for accurate mass database and MS/MS library search with optional retention time
- Add compounds, AM MS info, RT info and AM MS/MS spectra at multiple collision energies using the new PCDL Manager software
- Use create and edit PCDs and PCDLs on your personal PC (keep proprietary data in house!)

# Forensics/Tox Accurate Mass PCDL

“Broecker, Herre & Pragst” – MS/MS spectra for 2600 Cmpds

Extract MS/MS Spectra when running MFE



Identification via accurate mass MS/MS Lib Search

- The Forensics/Tox accurate mass PCD contains 7500 compounds
- New Forensics/Tox accurate mass PCDL contains **7900 MS/MS spectra for over 2600 compounds** from 3 collision energies mostly in positive mode.
- The **first** commercially available **accurate mass MS/MS library!**

# New METLIN AMRT PCD and PCDL B.04.00 MS/MS spectra for > 2300 endogenous metabolites !

MassHunter Personal Compound Database and Library for Metabolomics - D:\MassHunter\Library\AMRT\_RP\_Formula\_02\_17\_2010.cdb

Acquired spectra

Compound Name	Precursor Ion	Collision Energy	Ion Polarity	Ionization Mode	Instrument Type
Asparagine	133.06081	10	Positive	ESI	QTOF
Asparagine	133.06081	20	Positive	ESI	QTOF
Asparagine	133.06081	40	Positive	ESI	QTOF
Asparagine	131.04620	10	Negative	ESI	QTOF
Asparagine	131.04620	20	Negative	ESI	QTOF
Asparagine	131.04620	40	Negative	ESI	QTOF

Library spectra

Compound Name	Precursor Ion	Collision Energy	Ion Polarity	Ionization Mode	Instrument Type
Asparagine	133.06081	10	Positive	ESI	QTOF
Asparagine	133.06081	20	Positive	ESI	QTOF
Asparagine	133.06081	40	Positive	ESI	QTOF
Asparagine	131.04620	10	Negative	ESI	QTOF
Asparagine	131.04620	20	Negative	ESI	QTOF
Asparagine	131.04620	40	Negative	ESI	QTOF

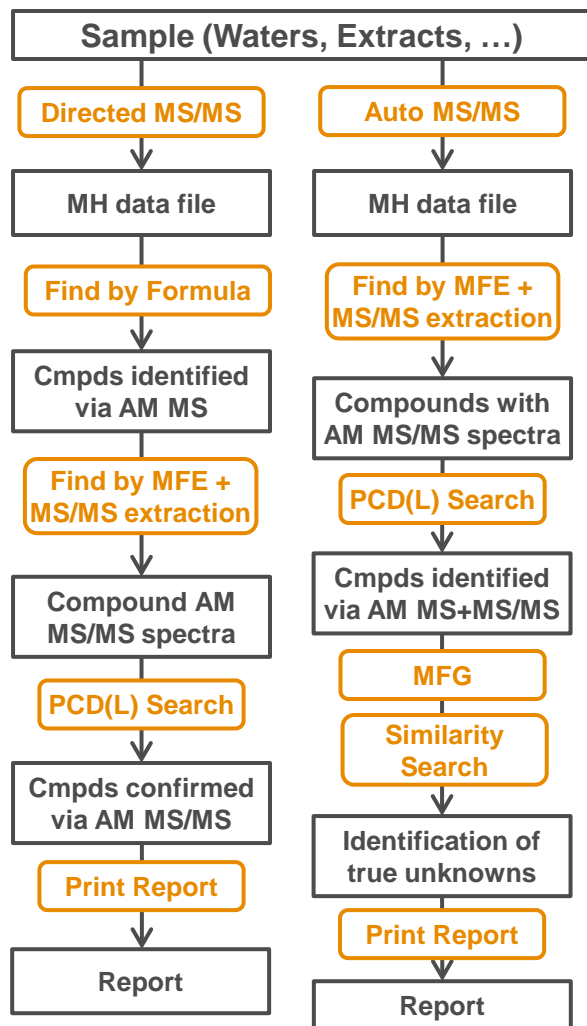
Single Search Results: 23187 hits

Compound Name	Formula	Mass	RT (min)	CAS	ChemSpider	METLIN	HMP	KEGG	LMP	IUPAC Name	Spectra #
Niacin (Nicotinic acid)	C6H5NO2	123.03203	0.646	59-67-6	240			C00253			6
Hydroxyproline	C5H9NO3	131.05824	0.349	51-35-4	257						6
Asparagine	C4H8N2O3	132.05349	0.346	70-47-3	14			C00152			6
Aspartic Acid	C4H7NO4	133.03751	0.373	56-84-8	15			C00049			6
Glutamine	C5H10N2O2	146.06914	0.342	56-85-9	18			C00064			6
Glutamic Acid	C5H9NO4	147.05316	0.349	56-86-0	19			C00025			6
p-Acetamidophenol (Acetaminophen, Tylenol)	C8H9NO2	151.06333		103-90-2	487						6

- Now contains ~ 45.000 endogenous metabolites
- New METLIN AMRT PCD added retention times for 700 compounds on a RP column. Additional RTs on a hydrophilic column in progress.
- New METLIN AMRT PCDL contains MS/MS spectra from over 4.600 compounds from up to 4 collision energies in positive and/or negative mode (~ 27.000 spectra total)

# MassHunter Workstation B.04.00 for TOF/Q-TOF

## Confident Screening + ID in Food and Environment



### • Targeted Workflow

- Highest productivity via automatic Finding, identifying and confirming targeted compounds via **Find by Formula** using accurate mass MS info
- Easily create a **Personal Compound Database and Library (PCDL)** from targeted compounds via **new PCDL Manager**
- Confirm identity via accurate mass MS/MS spectra library search in a PCDL via **new Directed MS/MS** in the first run!

### • Untargeted Workflow

- Highest productivity via automatic extraction of accurate mass MS and MS/MS info via **new Find by MFE with MS/MS spectral extraction** from Auto MS/MS data files.
- Automatically conduct a PCDL search and Molecular Formula Generation using MS *and (!)* MS/MS information
- Highest confidence via **new** combined scoring and viewing of results from AM DB search, AM library search and MFG.



# New 6550 iFunnel QTOF

## *10X Sensitivity Gain Enables Applications*

### Sensitivity

- Dramatically improved quantitative capabilities
- New Qual/Quan Workflows
- Non-targeted compound screening

### Comprehensive Performance Enhancements

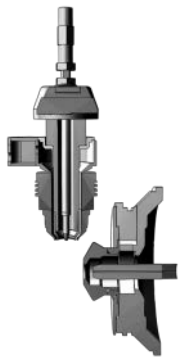
- Mass Resolution >40,000
- 50 spectra /sec MS and 33 spectra/sec MS/MS
- 5 orders of linear dynamic range
- <1 ppm MS mass accuracy; <2 ppm MS/MS
- Unrivalled sensitivity



# iFunnel Technology Captures 6x More Ions

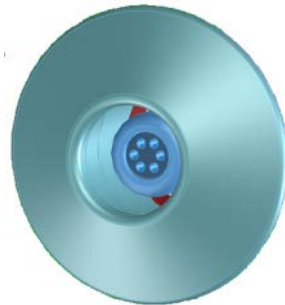
## Agilent Jet Stream

- Thermal confinement of ESI plume
- Efficient desolvation to create gas phase ions
- Creates an ion rich zone



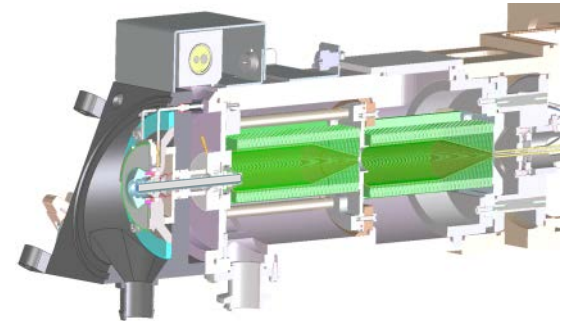
## Hexabore Capillary

- Samples 6 times more ion rich gas from the source with 6 capillaries
- Captures the majority of the gas from the source region



## Dual Ion Funnel

- Removes the gas but captures the ions
- Removes neutral noise
- Extends turbo pump life



# Agilent Jet Stream

## Thermal Gradient Focusing Technology

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Dramatic **Sensitivity Gains** for  
Premium TOF, Q-TOF, and Triple Quad

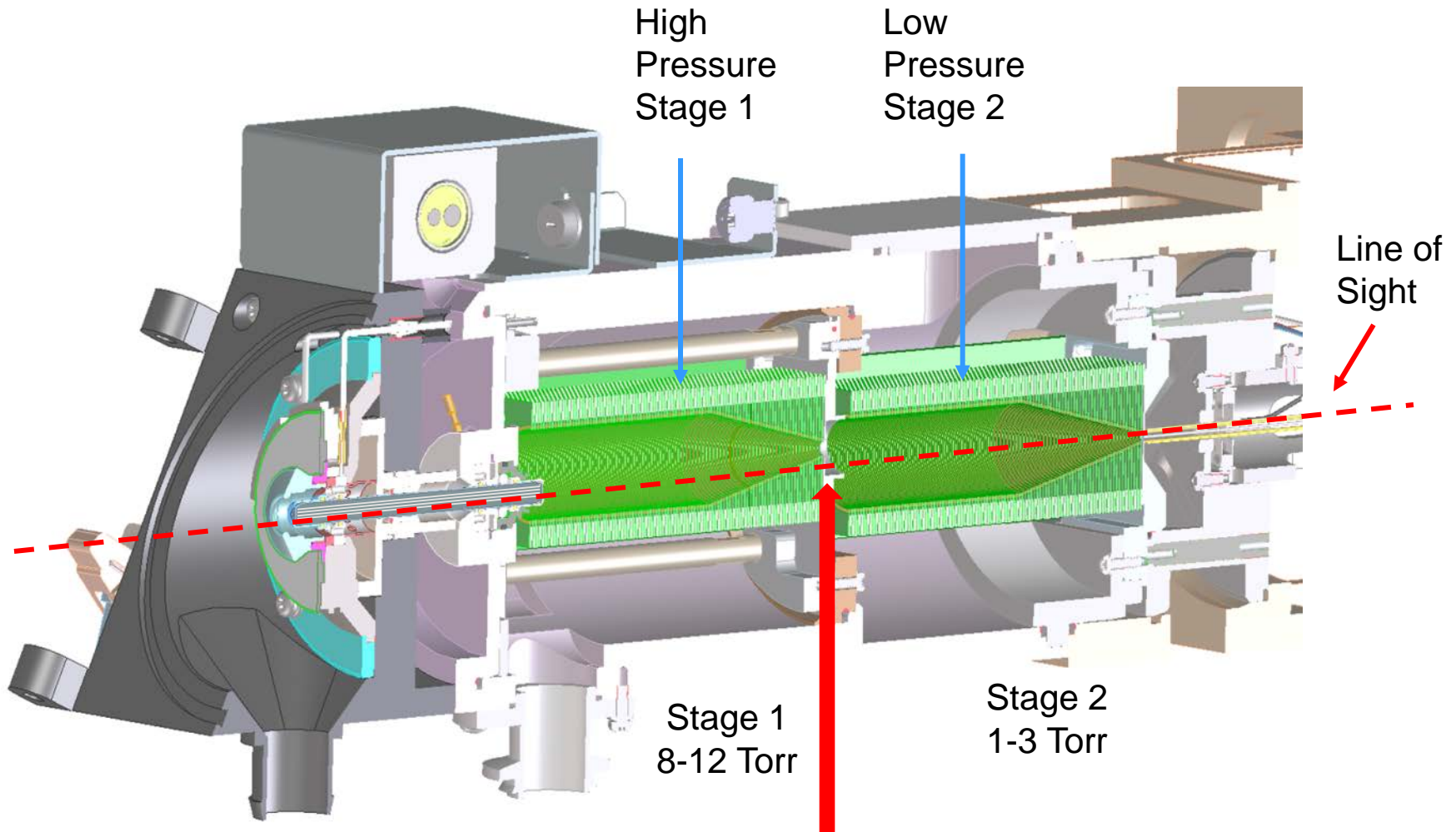
Ions Focused in a Collimated  
Thermal Confinement Zone

Improved Ionization Efficiency and  
Sampling

**Effective Across a Broad Range of  
Analyte Classes, including many  
APCI compounds**

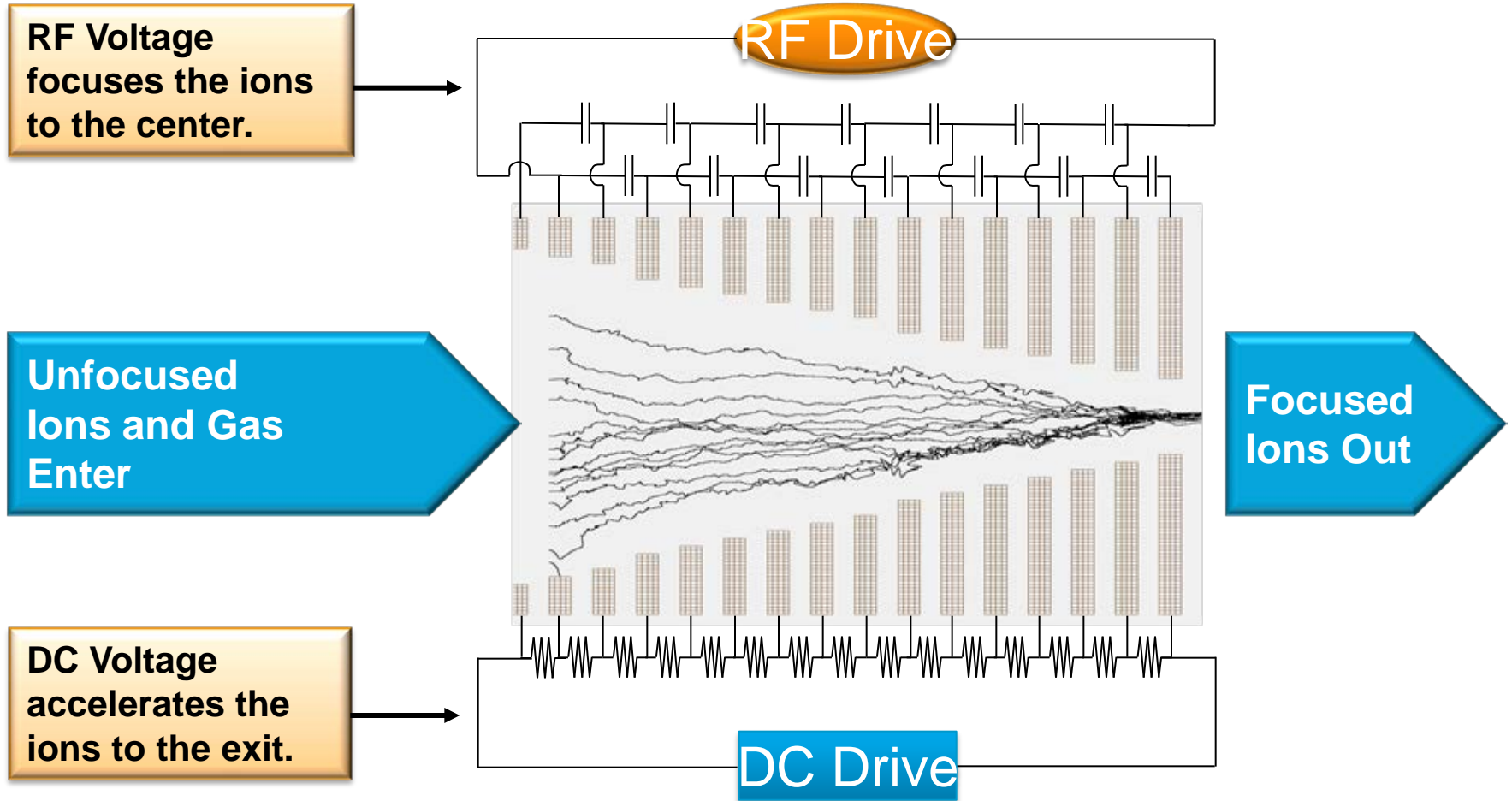


# Two Stage Ion Funnel Manages the Gas Load



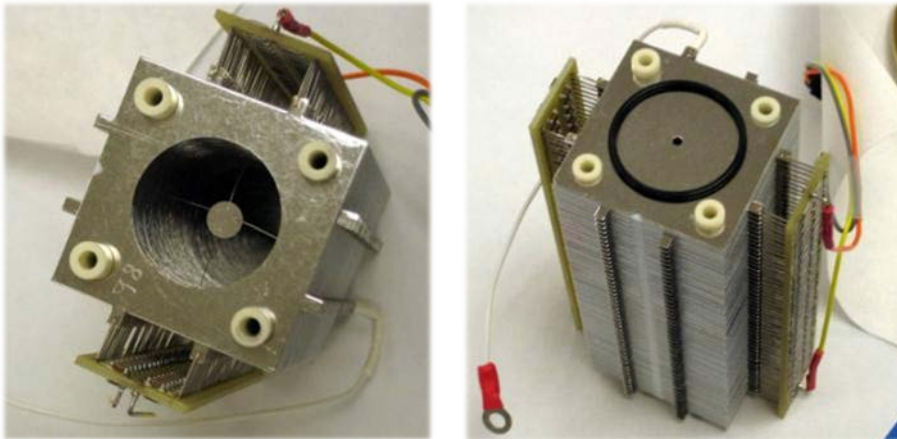
*Offset ion funnels to prevent neutrals from going straight through to MS*

# Ion Funnel Operation

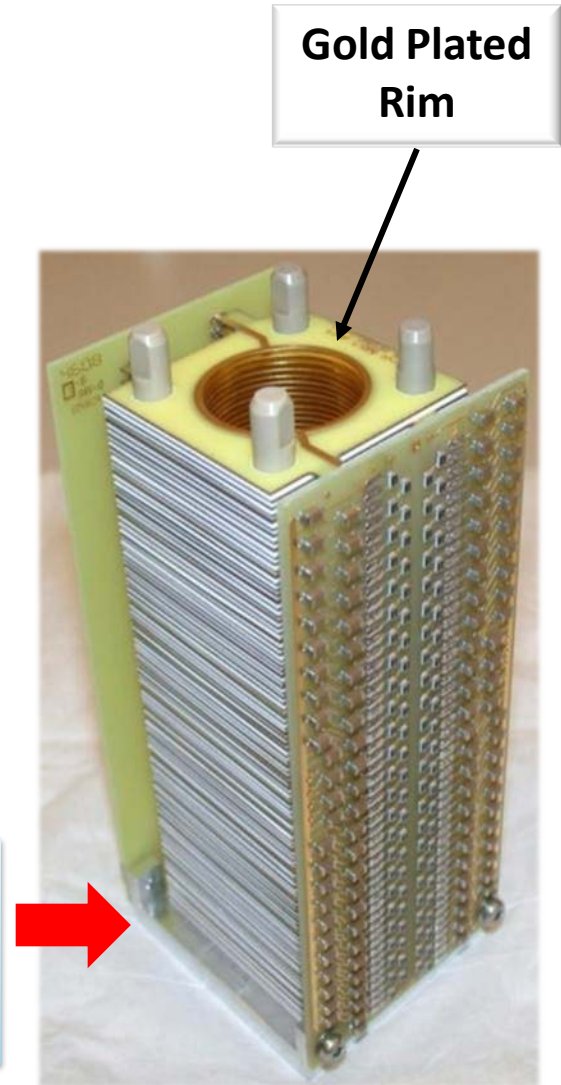


# Ion Funnel Construction

Previously, many metal plates made cleaning a priority because of the large, active surface area... The high capacitance also required larger power supplies to provide RF power



**The 6490 design uses printed circuit board technology giving a greatly reduces surface area. This low capacitance enables the use of small power supplies, and enables fast polarity switching**



# Simple and Easy Ion Funnel Cleaning Procedure

- As with all LC/MS systems routine cleaning is necessary periodically.
- The high pressure ion funnel should be cleaned periodically, although this could vary from 3 months to 1 year depending on the quantity and type of samples
- The high pressure ion funnel is easily removed
- Clean by sonicating the ion funnel assembly in 100% isopropanol for 15 minutes.



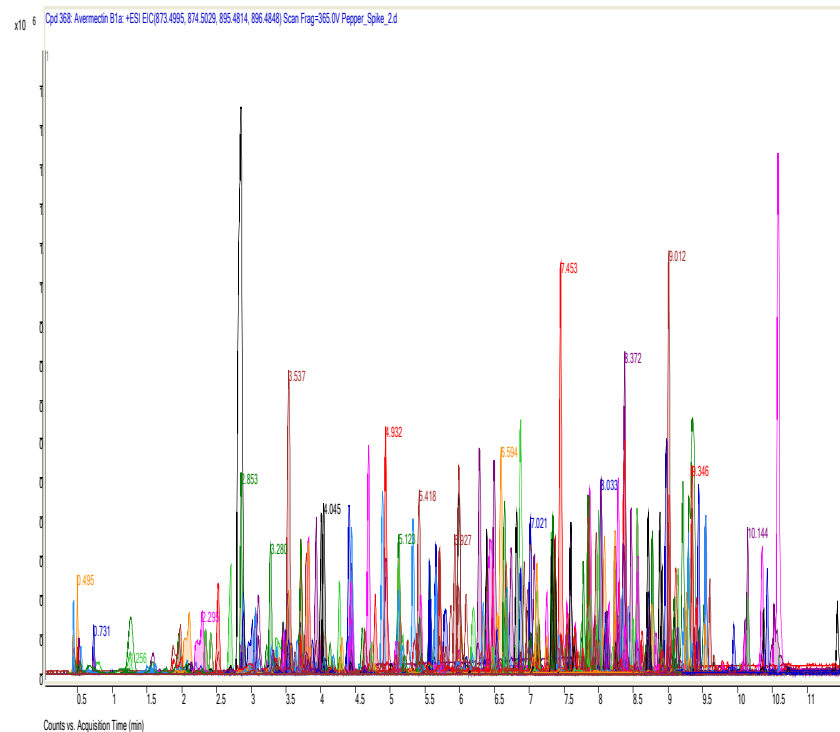
# Dramatically Improving Detection Levels for Non-Targeted Screening

## 10 ppb Detection of Low Response Compounds



### European Reference Lab for Pesticides

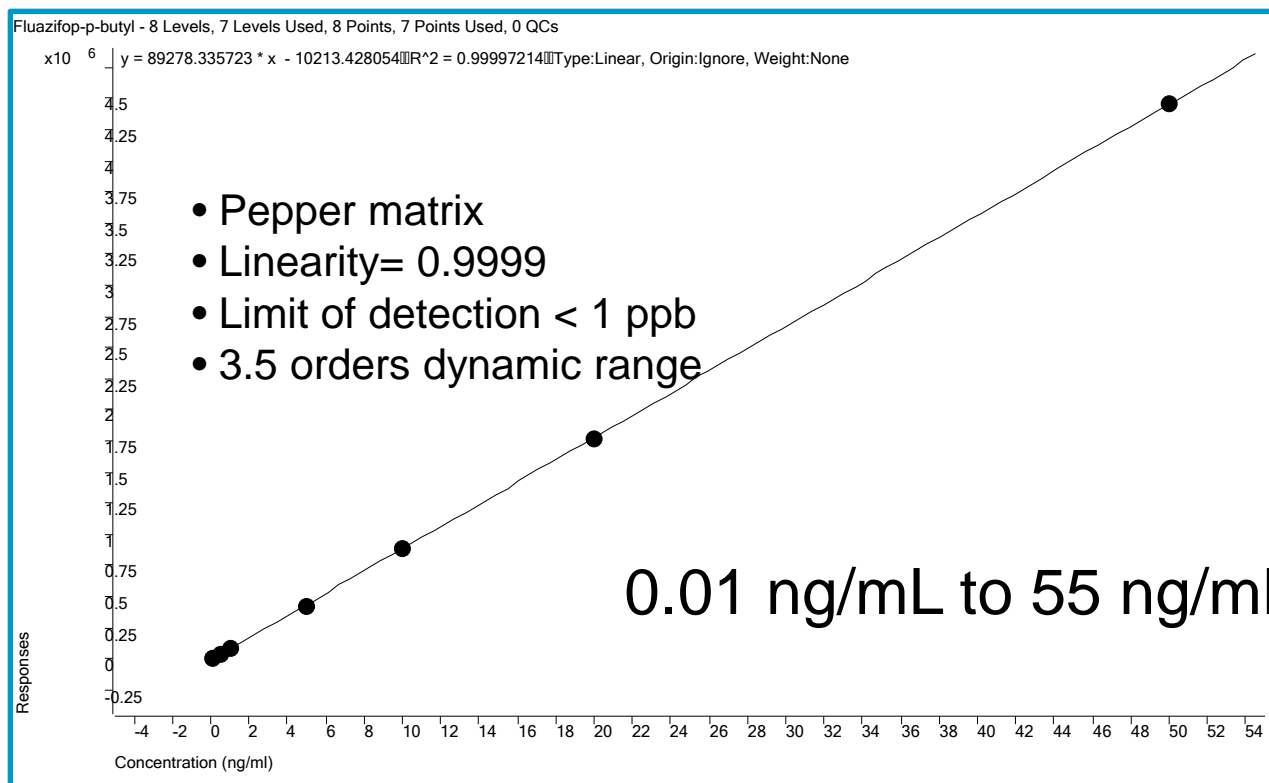
- 15% of tested pesticides have detection limits between 20 ppb to 100 ppb
- International actionable level is 10 ppb
- Challenge: Detect low responding compounds at <10 ppb using 6550 iFunnel QTOF



Chromatograms of 300 pesticides spiked in pepper extract at conc.10 ug/kg (10 ppb)



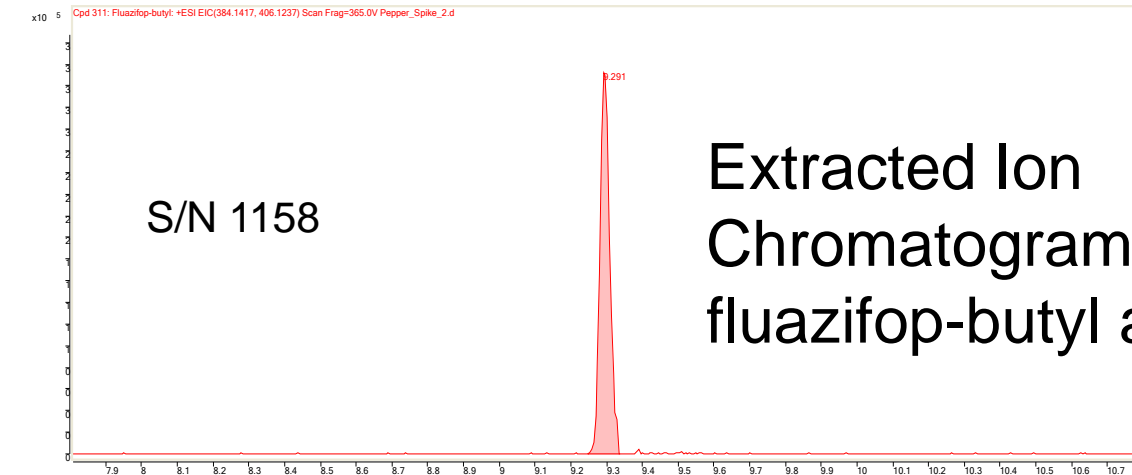
# 6550 Linearity and Precision for Fluazifop-butyl



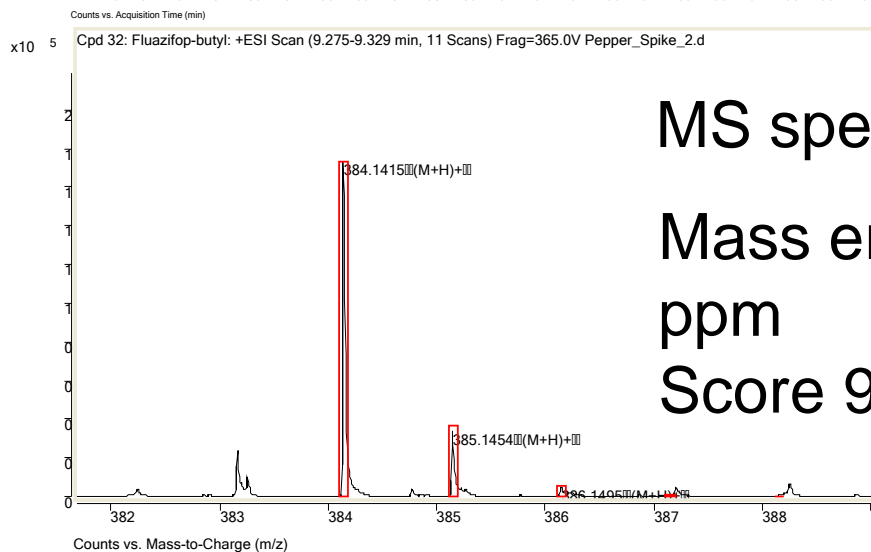
*Successfully Detected in Pepper at 1 ppb*

# Dramatic Increase in Pesticide Detection

## Over 10 Fold Gain in Detection for Fluazifop-butyl



Extracted Ion Chromatogram for fluazifop-butyl at 10 ppb



MS spectrum of fluazifop-butyl

Mass error ~0.5

ppm

Score 98

# Compound Detection Below 10 ppb



	Pepper	Pepper	Orange	Orange
Compound	6530	6550	6530	6550
Chlorfluazuron	Red	Green	Red	Green
Cymoxanil	Green	Green	Red	Green
Diuron	Green	Green	Green	Green
Fluazifop-butyl	Red	Green	Red	Green
Fluroxypr	Green	Green	Red	Red
Propaquizafop	Red	Green	Green	Green
Quizalofop-ethyl	Green	Green	Red	Green
Rotenone	Green	Green	Red	Green
Bromacil	Green	Green	Red	Green
Fenproximate	Green	Green	Red	Green
Tribenuron	Red	Green	Red	Green
Aldoxicarb	Green	Green	Green	Green

85% of all pesticides successfully detected by 6530 QTOF in tomato, pepper, leek, orange matrices



# THANK YOU!