7200 Series Q-TOF for GC/MS

A new analytical tool for solving complex analytical problems

June 2011

ASMS Conference on

Mass Spectrometry and Allied Topics

June 5-9, 2011

Colorado Convention Center, Denver, CO

7200 GC/Q-TOF Breakfast Seminar

Hospitality Suite

"There's Something Brewing at Agilent" BrewPub Theme

Heavy Matrix Hefeweizen

Super Sensitive Stout

Clearly Better Bitter

5975E SQ

5975C SQ

5975T LTM SQ

Agilent GC/MS & GC/MS/MS

More Choices – Better Solutions

220 IT

240 IT

7000 TQ

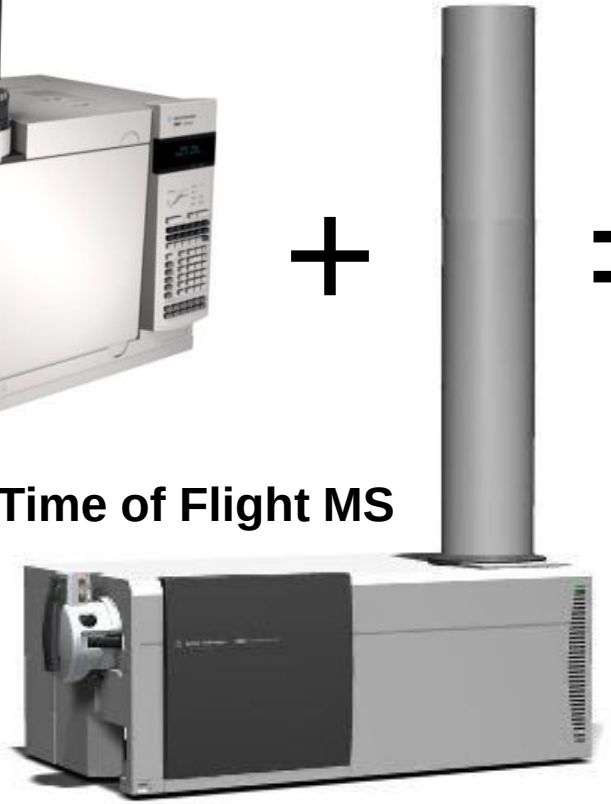
7200 Q-TOF NEW

What is it?

7890 + 7000 + 6500 = 7200 GC/Q-TOF

Triple Quadrupole MS

+



Time of Flight MS

=

Quadrupole Time of Flight MS

What Will The 7200 Q-TOF Do For You?

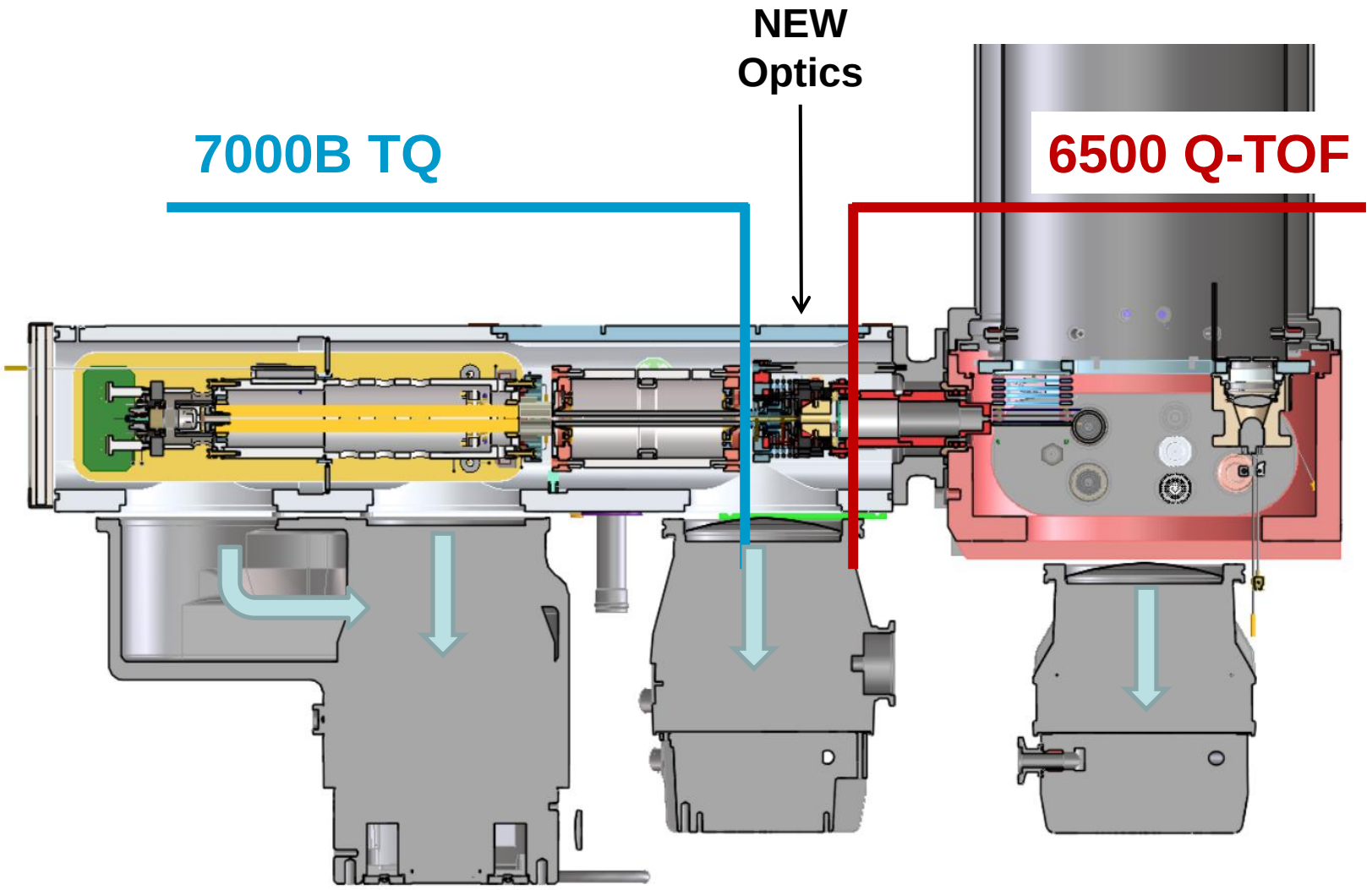
- TOF mode
  - High resolution full scan spectra
  - Accurate mass measurements
  - Fast full spectrum acquisition
- MS/MS mode
  - Product ion spectra – high resolution, accurate mass
  - Sensitivity > TQ product ion methods
- Ideal tool for solving complex analytical problems
- New tools for structural elucidation of unknowns and confirmation of non-targets

7890 + 7000 + 6500 = 7200 GC/Q-TOF

It's our newest GC/MS . . .
built upon many well proven parts:

Almost one thousand 7000 TQs
Over one thousand TOFs and Q-TOFs
Many thousand 7890 GCs

7200 Analyzer



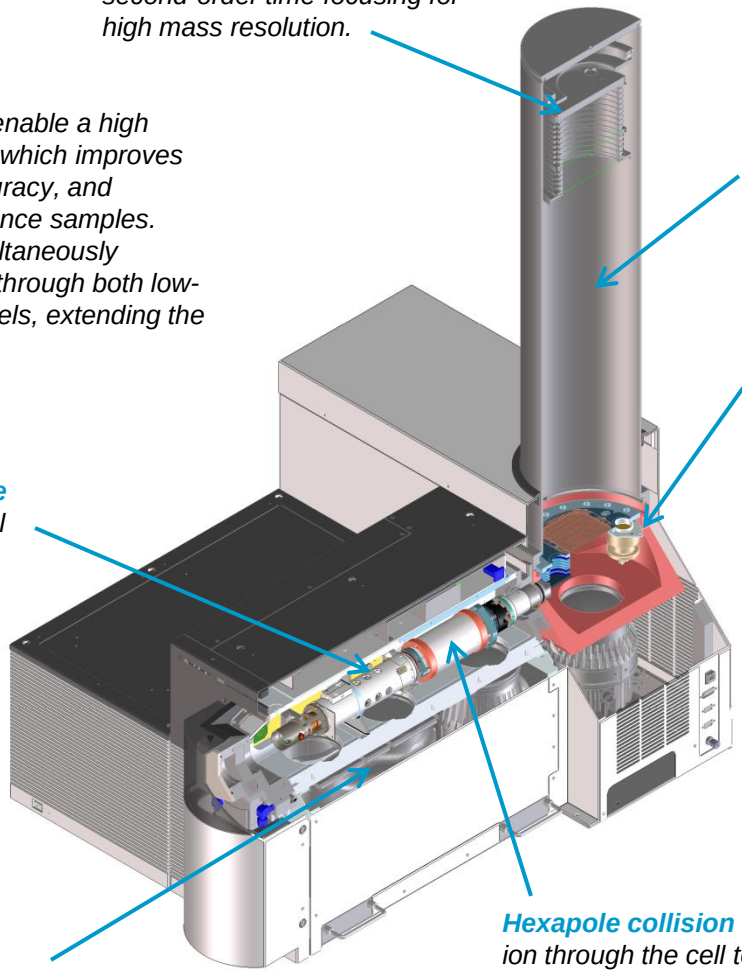
New . . . Yet Totally Proven

Dual-stage ion mirror *improves second-order time focusing for high mass resolution.*

Proprietary INVAR flight tube *sealed in a vacuum-insulated shell eliminates thermal mass drift due to temperature changes to maintain excellent mass accuracy, 24/7. Added length improves mass resolution.*

4GHz ADC electronics *enable a high sampling rate (32 Gbit/s) which improves the resolution, mass accuracy, and sensitivity for low-abundance samples. Dual gain amplifiers simultaneously process detector signals through both low-gain and high gain channels, extending the dynamic range to 105.*

Analog-to-digital (ADC) Detector*: Unlike time-to-digital (TDC) detectors which record single ion events,* ADC detection *records multiple ion events, allowing very accurate mass assignments over a wide mass range and dynamic range of concentrations.*

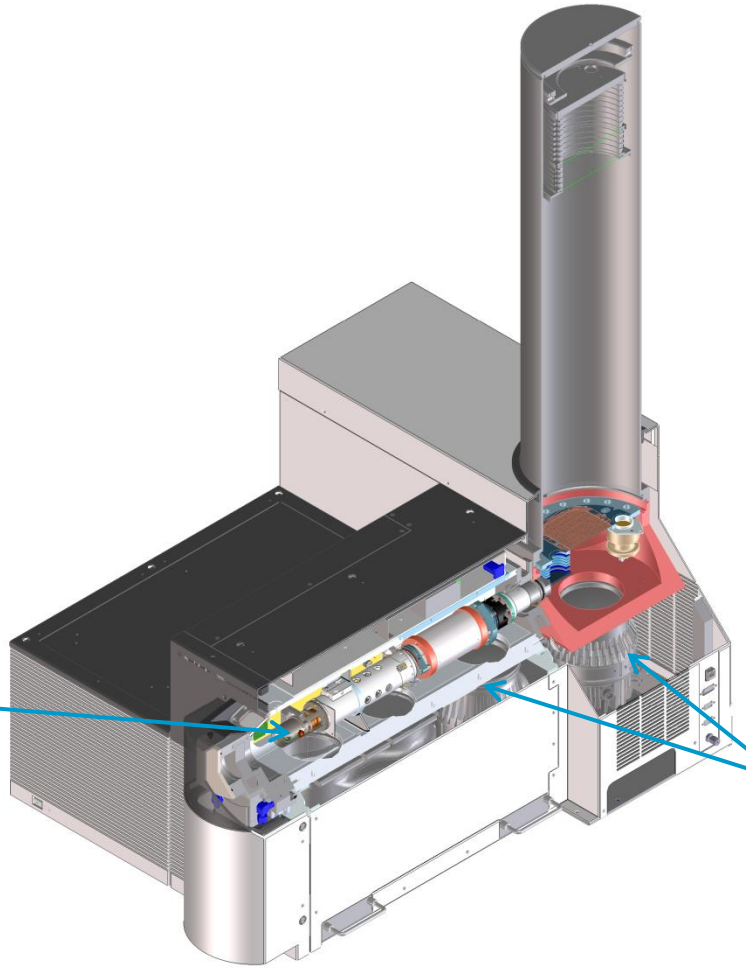


Hot, quartz monolithic quadrupole analyzer and collision cell *identical to the 7000 Quadrupole MS/MS*

Split-flow turbo *differentially pumps the ion source and quadrupole analyzer compartments*

Hexapole collision cell *accelerates ion through the cell to enable faster generation of high-quality MS/MS spectra without cross-talk*

Other New . . . And Improved



New ***Removable Ion Source*** *includes repeller, ion volume, extraction lens and dual filaments*

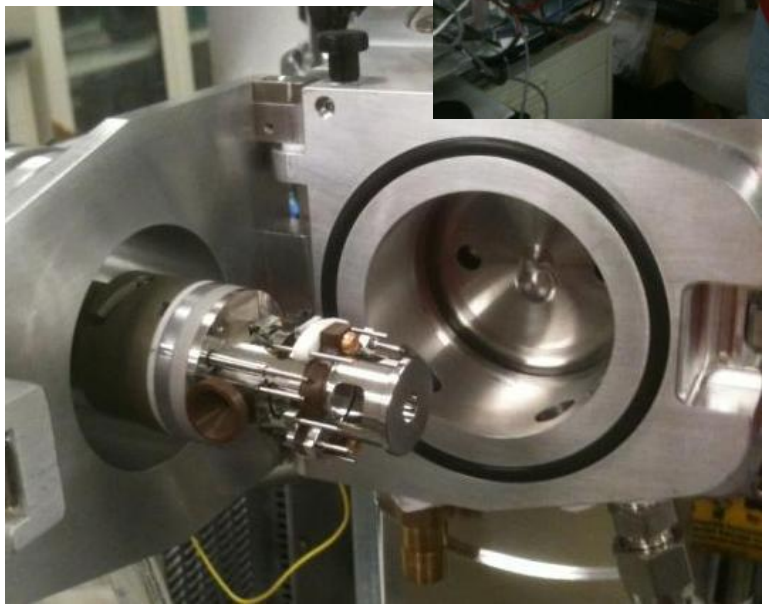
New ***Internal Reference Mass*** *can be delivered to the source at a low and high concentration*

Two 300L/s turbos *pump the focusing optics and flight tube*

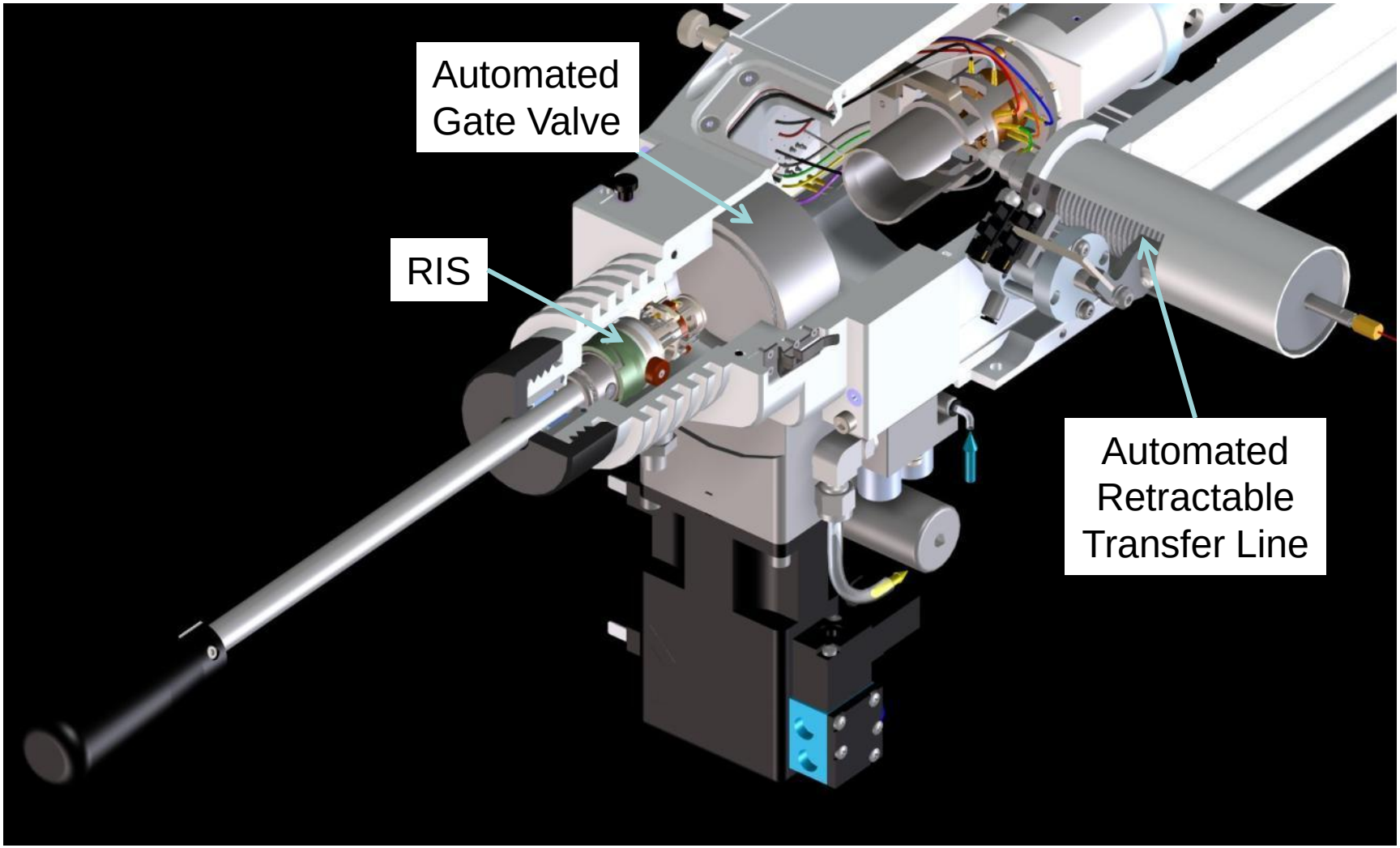
Removable Ion Source (RIS)

- Allows swap of complete ion source, including filaments, in ~30 minutes without venting

- Allows fast EI/CI source swapping without venting

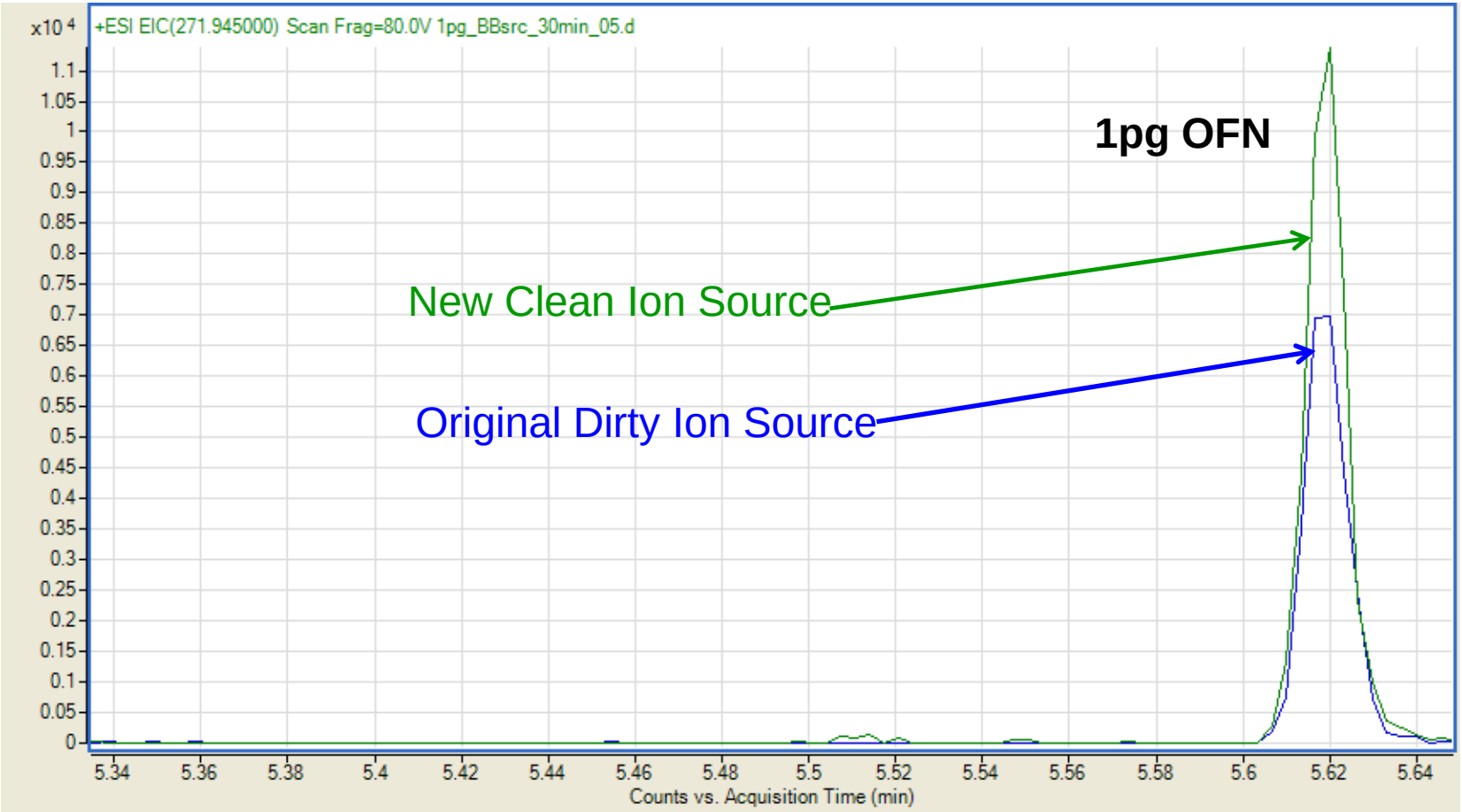


Removable Ion Source (RIS)



30 minute source swap with RIS

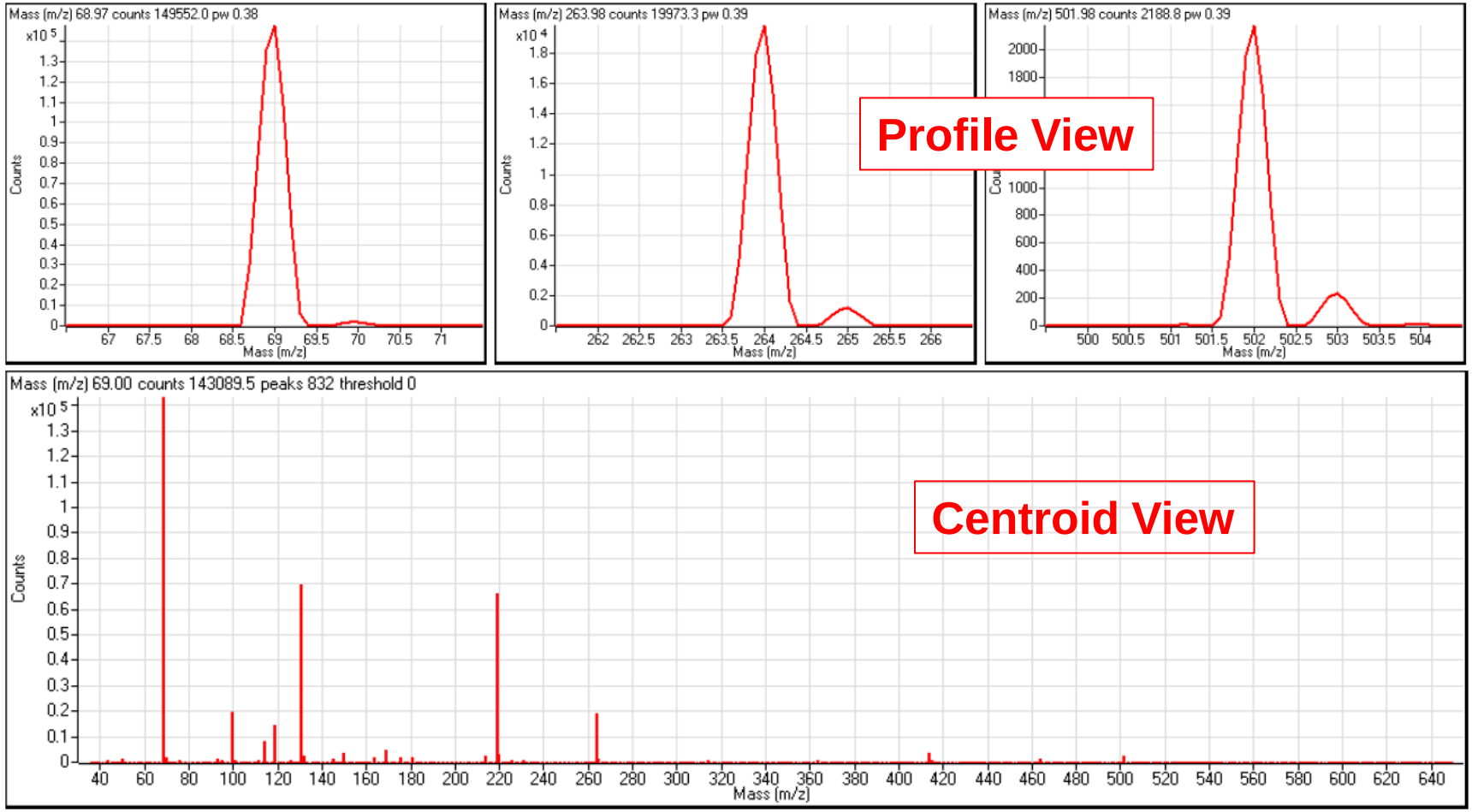
Vent→cool ion source→open chamber and replace/maintain source components→ close chamber→pump out→heat source→ stabilize vacuum and source temperature



Agilent Technologies

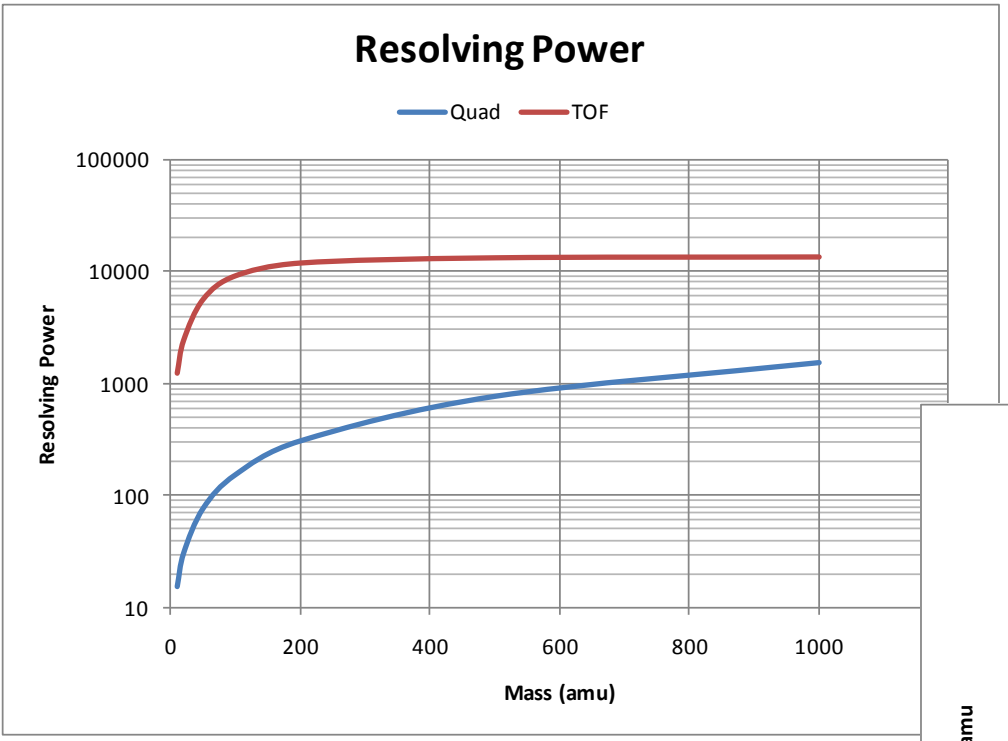
Spectral presentation (Tune File)

Most users think in “centroid”, but the MS operates in “profile”



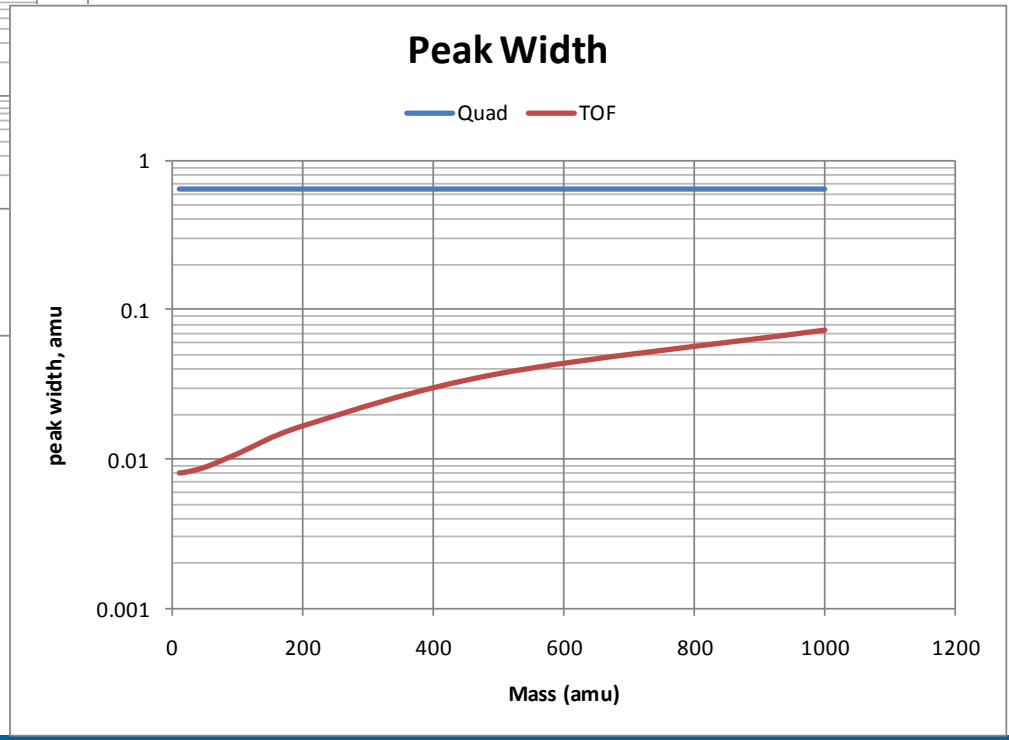
Agilent Technologies

Comparing Quad & TOF

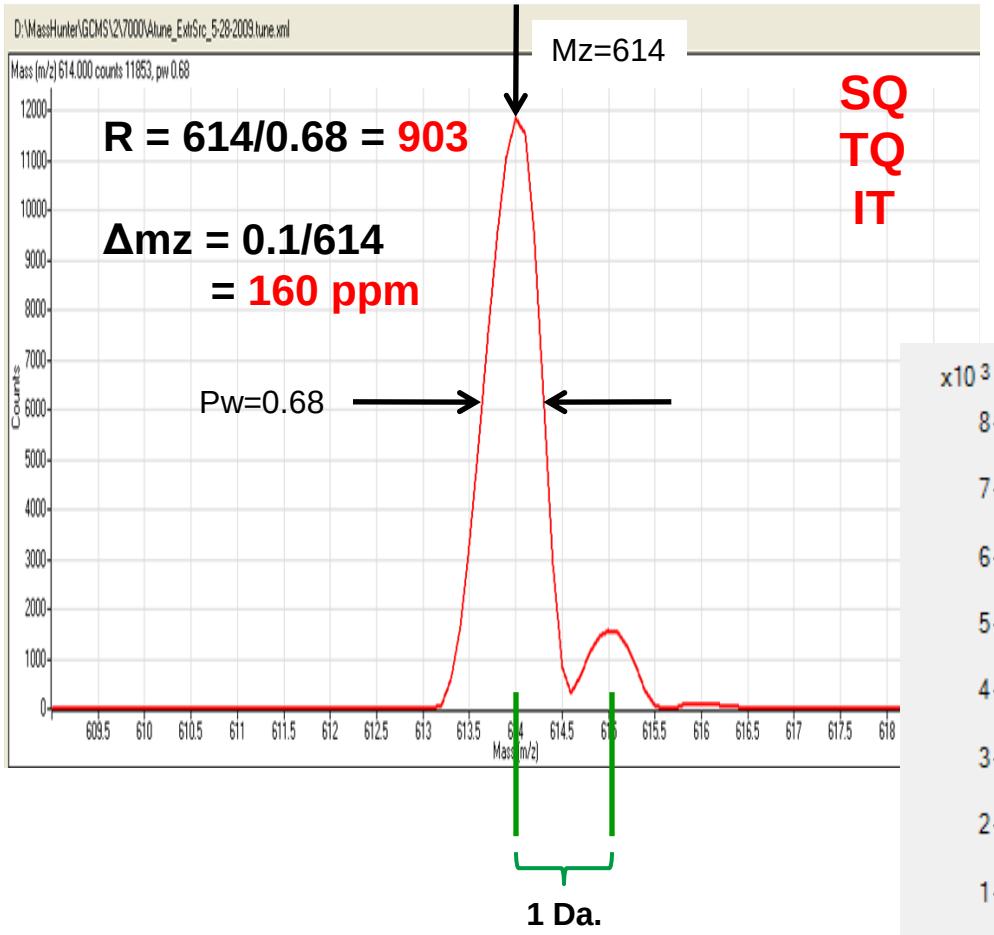


TOF has constant Resolving Power (peak-width changes with mass)

Quads operate with constant peak-width (Resolving Power changes with mass)



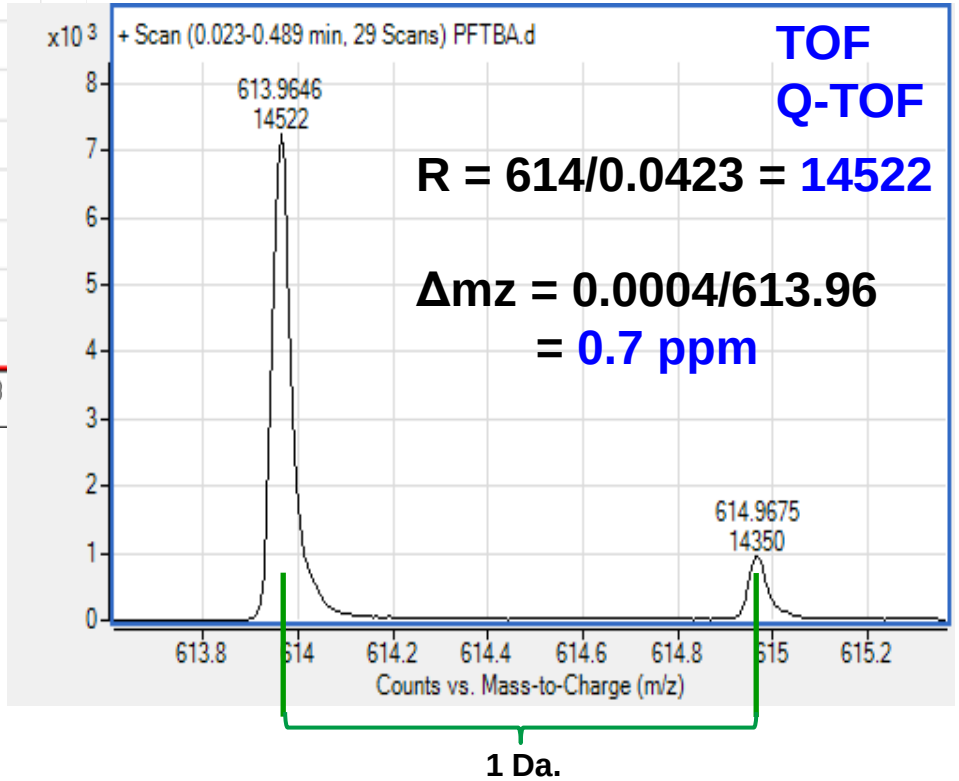
Resolving power & mass accuracy



Resolving Power:
R=mz/FWHM

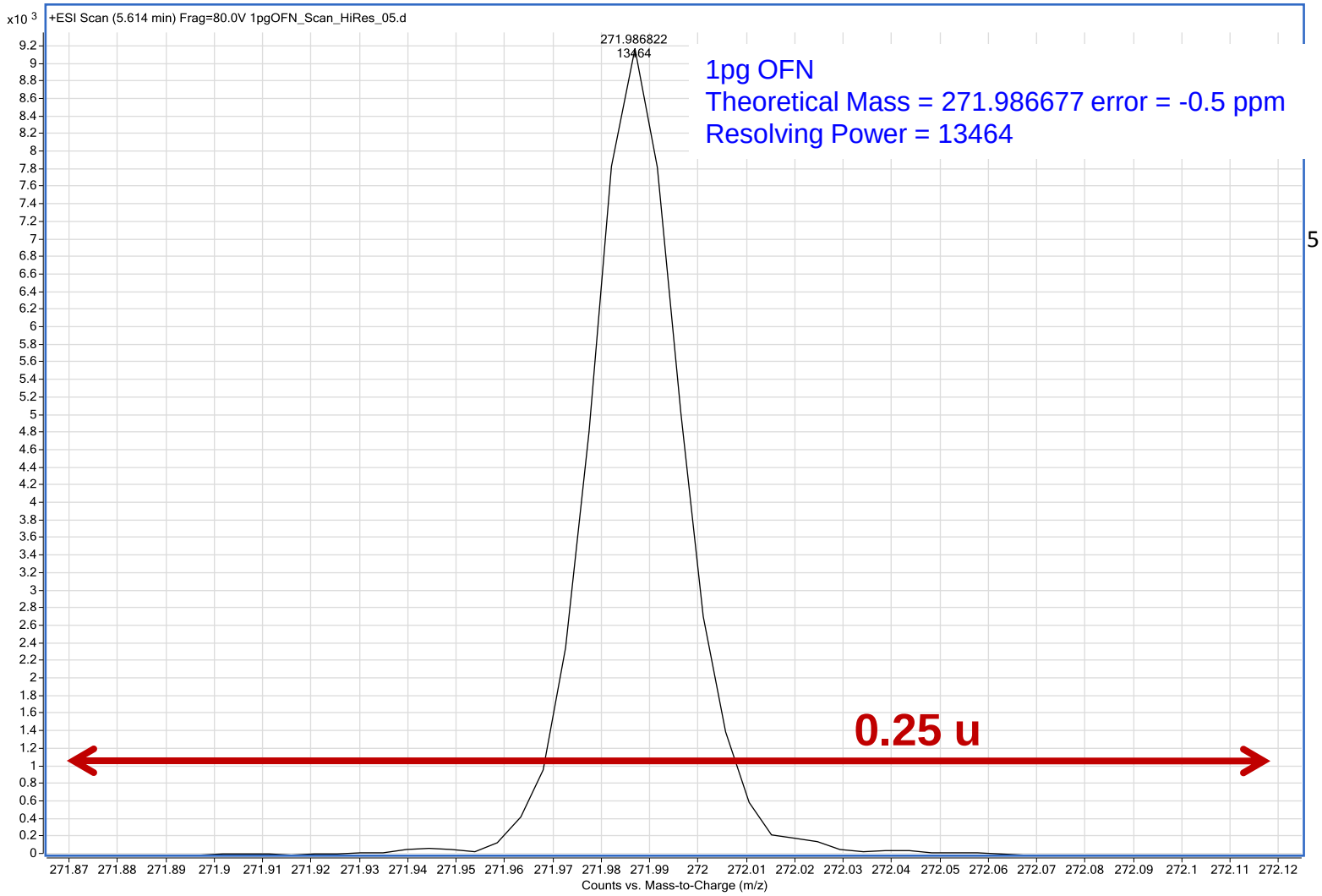
Mass Accuracy: $\Delta mz = dm/mz * 10^6$, parts per million (ppm)

PFTBA mass 614
C12F24N=613.964203

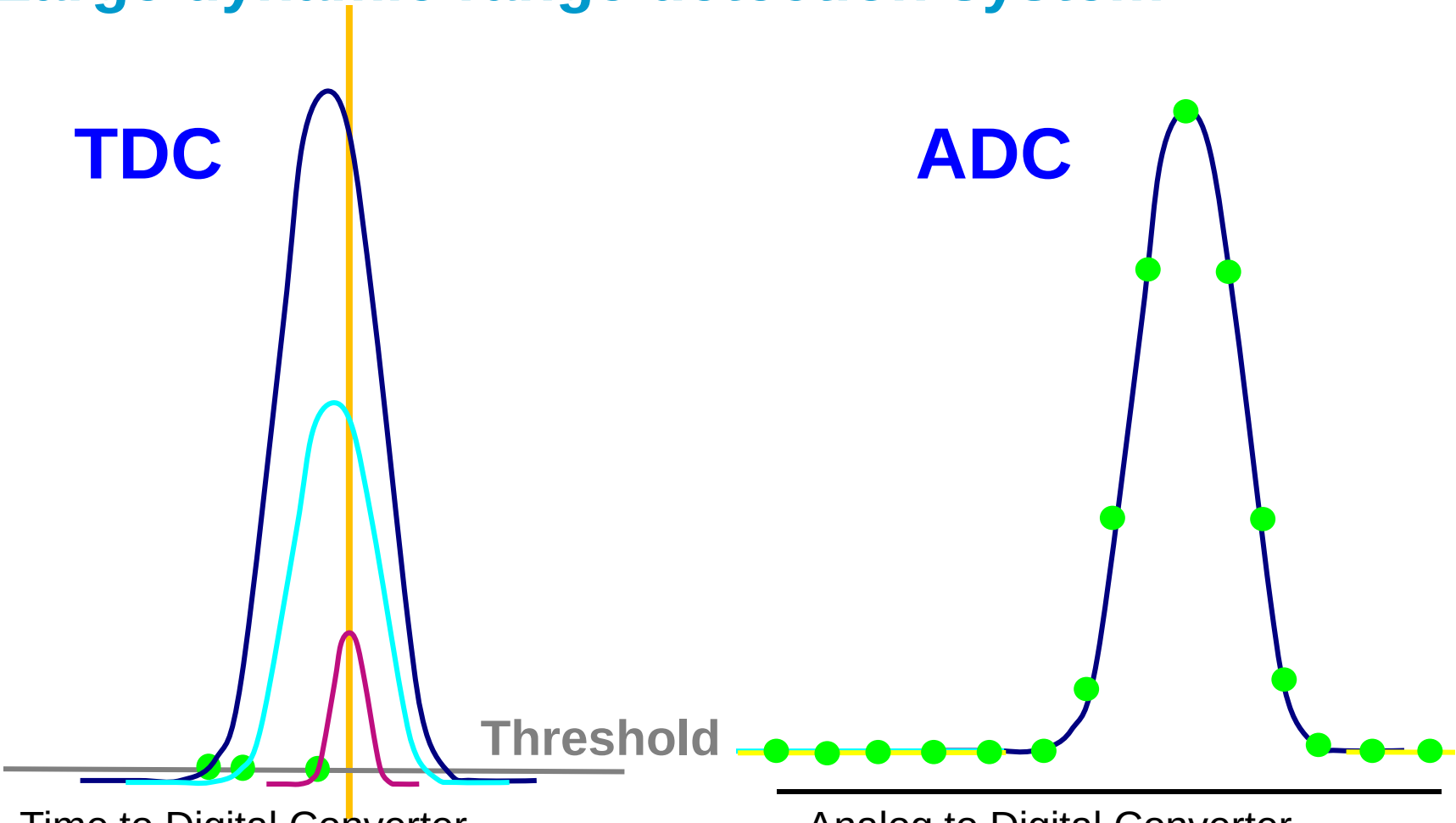


OFN Results

Later Prototype Q-TOF



Large dynamic range detection system

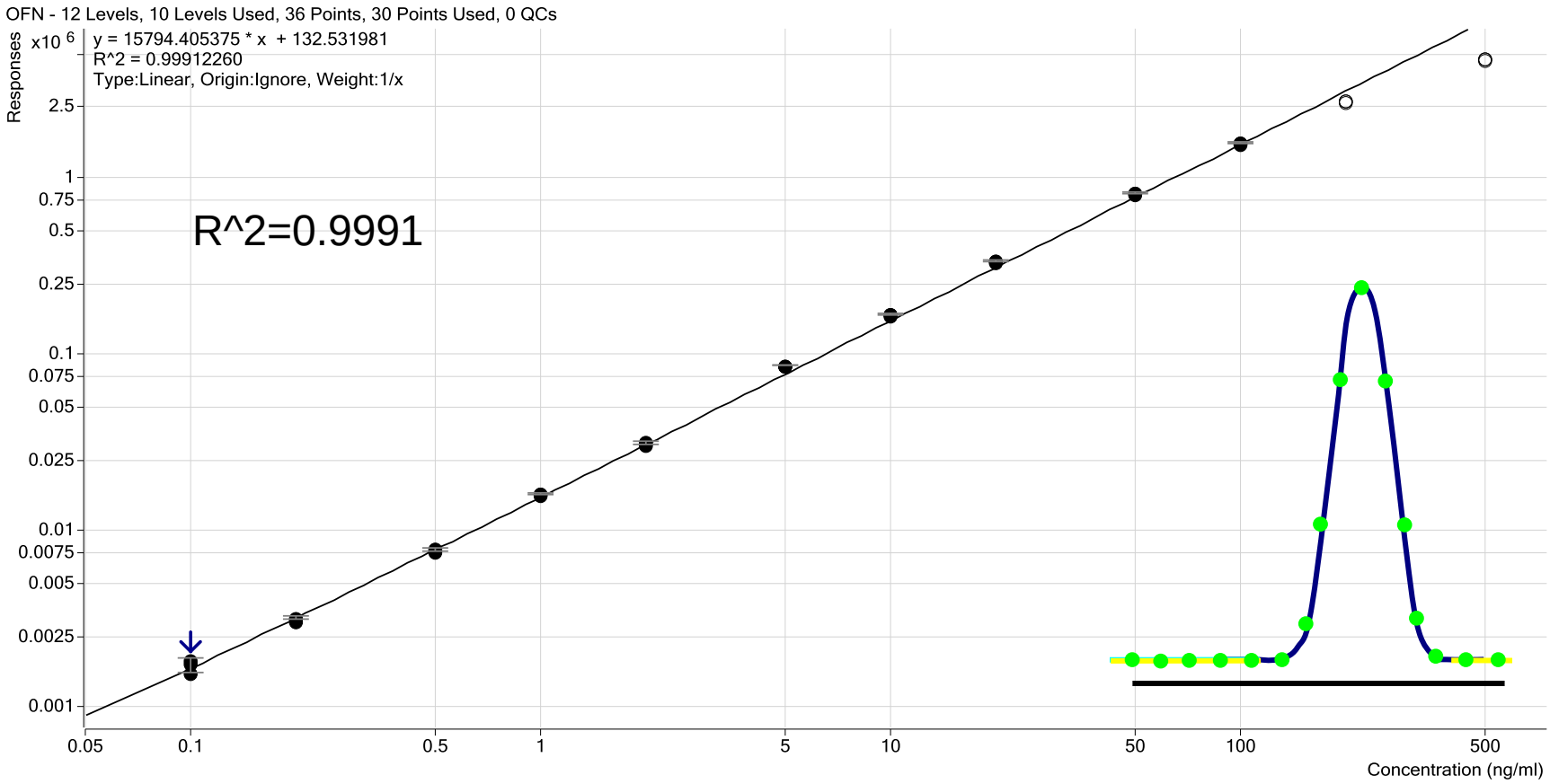


Time to Digital Converter
Counts “1” when above Threshold
1-2 Orders Magnitude Dynamic Range
2-8 Gbit/sec of information

Analog to Digital Converter
Measures each point
4-5 Orders Magnitude Dynamic Range
32 Gbit/sec of information

Response linearity and mass accuracy

ADC advantages



5 Hz acquisition, RIS

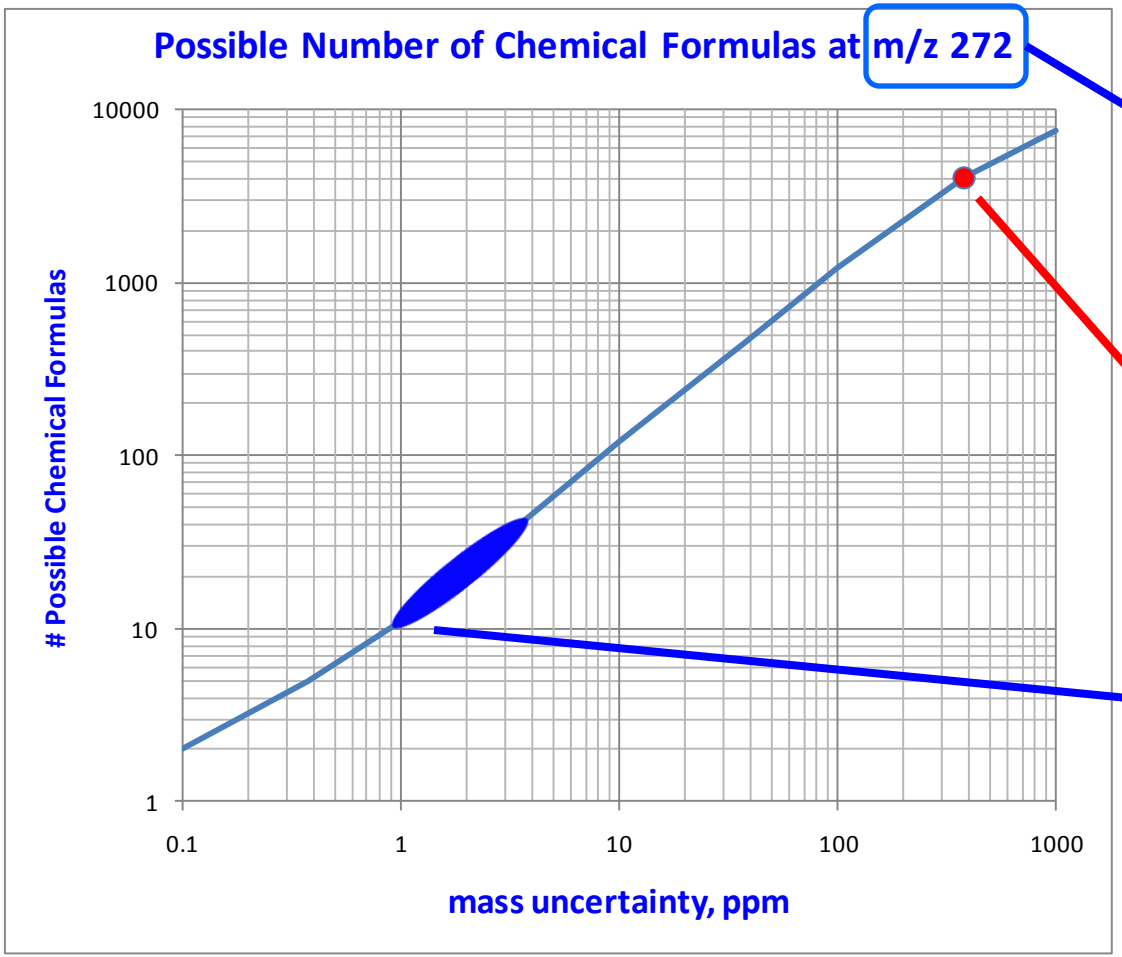
LOD about 0.01 pg

Accurate mass makes mass defect important

Type	Element	Symbol	Integer Mass	Exact Mass	Abundance	X+1 Factor	X+2 Factor	Mass Defect
X	Hydrogen	H	1	1.0078	99.99			0.0078
		D or ^{2}H	2	2.0141	0.01			0.0141
X+1	Carbon	^{12}C	12	12	98.91			0
		^{13}C	13	13.0034	1.1	$1.1n_C$	$0.0060n_C^2$	0.0034
X+1	Nitrogen	^{14}N	14	14.0031	99.6			0.0031
		^{15}N	15	15.0001	0.4	$0.37n_N$		0.0001
X+2	Oxygen	^{16}O	16	15.9949	99.76			-0.0051
		^{17}O	17	16.9991	0.04	$0.04n_O$		-0.0009
		^{18}O	18	17.9992	0.2		$0.20n_O$	-0.0008
X	Fluorine	F	19	18.9984	100			-0.0016
X+2	Silicon	^{28}Si	28	27.9769	92.2			-0.0231
		^{29}Si	29	28.9765	4.7	$5.1n_{Si}$		-0.0235
		^{30}Si	30	29.9738	3.1		$3.4n_{Si}$	-0.0262
X	Phosphorus	P	31	30.9738	100			-0.0262
X+2	Sulfur	^{32}S	32	31.9721	95.02			-0.0279
		^{33}S	33	32.9715	0.76	$0.8n_S$		-0.0285
		^{34}S	34	33.9679	4.22		$4.4n_S$	-0.0321
X+2	Chlorine	^{35}Cl	35	34.9689	75.77			-0.0311
		^{37}Cl	37	36.9659	24.23	$32.5n_{Cl}$		-0.0341
X+2	Bromine	^{79}Br	79	78.9183	50.5			-0.0817
		^{81}Br	81	80.9163	49.5		$98.0n_{Br}$	-0.0837
X	Iodine	I	127	126.9045	100			-0.0955

Many possible formulas with an MSD or IT

But only a few with TOF



Octafluoronaphthalene (CAS 313-72-4)

$C_{10}F_8$ = 271.98667

mass uncertainty		# of Possible Formulas
ppm	amu	
1000	0.3	7657
368	0.1	4050
100	0.03	1223
37	0.01	466
10	0.003	120
4	0.001	43
1	0.0003	11
0.4	0.0001	5
0.1	0.00003	2

Formulas made of: C,H,N,O,F, & Cl

Accurate mass reduces risk of investing effort on the wrong molecule

Internal Reference Mass (IRM)

- The goal for the 7200 is for easy and reliable ~2-5ppm mass accuracy under all conditions
  - Agilent has developed a proprietary Internal Reference Mass (IRM) delivery system for “on the fly” mass axis correction
    - IRM is the use of known background ions to “lock” the mass axis for each scan
    - Requires reliable IRM calibration signals with and without matrix

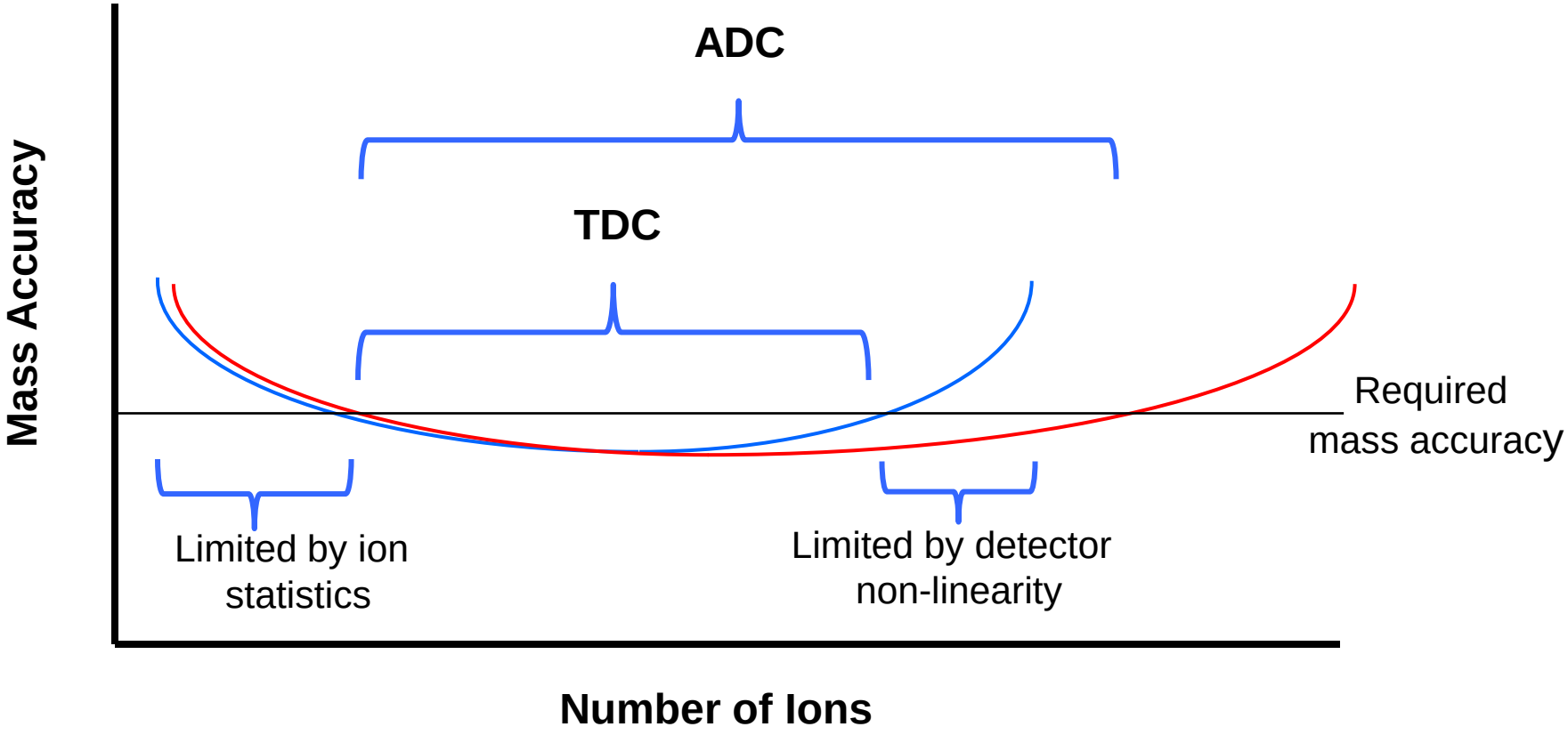
7200 provisional instrument performance

Specifications…

- Resolving Power: >10K at m/z 272 (>13K typical)
- Mass Accuracy: <5 ppm at m/z 272 (<2ppm typical)
- MS Sensitivity: 1 pg OFN S/N > 400:1
- Dynamic Range: > 3 orders of magnitude
- Quad Mass range: 20-1050 Da (0.7-4.0 Da FWHM)
- TOF Mass range: 20-1700 Da
- Spectral Rate: 1-50 spectra/sec

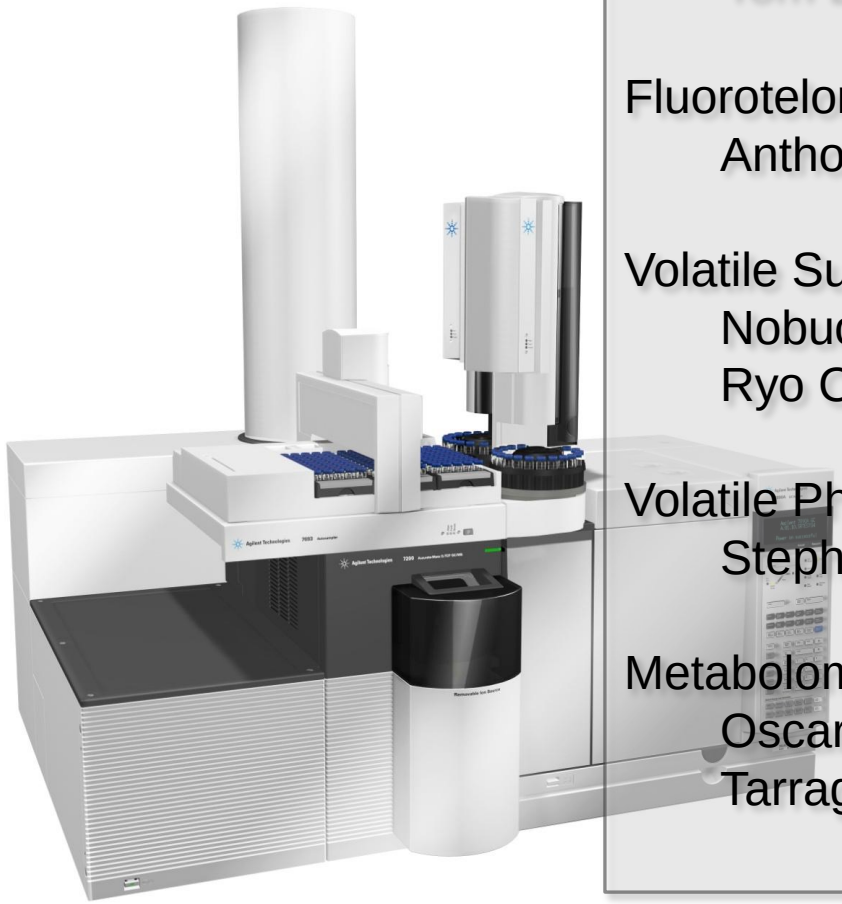
All specifications subject to change

Mass accuracy



7200 Series Q-TOF for GC/MS

How is this new capability used - application results



Pesticides in Food

Tom Doherty, Phil Wylie, Chris Sandy, Bill Russ

Fluorotelomer Alcohols in Biosolids (PCI)

Anthony Macherone

Volatile Sulfur-containing Compounds in Beverages

Nobuo Ochiai, Kikuo Sasamoto – Gerstel KK, Japan

Ryo Ogasawara, Hajime Kawakami – Agilent

Volatile Photodegradation Products in Beer

Stephan Baumann

Metabolomics

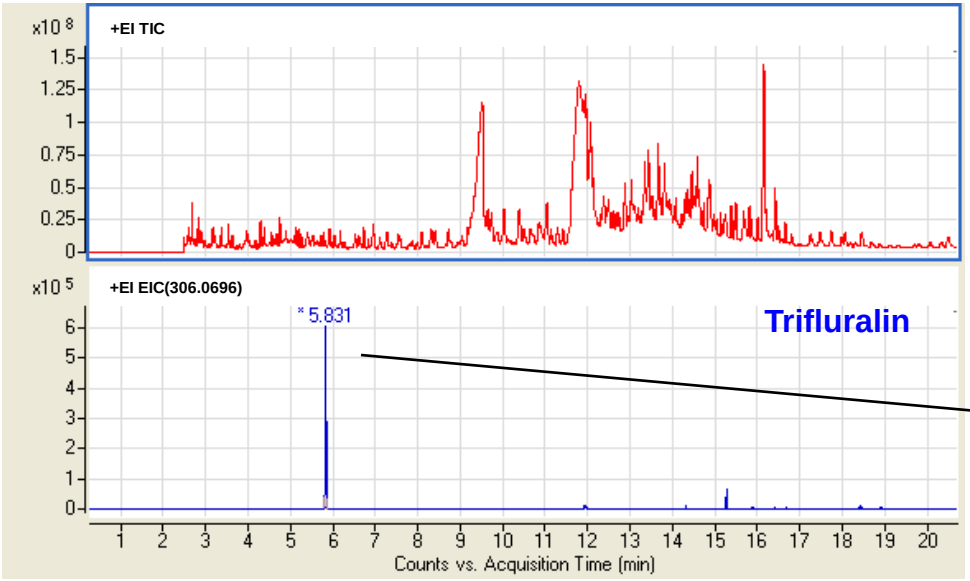
Oscar Yanes, Maria Vinaixa, Jesus Breznes – Tarragona University, Spain

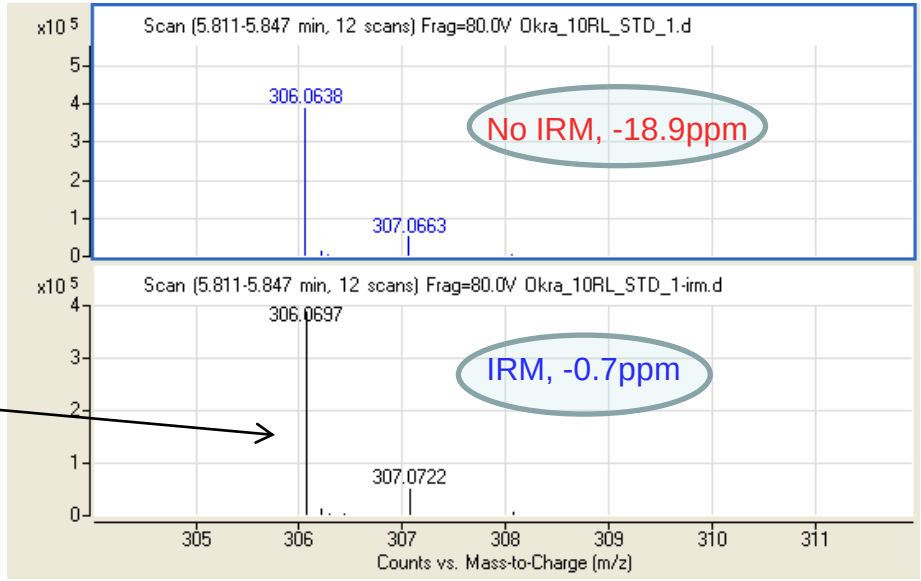
Pesticides in Food

Internal reference mass correction in matrix

100ppb pesticides in Okra extract

			Measured Accurate Mass (Da)		Mass Error, ppm	
Analyte	RT	Theoretical Mass	No IRM	With IRM	No IRM	With IRM
Trifluralin	5.83	306.0696	306.0638	306.0698	-18.9	0.7
Ethion	13.03	230.9732	230.9689	230.9744	-18.6	5.2
Iprodione	14.26	314.0094	314.0030	314.0101	-20.4	2.2
Indoxacarb	18.06	527.0702	527.0603	527.0730	-18.8	5.3

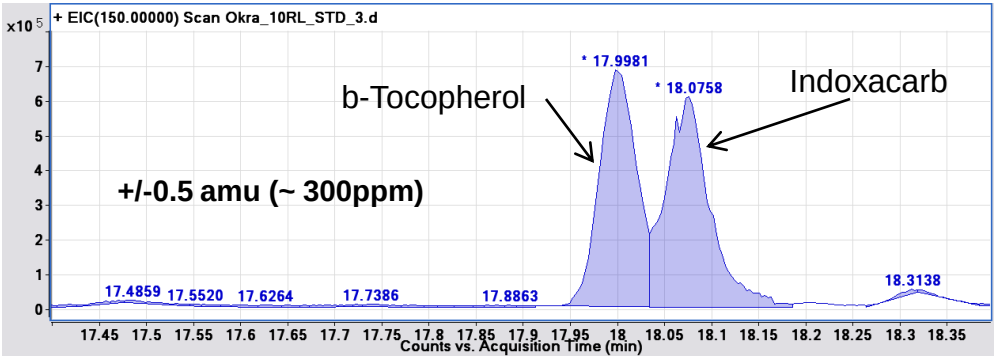


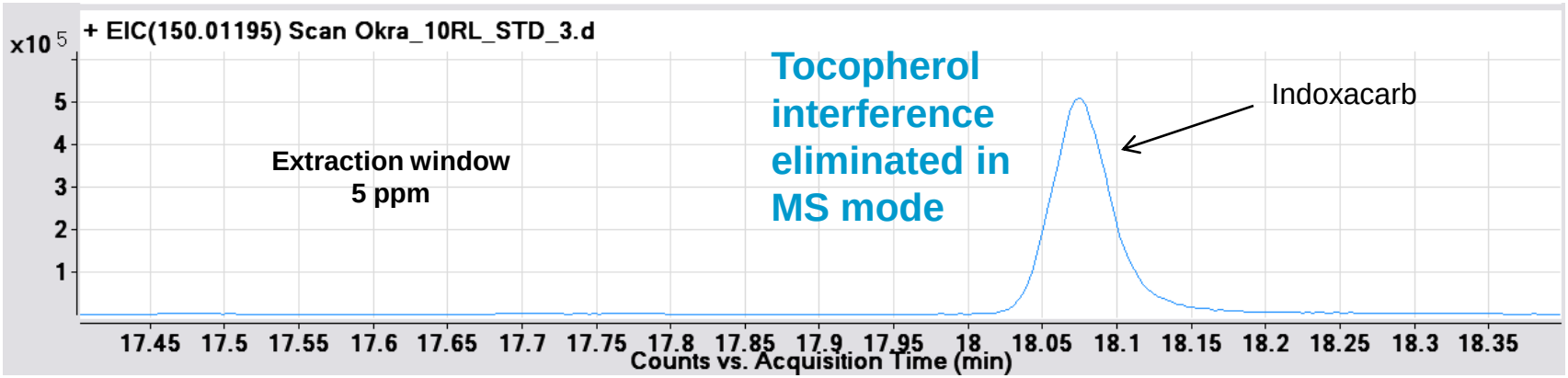


TOF Accurate Mass to Eliminate Matrix Interferants

Okra QuEChERS Extract
Matrix interferant ion (b-Tocopherol)
150.06839 Da
Analyte Indoxacarb ion (100pg)
150.01195 Da (fragment ion)

Δm = 0.0564 Da.

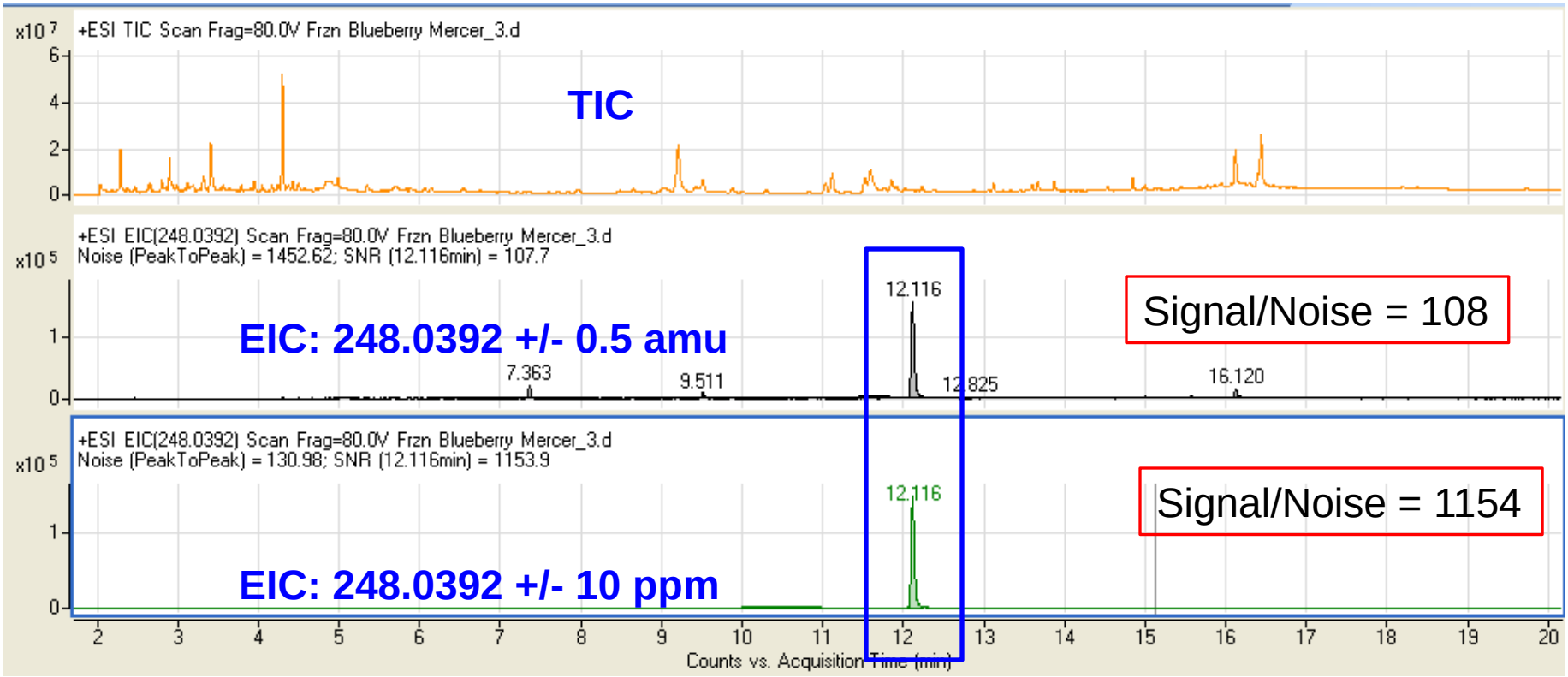




If even more selectivity is needed, option of MS/MS
MS/MS with high resolution and accurate mass!

Fludioxonil in Frozen Blueberry Extract

38 ppb in extract



Why add ‘Q’ to TOF to make Q-TOF?

Add ‘Q+CID’ to TOF solution

Sometimes the combined power of

GC Resolution (Agilent)

+

MS Resolving Power (Agilent)

Is not enough based upon:

Small ΔMass Defect (Nature)

+

Intense Matrix Ions (Sample)

High resolution MS/MS can solve some of these problems

How is it used?

Structure elucidation

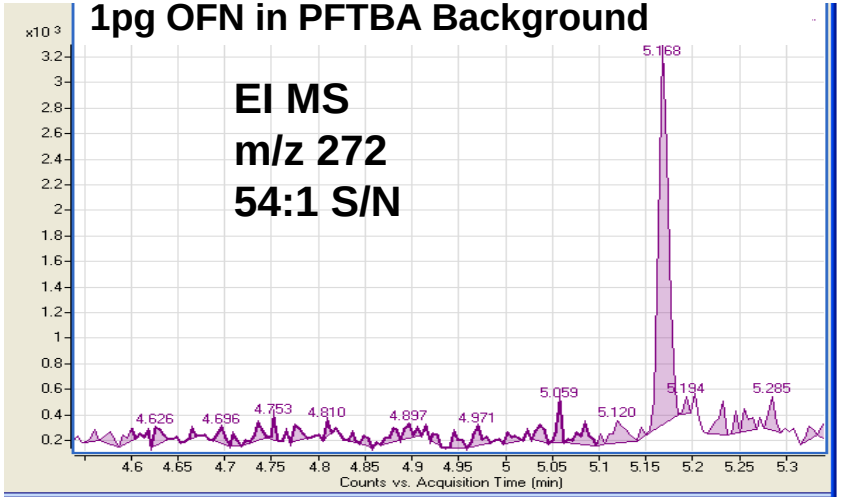
- Structural Elucidation from product Ion spectra using high resolution and accurate mass
- Start with full scan EI spectrum
- Use CID on each fragment mass to confirm structure of fragment
  - Select Fragment 1 to be precursor 1 $\xrightarrow{\text{CID}}$ Product ions
  - Select Fragment 2 to be precursor 2 $\xrightarrow{\text{CID}}$ Product ions

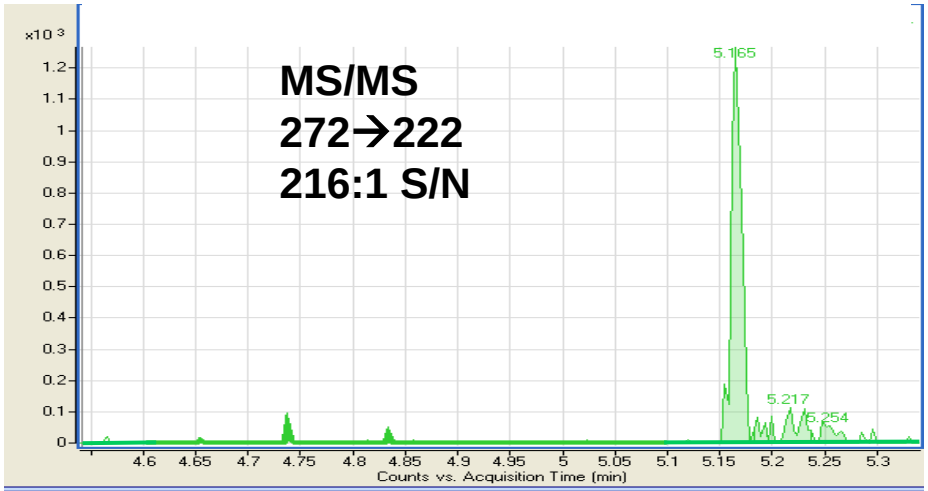
Precursor-product ion relationship is documented and ion molecular formula confirmed by accurate mass

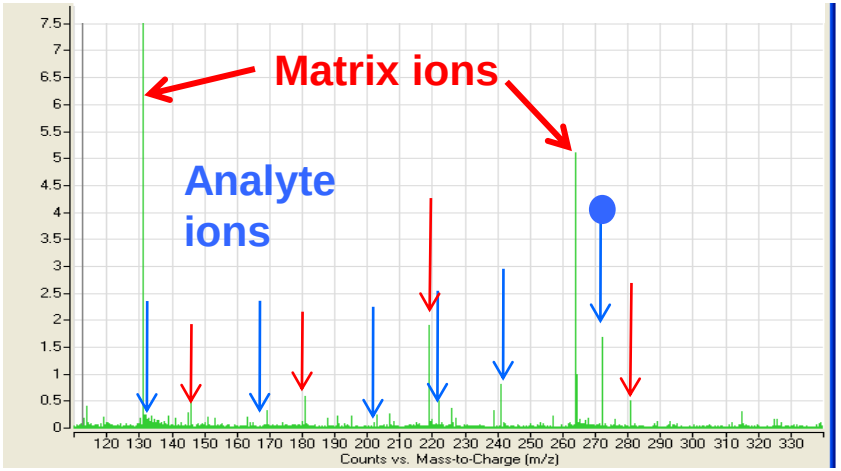
Requires multiple analyses and much more sensitive than NMR Will not replace NMR, but will complement nicely

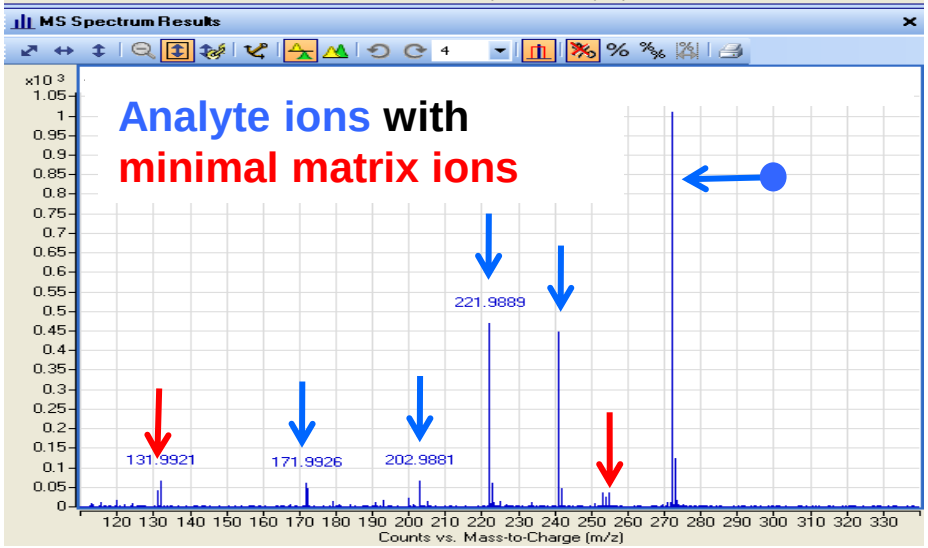
MS/MS chemical noise reduction

If resolution and accurate mass are not enough





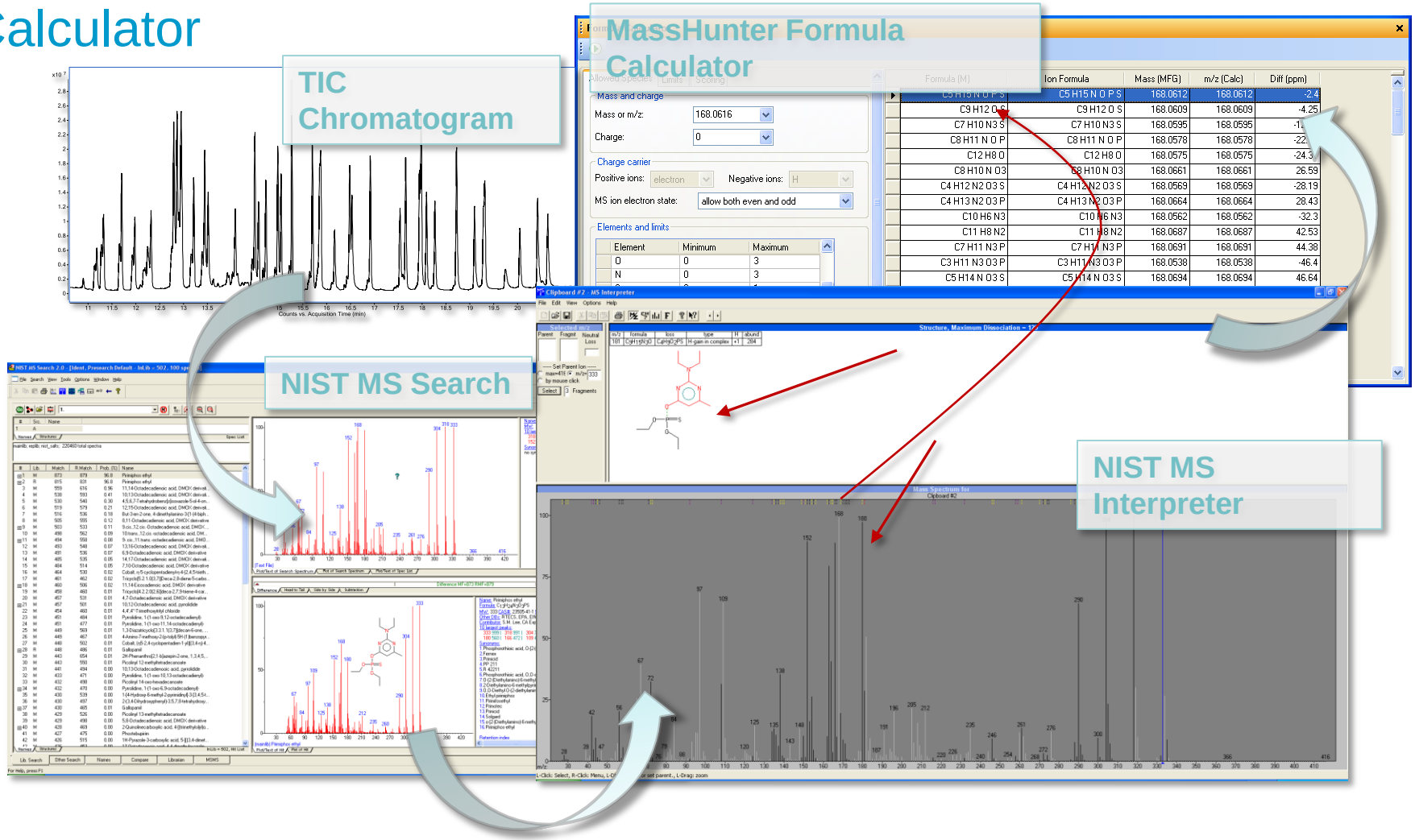




Agilent Technologies

Accurate Mass Library Workflow

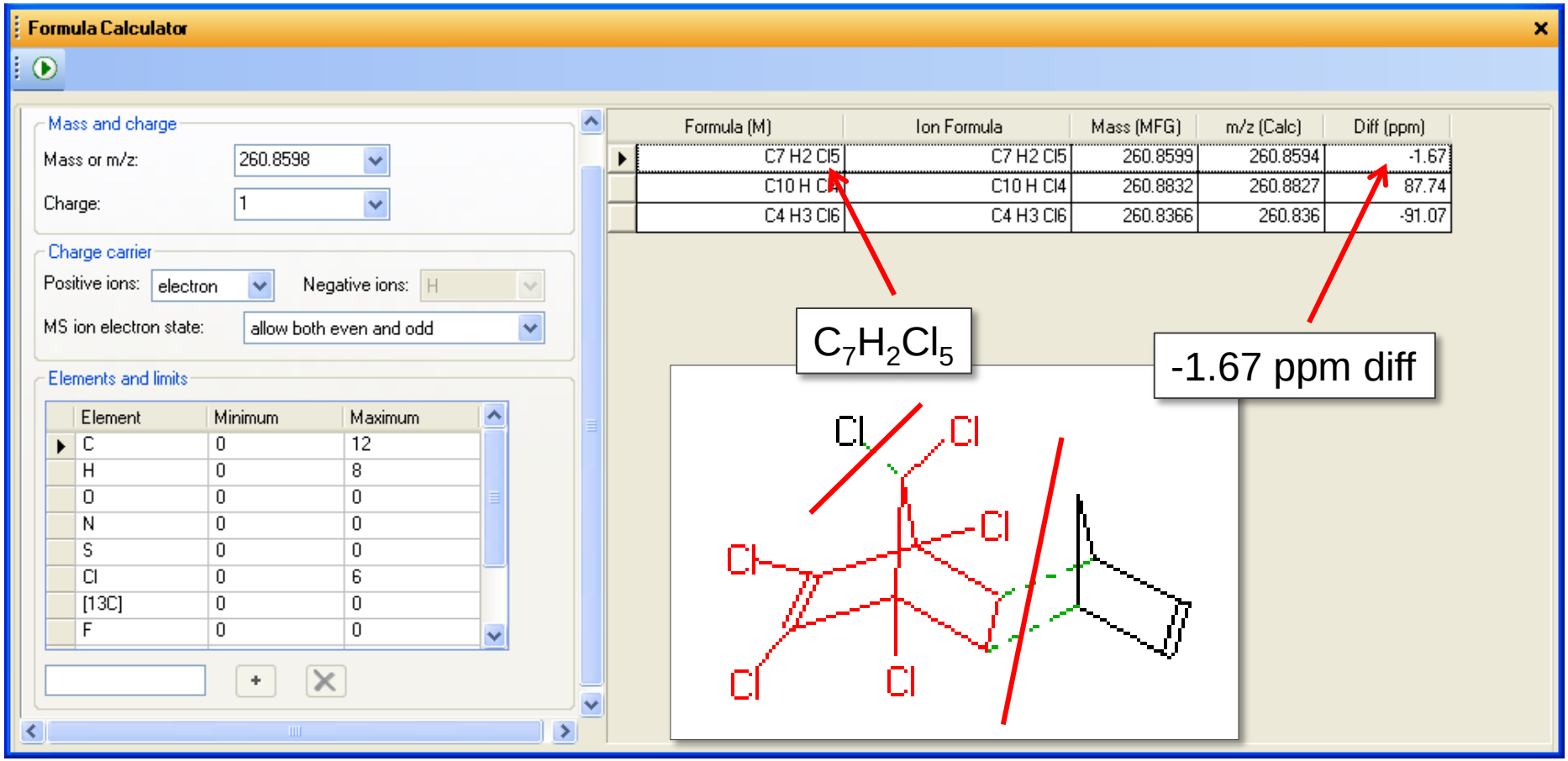
Using NIST MS Interpreter and MassHunter Qual Formula Calculator



Agilent Technologies

Formula Calculator

Determine all possible formulas consistent with measured mass



Fragment ion mass with high mass accuracy

Helps unambiguously identify corresponding formula and hence exact mass of a fragment

Most probable fragment ion

	Molecular Ion		Fragment Ions							
			1		2		3		4	
Pesticide	**m/z**	**Formula**	**Δ ppm**	**Formula**	**Δ ppm**	**Formula**	**Δ ppm**	**Formula**	**Δ ppm**	**Formula**
Chlorpyrifos-methyl	320.8944	C7H7Cl3NO3PS	-0.7	**C7 H7 Cl [37Cl] N O3 P S**	0.0	C7 H7 Cl2 N O3 P S	0.0	C2 H6 O2 P S		
			215.4	**C6 H2 Cl3 N O2 P S**						
Dichlorvos	219.9454	C4H7Cl2O4P	1.6	C4H7ClO4P	-0.9	C2H6O3P	3.7	**C4 H7[37Cl] O4 P**		
							336.5	**C3 H2 Cl2 O3 P**		
Endosulfan sulfate	419.8112	C9 H6 Cl6 O4 S	-2.1	C9 H6 Cl4[37Cl] O4 S	-0.7	C5 Cl5[37Cl]	0.0	C5 Cl4[37Cl]2		
							-220.9	**C8 H3 Cl5**		
Propachlor	211.0758	C11 H14 Cl N O	-1.0	C10 H11 Cl N O	1.1	C11 H14 N O	1.8	**C8 H8 Cl N O**	-3.9	C6 H5
									771.6	**C2 H2 Cl O**
Fluazifop-p-butyl	383.1339	C19 H20 F3 N O4	-2.2	C19 H20 F2 N O4	-1.1	C14 H11 F3 N O2	-1.3	C12 H7 F3 N O	2.1	**C6 H3 F3 N**
									-494.2	**C7 H14 O3**
Triazophos	313.0645	C12 H16 N3 O3 P S	-1.4	**C10 H12 N3 O3 P S**	-2.7	**C8 H8 N3 O3 P S**	-0.6	C8 H7 N3 O	-1.9	**C8 H8 N3 O**
			-47.7	**C11 H14 N2 O3 P S**	-54.1	**C9 H10 N2 O3 P S**				

Examples from building accurate mass pesticide library

Fluorotelomer Alcohols in Biosolids

Fluorotelomer Alcohols

- Source unknown, but probably intermediate degradation products of fluorinated polymers
- Oxidize to form fluorinated carboxylic acid, some of which are toxic
- Methods needed for studying their transport and fate in the environment
- Have the form $F_3C(CF_2)_{N-1}(CH_2)_MOH$
- *N:M FTOH* is the shorthand notation
- Positive CI, 20% CH_4

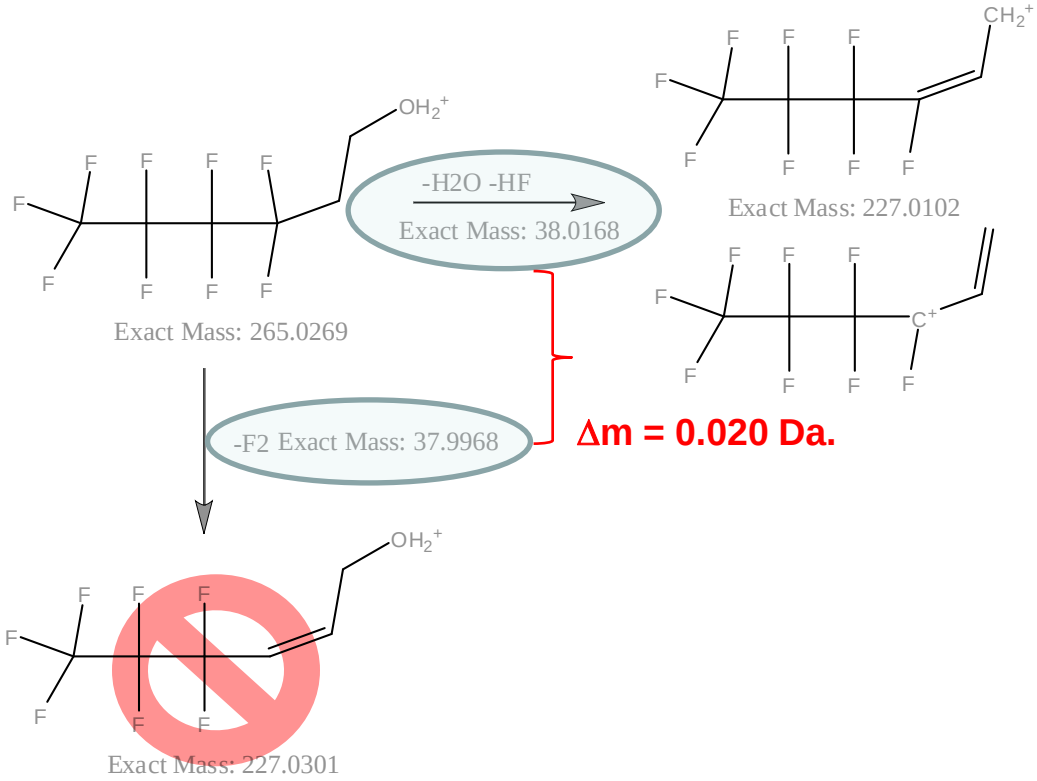
Fluorotelomer Alcohol Mass Accuracy

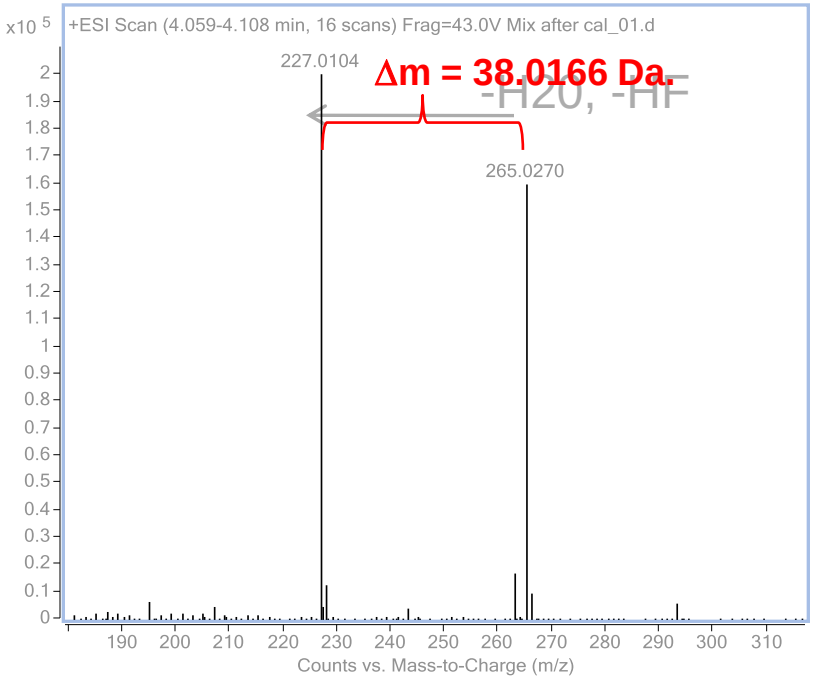
Protonated Molecular Ion (PCI)

Acronym	Formula	Exact Mass + H	Observed Mass	Δ ppm
4:2 FTOH	$C_6H_5F_9O$	265.0269	265.0270	-0.38
6:2 FTOH	$C_8H_5F_{13}O$	365.0206	365.0206	0
8:2 FTOH	$C_{10}H_5F_{17}O$	465.0142	465.0140	0.43
10:2 FTOH	$C_{12}H_5F_{21}O$	565.0078	565.0078	0
7:2 sFTOH	$C_9H_5F_{15}O$	415.0174	415.0190	-3.85
5:1 FTOH	$C_6H_3F_{11}O$	301.0081	301.0079	0.66
6:1 FTOH	$C_7H_3F_{13}O$	351.0049	351.0050	-0.28
7:1 FTOH	$C_8H_3F_{15}O$	401.0017	401.0016	0.25
8:1 FTOH	$C_9H_3F_{17}O$	450.9985	450.9985	0
9:1 FTOH	$C_{10}H_3F_{19}O$	500.9953	500.9956	-0.60
10:1 FTOH	$C_{11}H_3F_{21}O$	550.9921	550.9922	-0.18
11:1 FTOH	$C_{12}H_3F_{23}O$	600.9889	600.9896	-1.16
MeFOSE	$C_{11}H_8F_{17}NO_3S$	558.0026	558.0042	-2.87
EtFOSE	$C_{12}H_{10}F_{17}NO_3S$	572.0183	572.0167	2.80

Fluorotelomer Neutral Loss Mechanism Inferred

PCI, methane

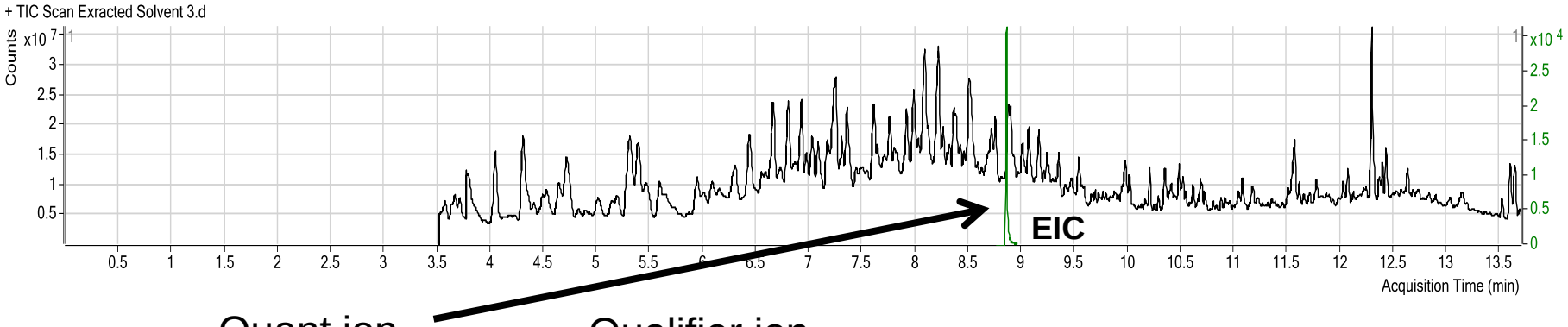




Acronym	Observed Base Peak m/z	Molecular ion -F_2 m/z	Δppm	Molecular ion -H_20, -HF m/z	Δppm
4:2 FTOH	227.0104	227.0301	86.77	227.0102	-0.88

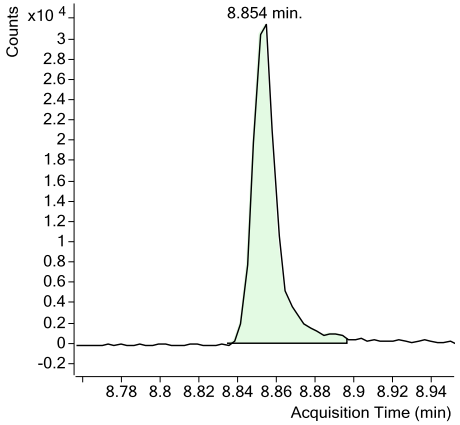
11:1 FTOH Spiked in Biosolid Extract

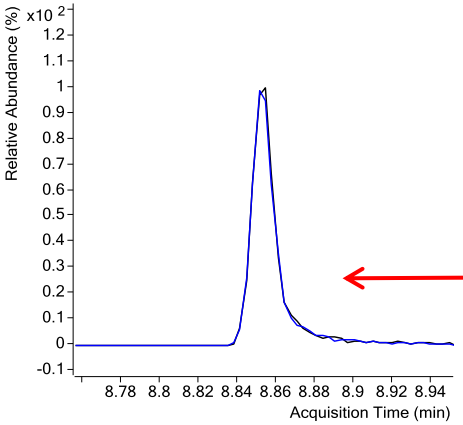
PCI, methane



Quant ion
m/z = 580.9784

Qualifier ion
m/z = 600.9845



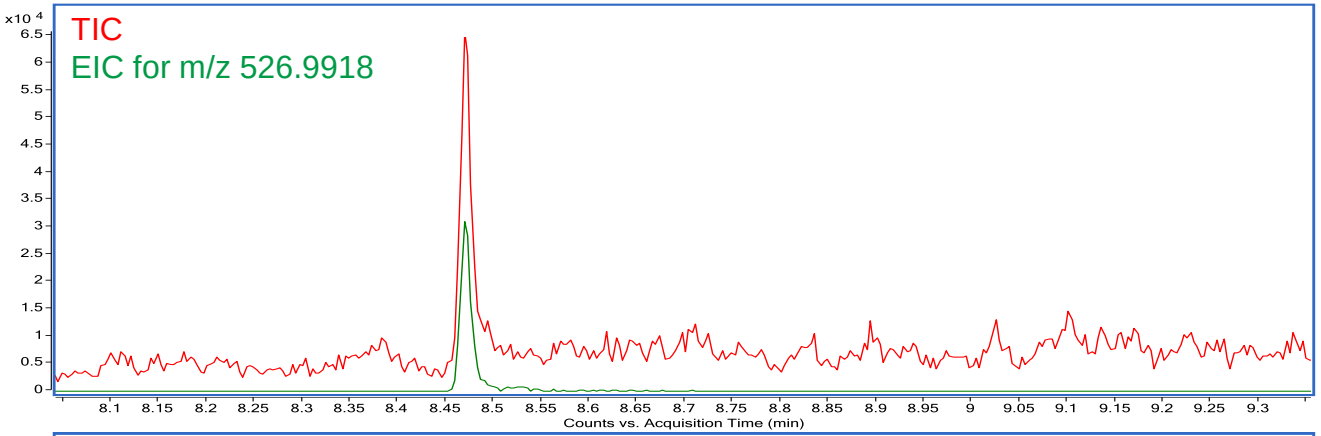


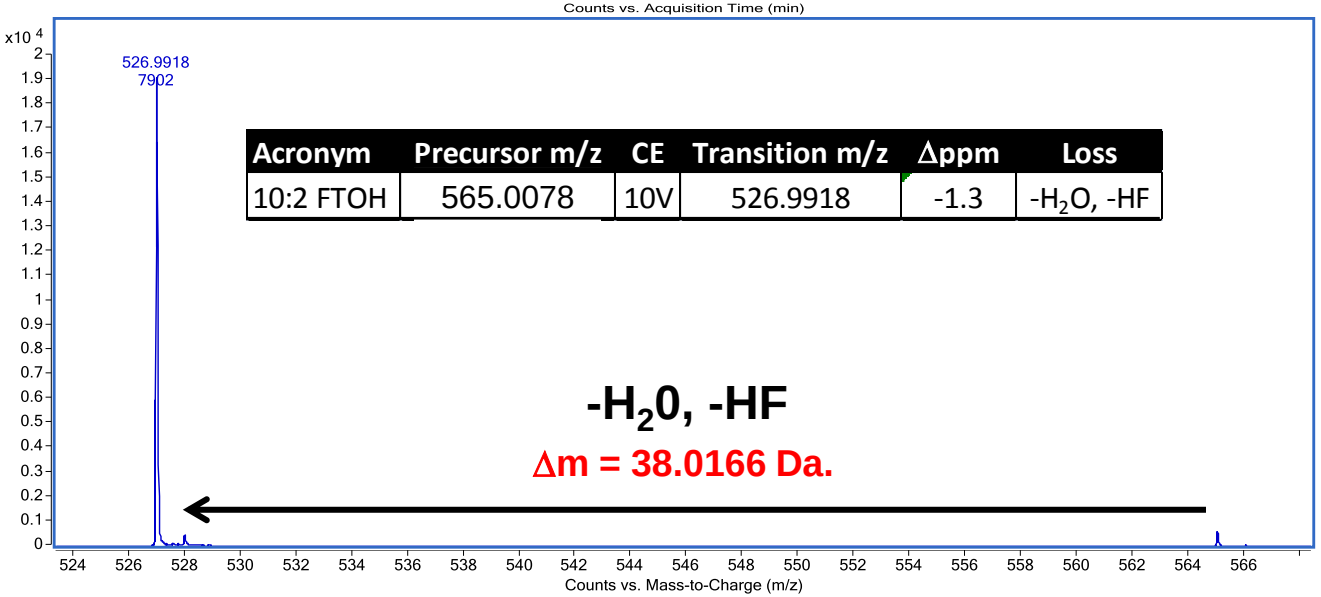
Spiked at 50 pg/ml level

Excellent qualifier ratio in the presence of nearly 10^3 excess of matrix. EIC of m/z=580.9784 overlaid on m/z=600.9845

10:2 FTOH Fluorotelomer Alcohol MS/MS

PCI, methane





Acronym	Precursor m/z	CE	Transition m/z	Δppm	Loss
10:2 FTOH	565.0078	10V	526.9918	-1.3	$-H_2O$, -HF

$-H_20$, -HF

Δm = 38.0166 Da.

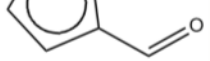
Identification and Quantification of Sulfur-Containing Compounds in Beverages

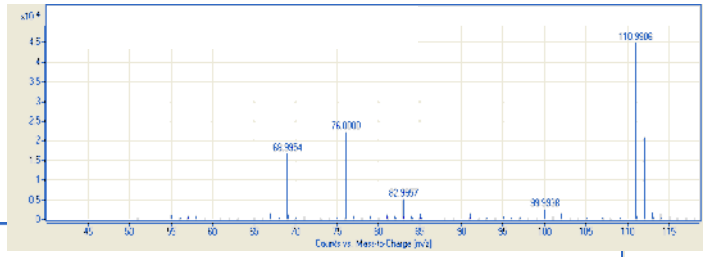
Compounds affecting taste and flavor

- 2-formyl thiophene and 2-acetyl thiazole are common contaminants
- Low sensory threshold and can have negative effect on product flavor or aroma
- Easy to separate from each other
- Often requires sophisticated extraction/enrichment procedures and/or powerful 2D GC techniques for separation from matrix for quantitation
- Method highlights
  - Simple L/L extraction in dichloromethane (10:1 enrichment)
  - 1:10 split injection with SSL inlet
  - DB-5MS column 30 m x 0.25 mm x 0.25 µm

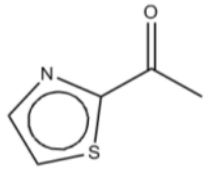
Standards at 100 pg On Column

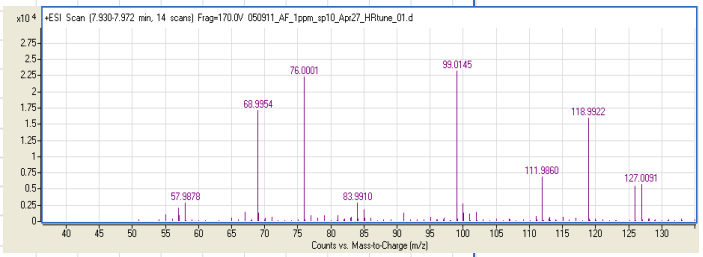
2-formyl thiophene
Formula C_5H_4OS
MW: 112



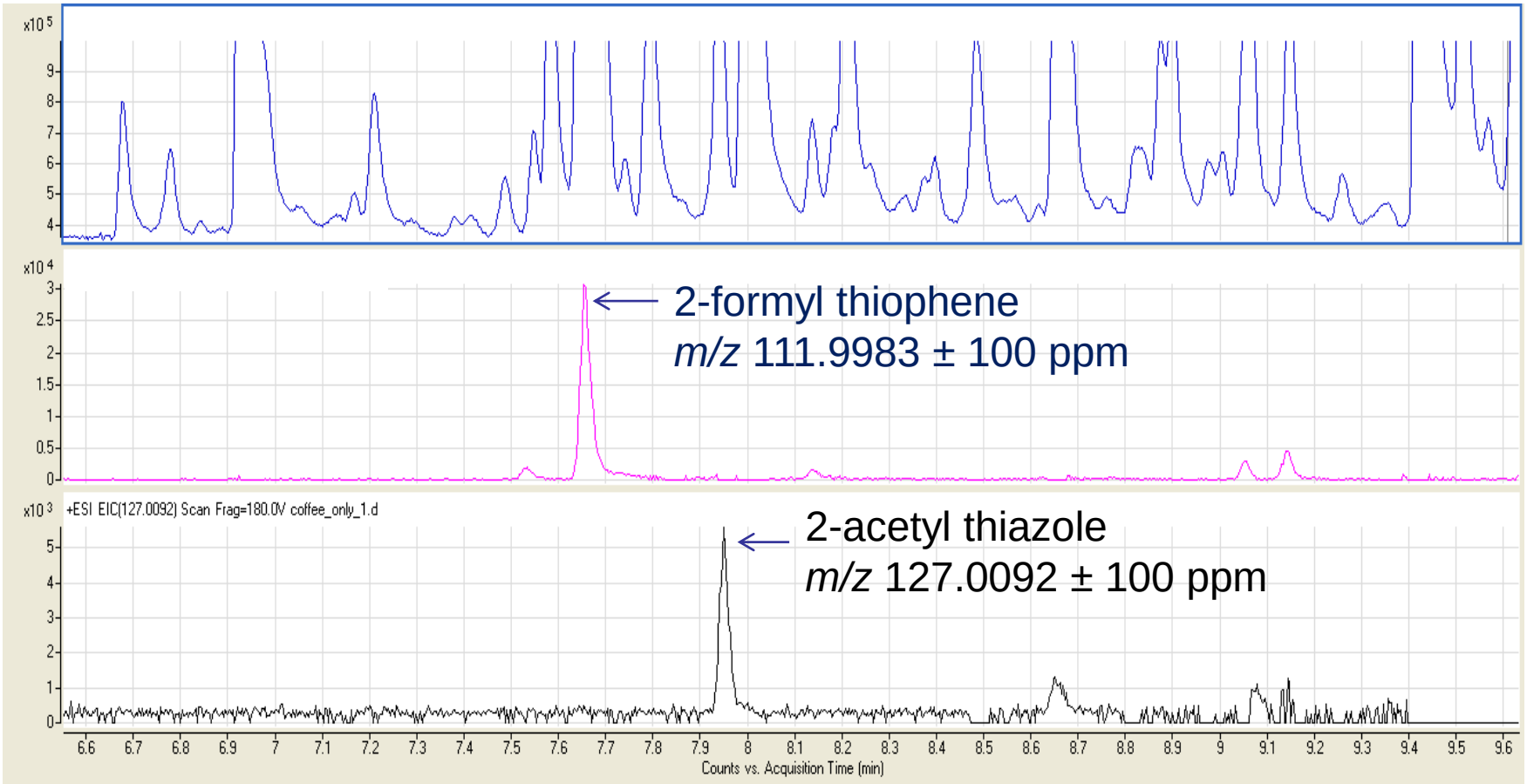


2-acetyl thiazole
Formula C_5H_5NO
MW: 127



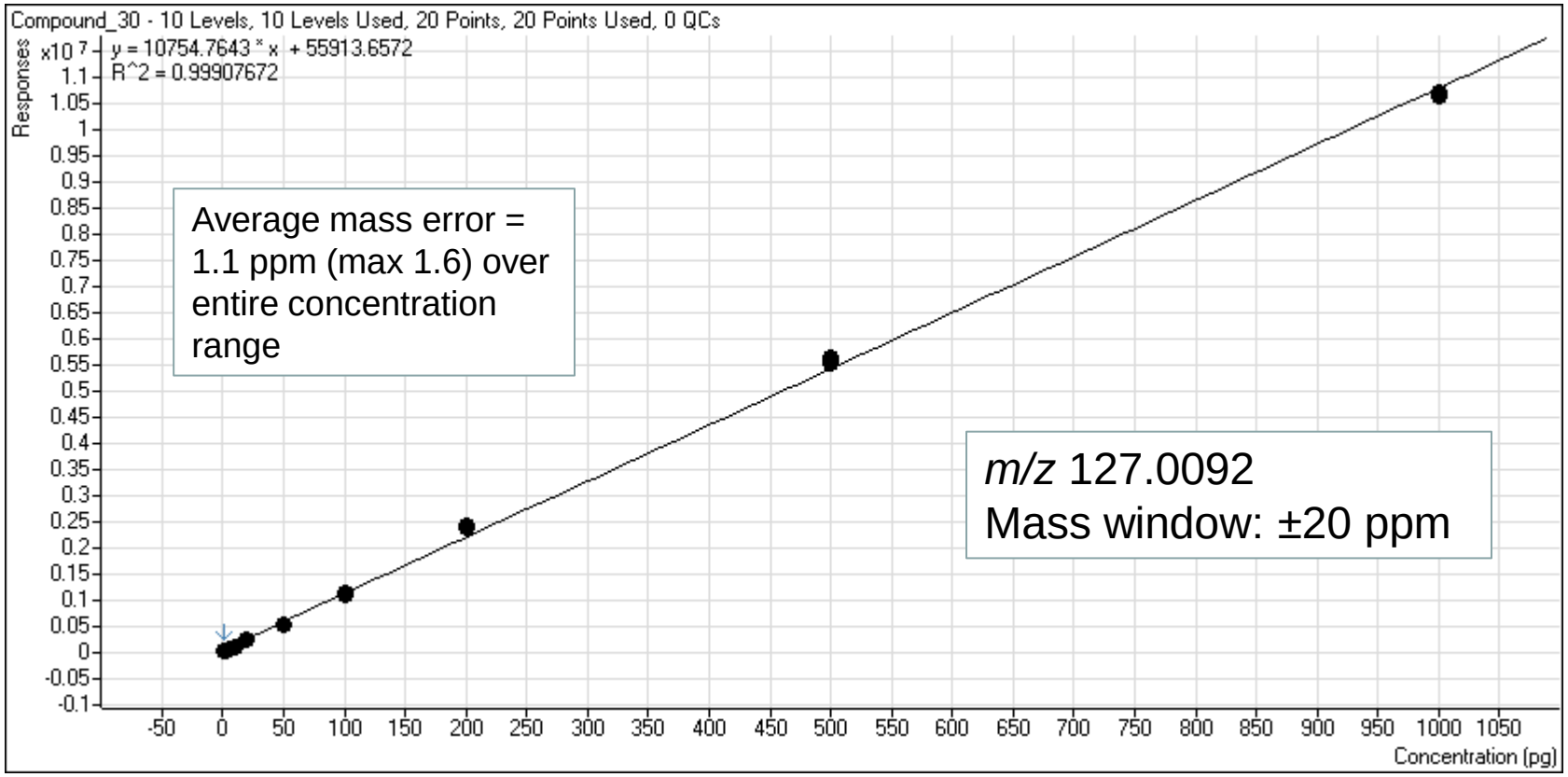


TIC and EICs of Coffee Extract



2-Acetyl Thiazole calibration

STD addition calibration curve for 2-acetyl thiazole in spiked coffee
(STD amount: 1, 2, 5, 10, 20, 50, 100, 200, 500, 1000 pg)



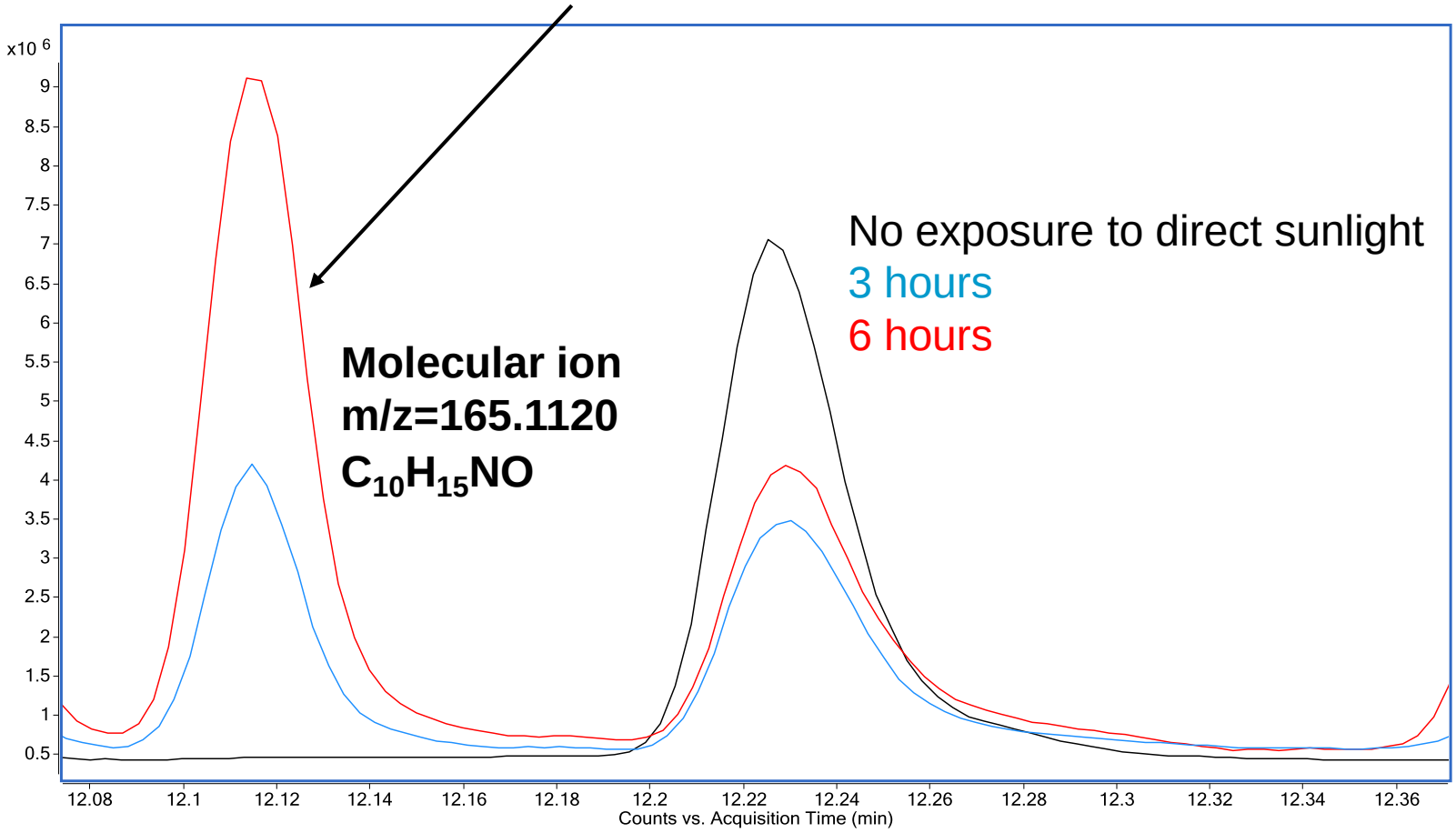
Photodegradation Products in Beer

Photodegradation Products in Beer

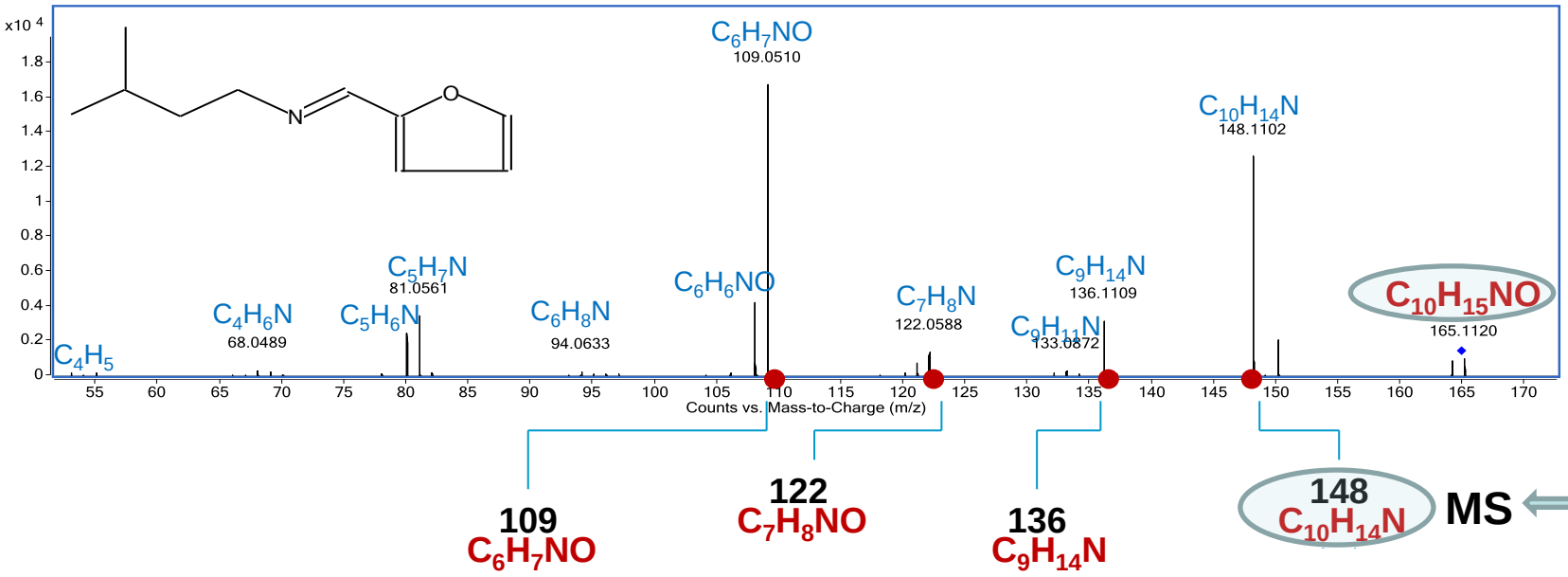
- Completely **untargeted** (initially) study of beer photodegradation
- Method highlights
  - 30 min extraction at 30 ˚C using manual SPME holder and conditioned 50/30 µm DVB/Carboxen/PDMS StableFlex SPME fiber (Supelco), no agitation
  - Desorption at 300 ˚C for 2 min in the SSL injector; 1:10 split
  - Agilent J&W column DB-5MS 30 m x 0.25 mm x 0.25 µm

Changes in the Chromatogram

Appears following the exposure of the sample to direct sunlight. Peak height is dependent on the duration of exposure to the sun



Summary of MS/MS Experiments



109
C_6H_7NO

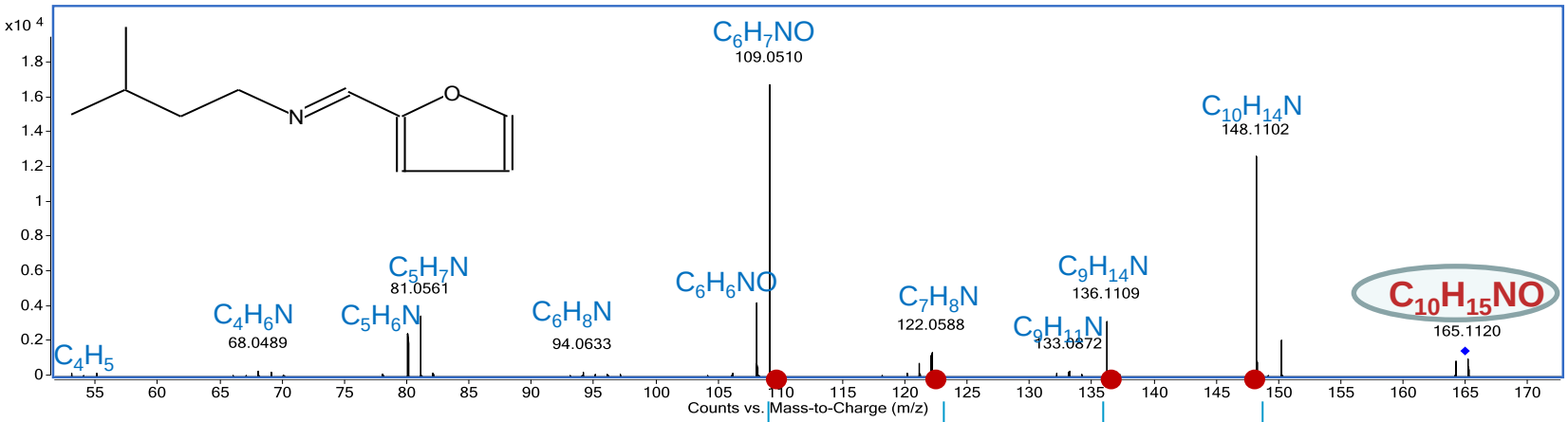
122
C_7H_8NO

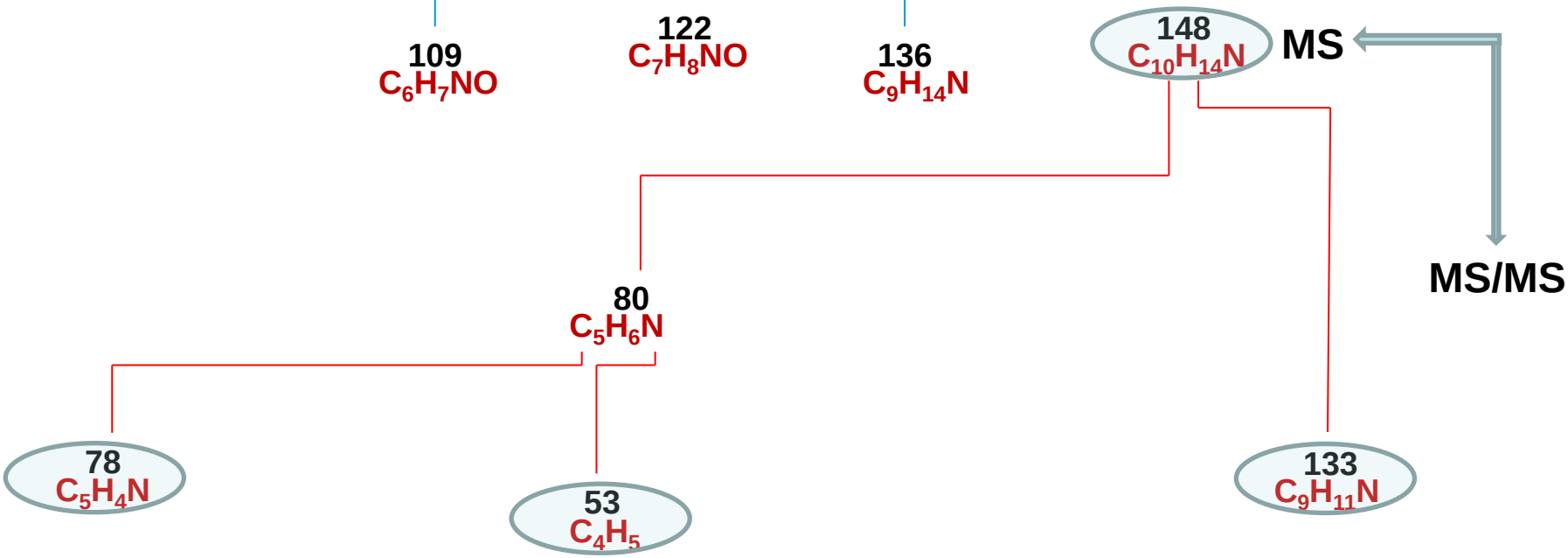
136
$C_9H_{14}N$

148
$C_{10}H_{14}N$

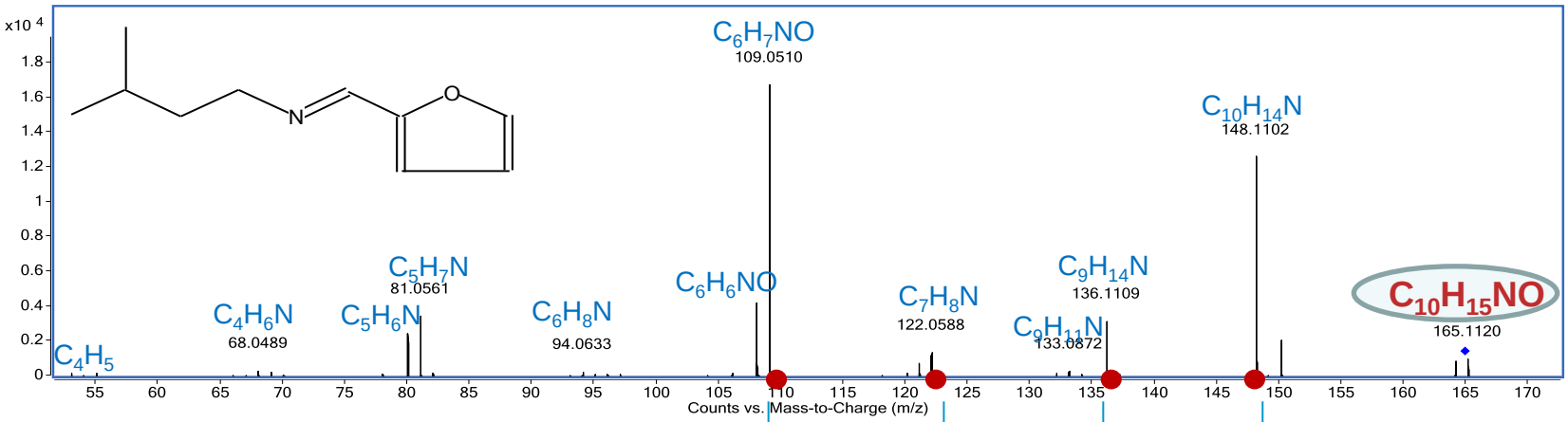
MS

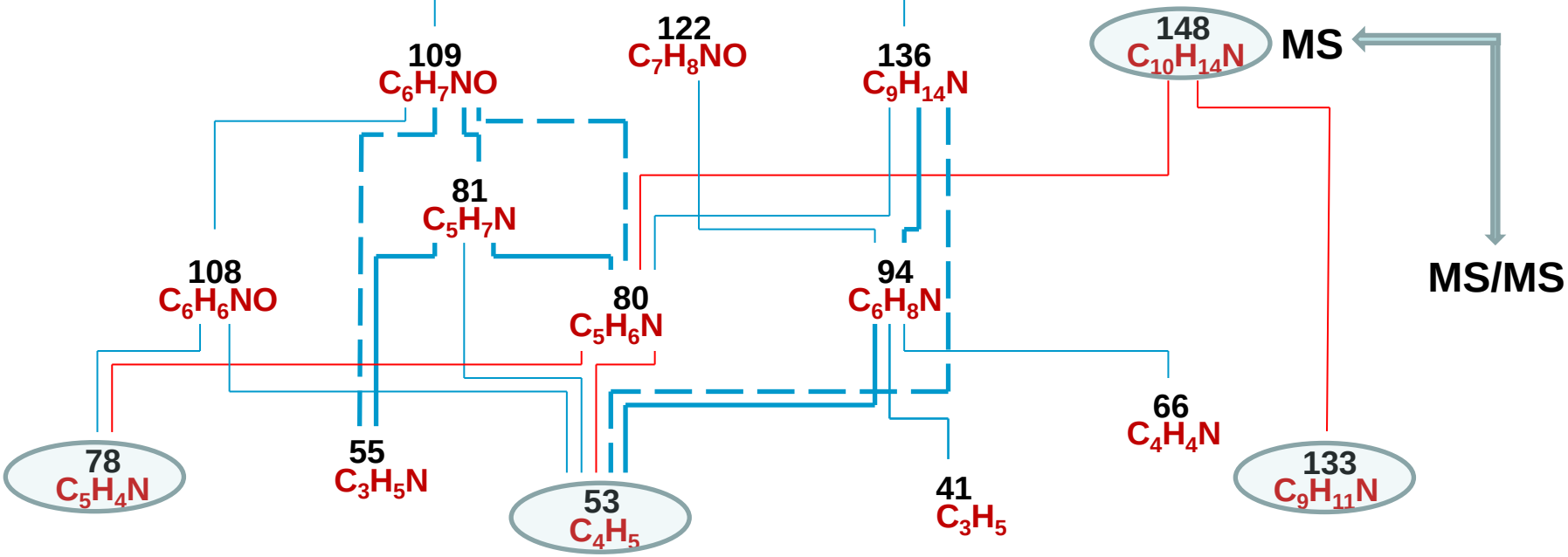
Summary of MS/MS Experiments





Summary of MS/MS Experiments

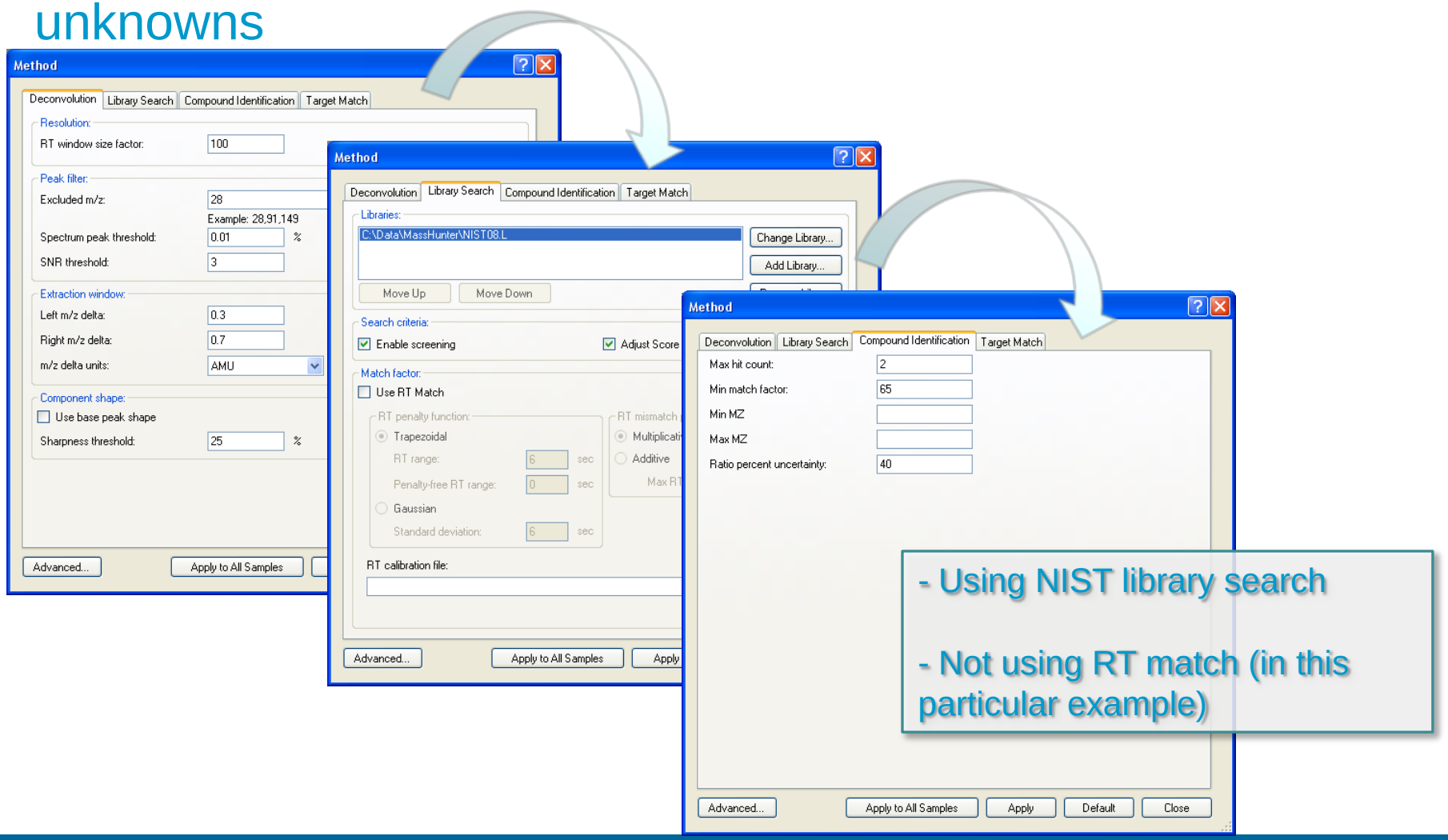




Metabolomics: Unknowns Analysis Tool to Identify Components of Bovine Plasma

Unknowns Analysis (MassHunter Quant)

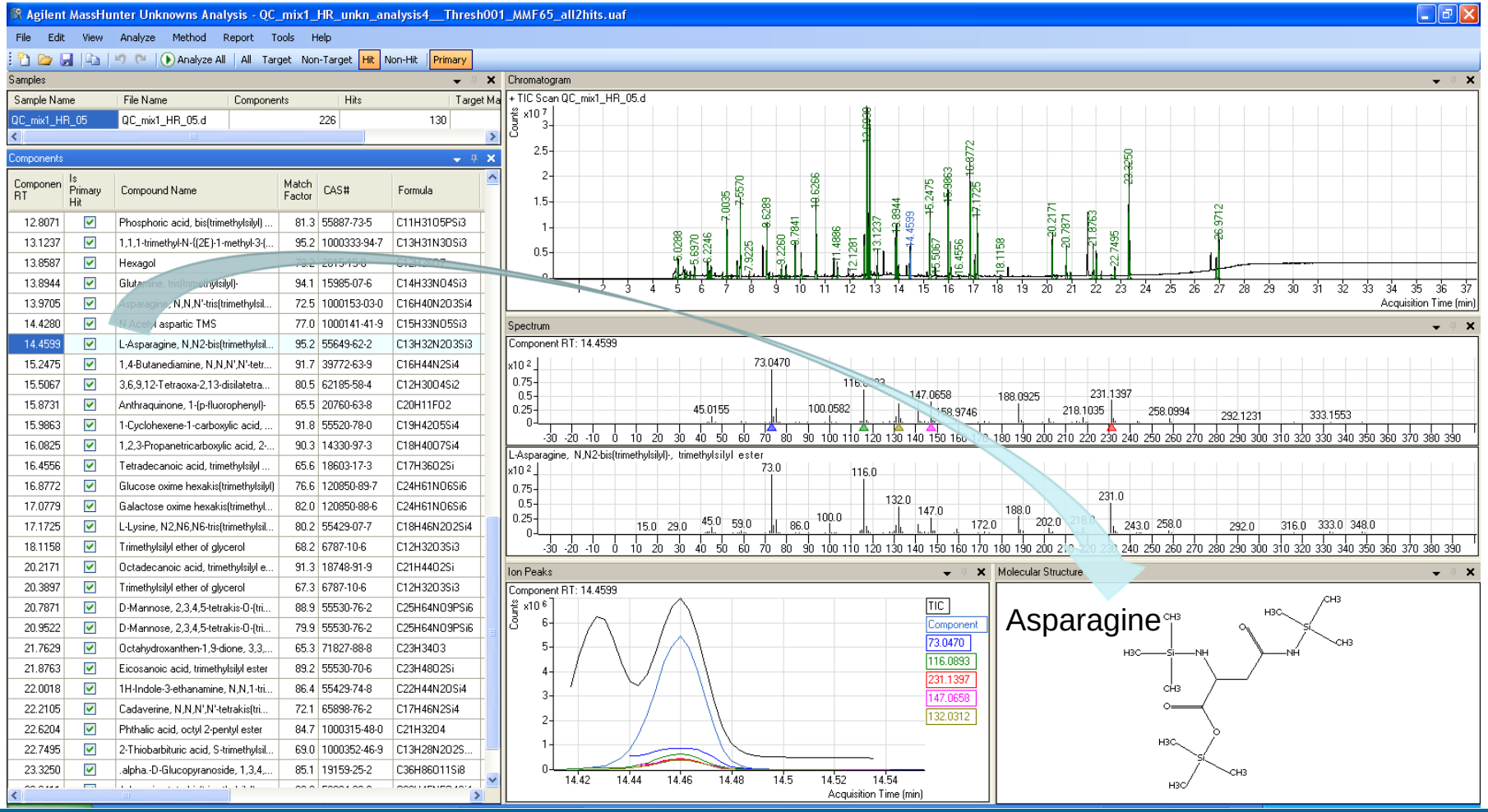
Using deconvolution and spectral library matching to identify unknowns



Agilent Technologies

Unknowns Analysis (MassHunter Quant)

Using deconvolution and spectral library matching to identify unknowns



Bovine plasma Unknowns Analysis results (partial)

Component RT	Compound Name	CAS#	Formula	Match Factor
9.73	L-Isoleucine, N-(trimethylsilyl)-, trimethylsilyl ester	7483-92-3	C12H29NO2Si2	78.22
9.81	L-Proline, 1-(trimethylsilyl)-, trimethylsilyl ester	7364-47-8	C11H25NO2Si2	75.45
10.03	Butanedioic acid, bis(trimethylsilyl) ester	40309-57-7	C10H22O4Si2	81.68
10.11	2-Phenyl-1-(p-tolyl)benzimidazole	3510-25-6	C20H16N2	58.53
10.21	Methyl 8-methyl-decanoate	1000336-49-1	C12H24O2	61.59
10.43	Phosphoric acid, 2-isothiocyanatoethyl bis(trimethylsilyl) ester	56051-85-5	C9H22NO4PSSi2	51.03
10.63	Serine tritms	64625-17-8	C12H31NO3Si3	85.27
10.68	Nonanoic acid, trimethylsilyl ester	82326-11-2	C12H26O2Si	88.03
10.85	Glycine, N-formyl-N-(trimethylsilyl)-, trimethylsilyl ester	55517-31-2	C9H21NO3Si2	50.55
10.96	N,O,O-Tris(trimethylsilyl)-L-threonine	2--2-7537	C13H33NO3Si3	78.77
11.15	Dodecyl trifluoroacetate	1000351-74-5	C14H25F3O2	64.8
11.29	Decanedioic acid, bis(tert-butyldimethylsilyl) ester	104255-98-3	C22H46O4Si2	71.42
11.48	Glyoxime, bis(trimethylsilyl)-	54731-39-4	C8H20N2O2Si2	51.54
11.7	2,4(1H,3H)-Pyrimidinedione, dihydro-1,3-bis(trimethylsilyl)-	74810-47-2	C10H22N2O2Si2	63.24
11.91	2-Piperidone, 1-(trimethylsilyl)-3-[(trimethylsilyl)amino]-	32565-12-1	C11H26N2OSi2	51.39
11.95	Decanoic acid, trimethylsilyl ester	55494-15-0	C13H28O2Si	73.52
12.05	Cycloheptasiloxane, tetradecamethyl-	107-50-6	C14H42O7Si7	54.25
12.19	(Z,Z)-3-Methyl-3H-cyclonona(def)biphenylene	110823-80-8	C18H14	51.04
12.29	Butanedioic acid, [(trimethylsilyl)oxy]-, bis(trimethylsilyl) ester	38166-11-9	C13H30O5Si3	68.14
12.33	Pyrazine, 3,6-dihydro-3,6-dimethyl-2,5-bis(trimethylsilyloxy)-	1000156-30-2	C12H26N2O2Si2	50.63
12.49	3,6,9,12-Tetraoxa-2,13-disilatetradecane, 2,2,13,13-tetramethyl-	62185-58-4	C12H30O4Si2	68.69
12.59	2-Hydroxymandelic acid, ethyl ester, di-TMS	1000071-88-8	C16H28O4Si2	53.02
12.72	L-Proline, 5-oxo-1-(trimethylsilyl)-, trimethylsilyl ester	30274-77-2	C11H23NO3Si2	70.45

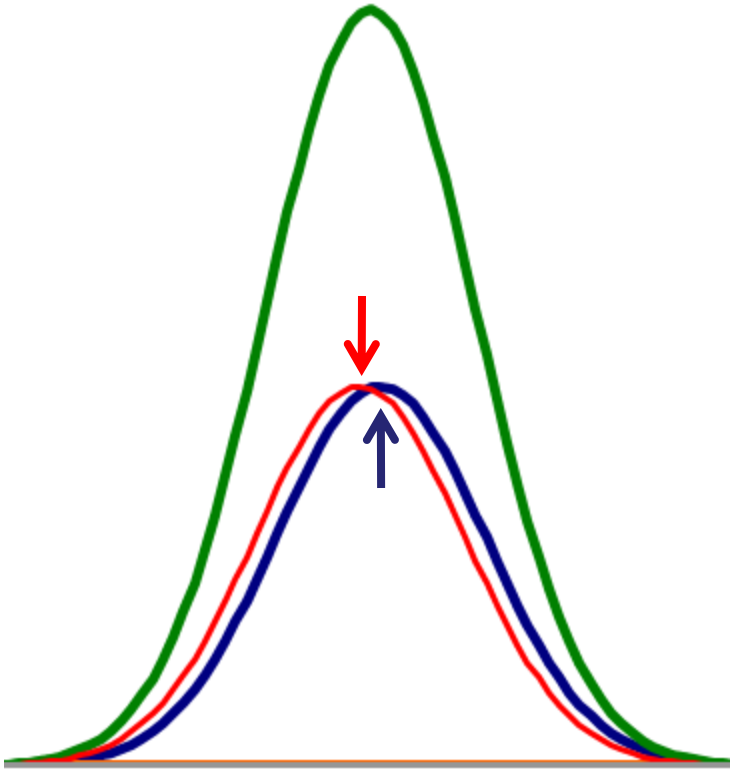
What about TOF *SPEED?*

TOF always collects full mass range
Q-TOF always display full product ion spectrum

- Acquisition Rate: transients (pulses) /second
  - 10,000 transients/second
- Sum of transients = Spectral Rate:
  - Typical max rate: 25-200 spectra/sec (**Hz**) to disk
  - Usable rate is limited by signal level (ion count)
- New analysis opportunities for GC/MS:
  - High Throughput: ~20 Hz
  - Ultra high resolution GC: ~ 40Hz
  - GCxGC: ~50-200 Hz

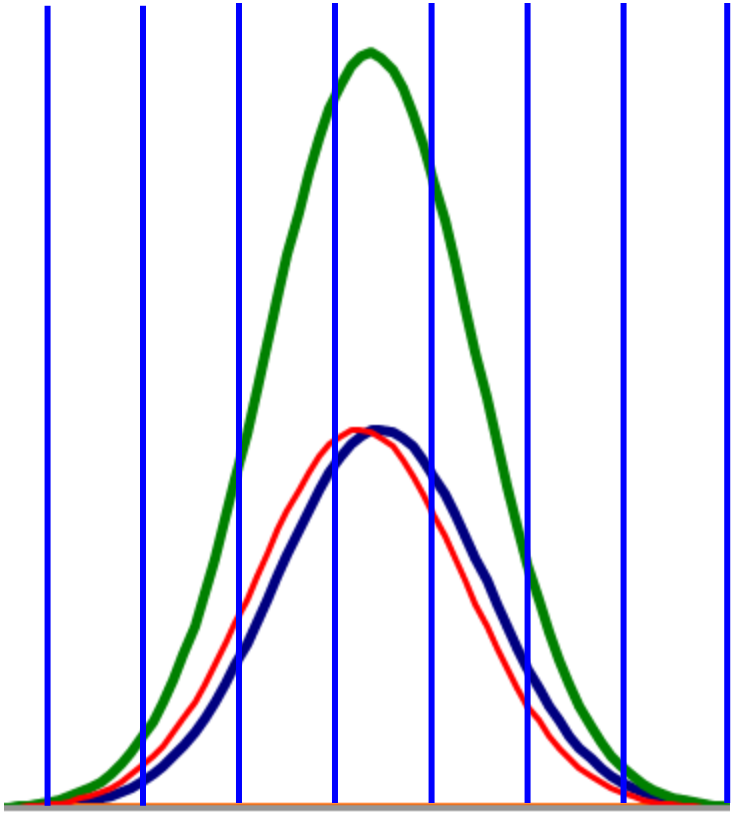
"*Speed*" enhances deconvolution

Deconvolution Requires Time Offset



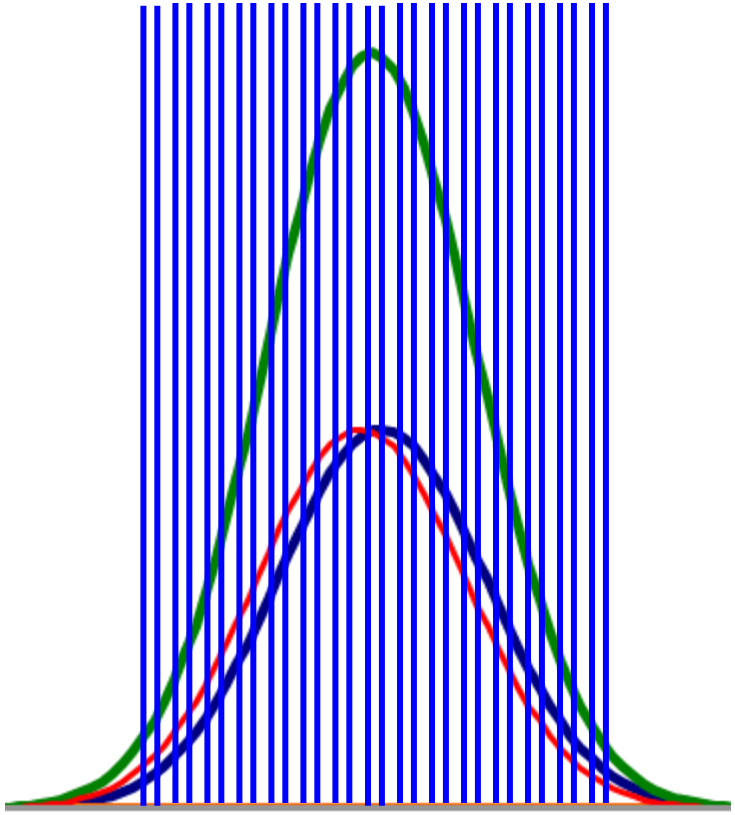
Time

High data rate = better deconvolution



Time

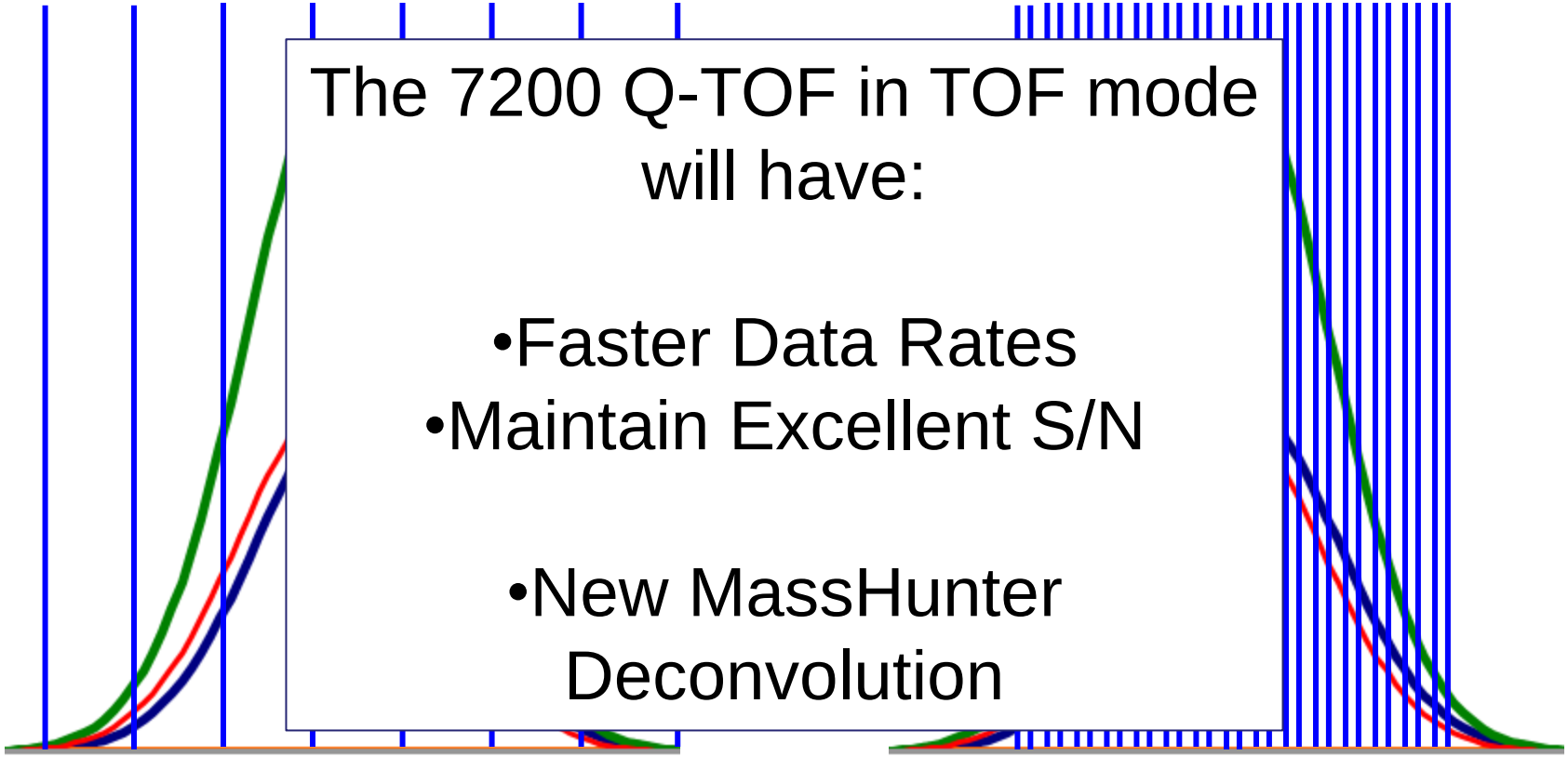
Slow data rate will not pick each peak apex



Time

Fast data rate will allow deconvolution of closely eluting peaks

High data rate = better deconvolution



And What about Q-TOF File Size?

- Typical file sizes for pesticide analysis
  - MSD SIM – 0.8-1 MB/18-min run
  - MSD scan – 3-5 MB/40-min run
  - TQ MRM – 5 MB/20-min run
  - TQ scan – 8 MB/20-min run
  - IT MS/MS – 2.5 MB/45-min run (99 compounds)

  - **TOF or Q-TOF Typical run**
    - **800-1200 MB/20-min run at 5 Hz, profile**
    - **Centroid only reduces 5-10X**

Note: File size depends on the threshold, number of target compounds, number of masses/compound, and runtime etc.

- Can accurate mass measurements be made in a real matrix?
- What are the limitations?

Successful Applications Require the Correct Combination of:

GC Resolution (Agilent)

+

MS Resolving Power (Agilent)

+

ΔMass Defect (Mother Nature)

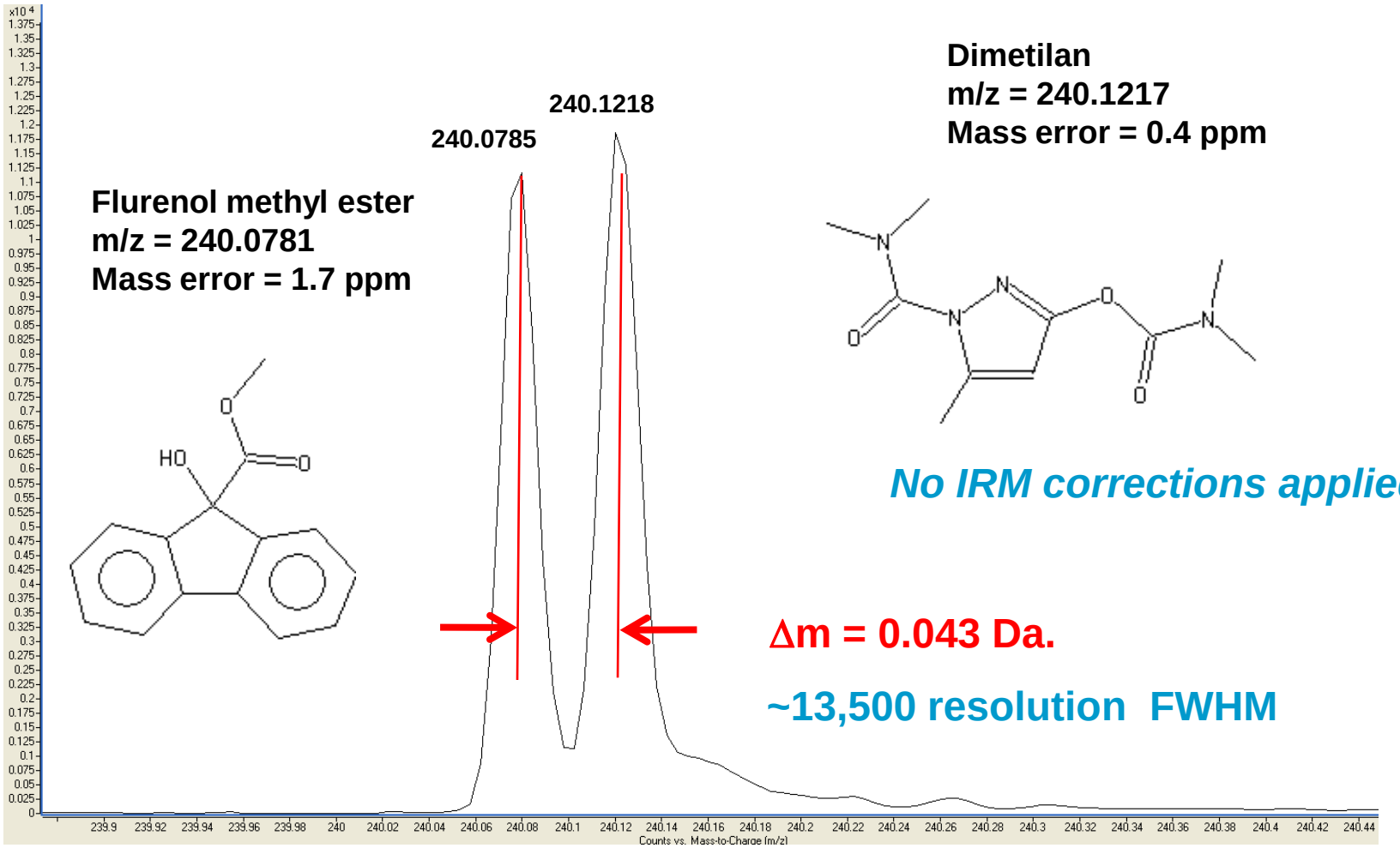
+

Relative Ion Intensities (Sample)

We may have a little to learn about these new apps.

How much “R” and “Defect” is enough?

Intensity Ratio = 1:1

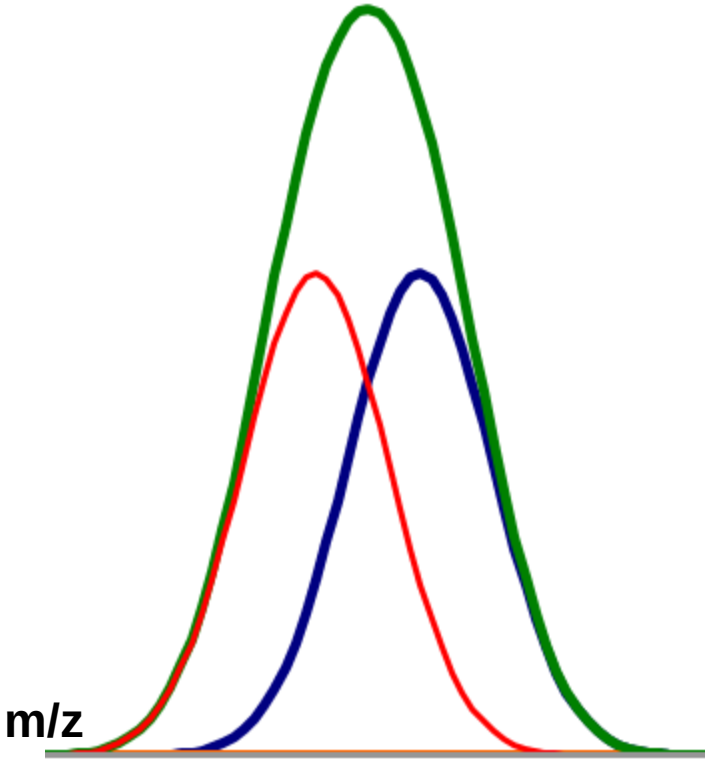


No IRM corrections applied

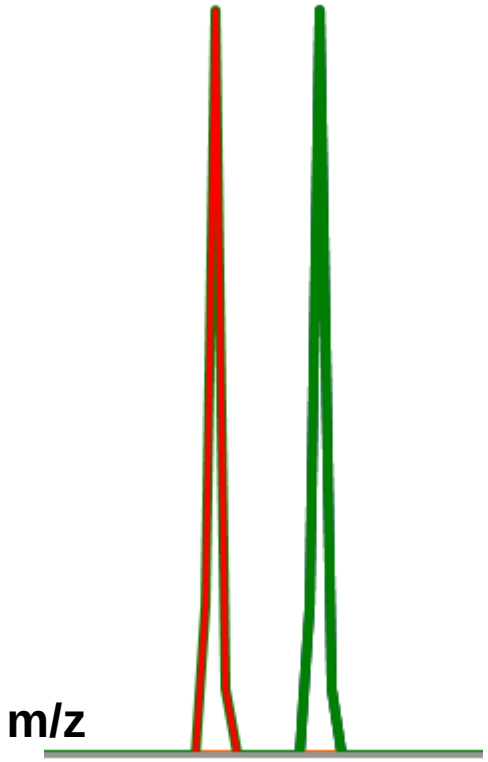
Δm = 0.043 Da.

~13,500 resolution FWHM

Intensity affects the rResult



Two mass peaks with FWHM 0.7 u with 0.5 u between centroided m/z value

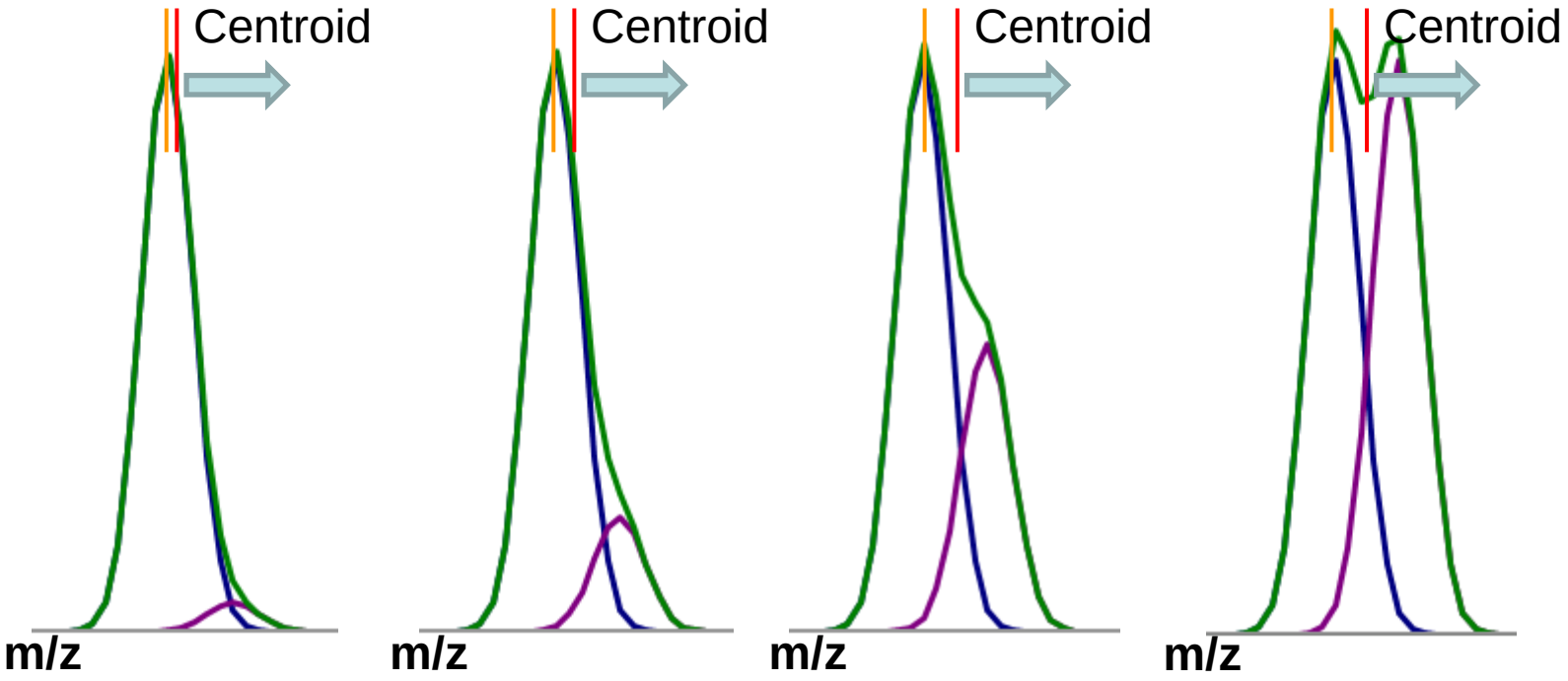


Two mass peaks with FWHM 0.05 u with 0.5 u between centroided m/z value

GC or MS:

Relative intensity affects the result

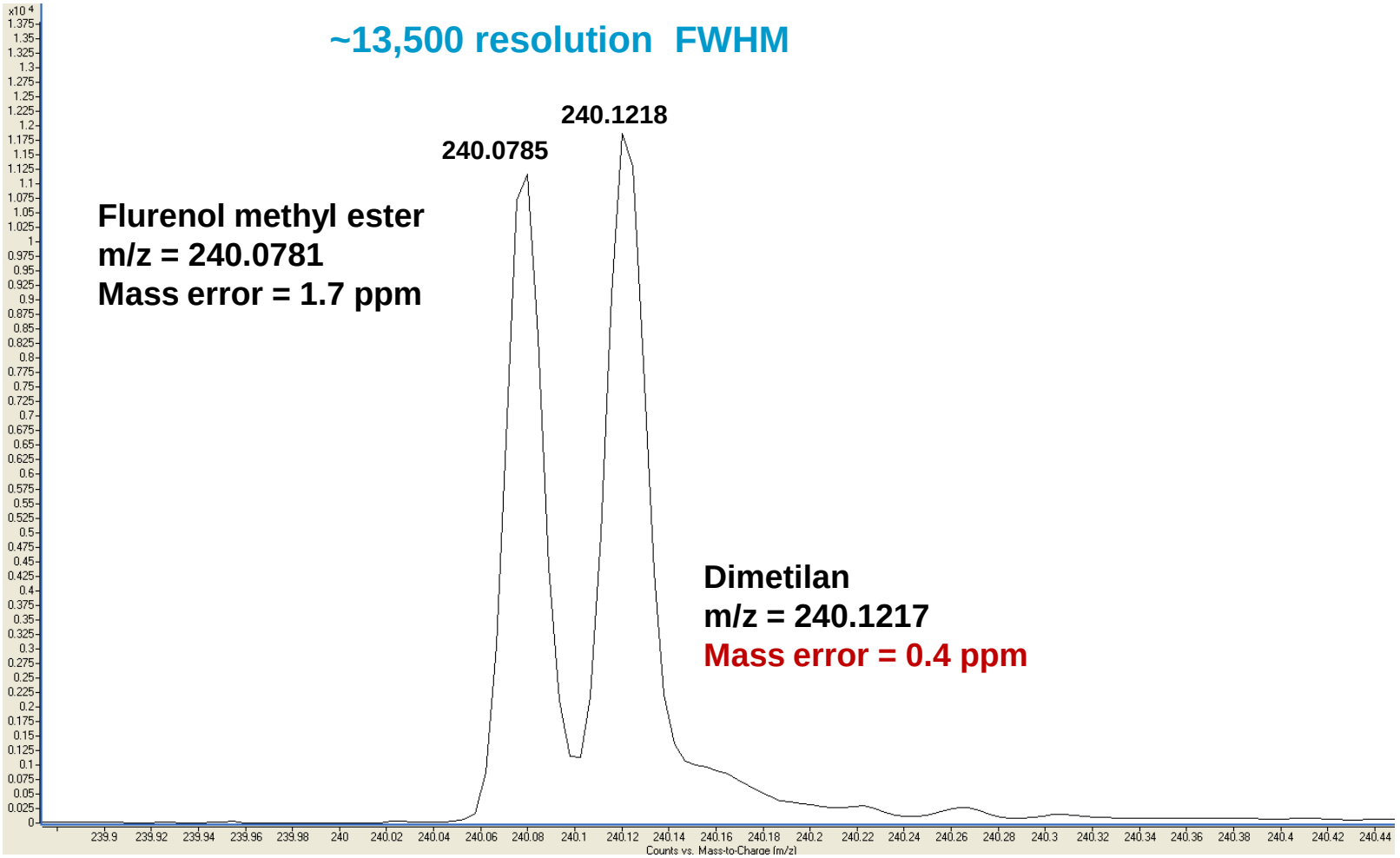
Profile view of mass peaks



Centroid view of mass peaks obscures this fact

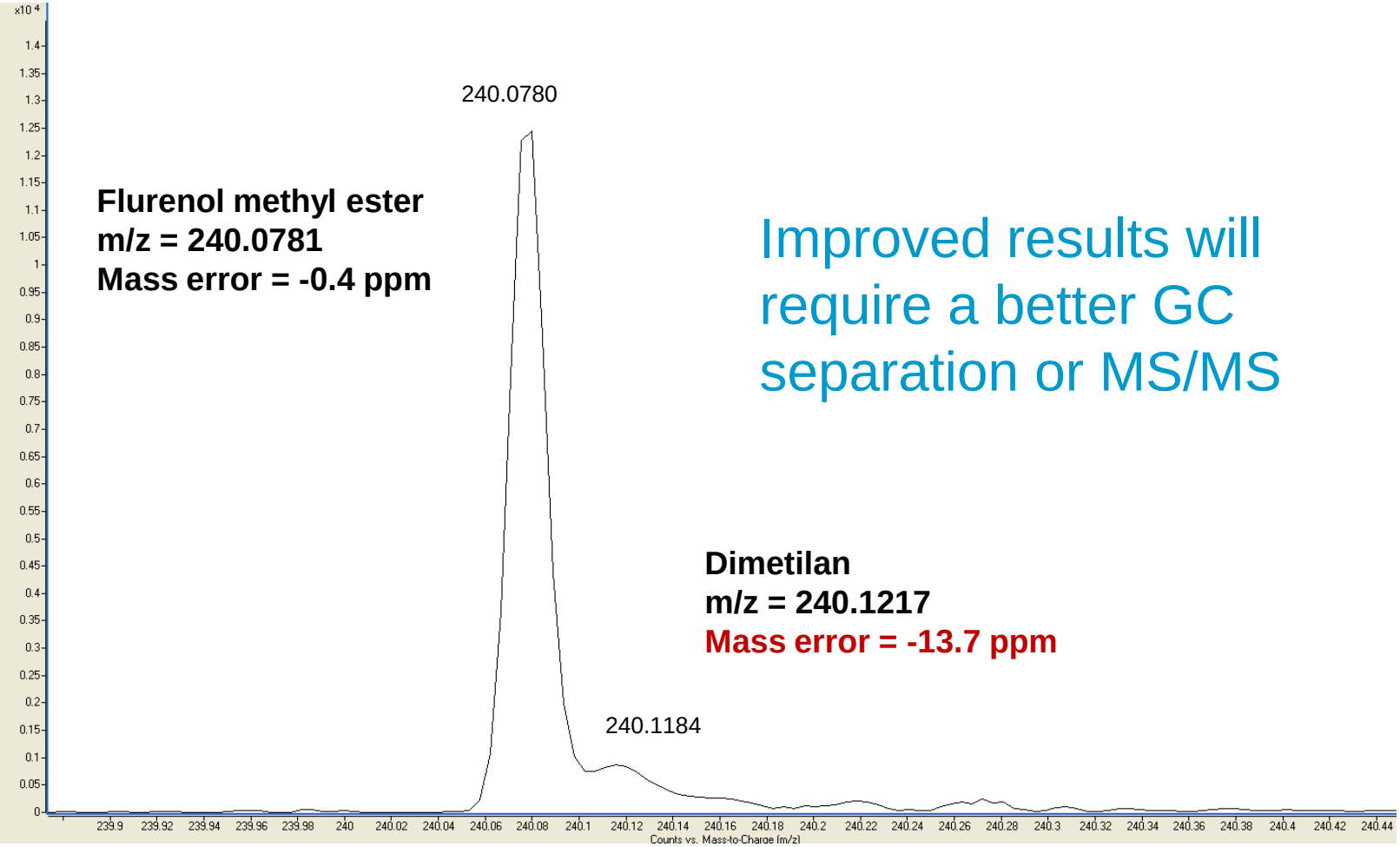
How much “R” and “Defect” is enough?

Intensity Ratio = 1:1



How much “R” and “Defect” is enough?

Intensity Ratio = 1:0.02



Flurenol methyl ester
m/z = 240.0781
Mass error = -0.4 ppm

Dimetilan
m/z = 240.1217
Mass error = -13.7 ppm

Improved results will require a better GC separation or MS/MS

Future Webinars: Balancing Performance Criteria

- Resolving Power: >10K at m/z 272 (>13K typical)
- Mass Accuracy: <5 ppm at m/z 272 (<2ppm typical)
- MS Sensitivity: 1 pg OFN S/N > 400:1
- Dynamic Range: > 3 orders of magnitude
- Quad Mass range: 20-1050 Da (0.7-4.0 Da FWHM)
- TOF Mass range: 20-1700 Da
- Spectral Rate: 1-50 spectra/sec

All specifications subject to change

Key Features of the 7200

1. Internal Reference Mass for routine sub 5ppm mass accuracy even in heavy matrix
2. Removable Ion Source

   (including filaments)
3. Q-TOF MS/MS:
   - Chemical noise reduction
   - Selectivity
   - Structural information
   - Method development
4. Removable Ion Source for quick source cleaning and EI/CI swapping without breaking vacuum
5. Software tools – formula calculator

5975E SQ

5975C SQ

5975T LTM SQ

Agilent GC/MS & GC/MS/MS

More Choices – Better Solutions

220 IT

240 IT

7000 TQ

7200 Q-TOF NEW