Extracting More Analytes from Complex Samples using Agilent's GC/TQ and GC/Q-TOF

GC/TQ (Triple Quad):

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GC/Q-TOF (Quad-Time-of-Flight):

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GC/MS Marketing Manager

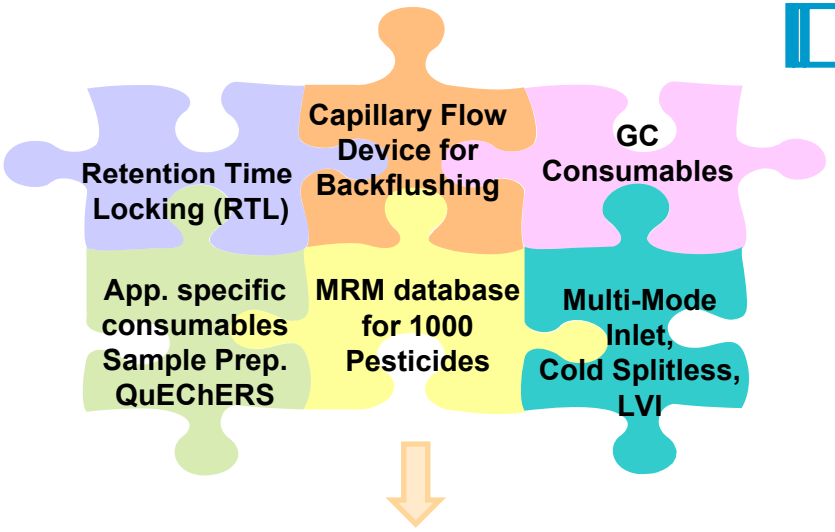
Extracting More Analytes from Complex Samples using Agilent's Pesticide GC/TQ Analyzer

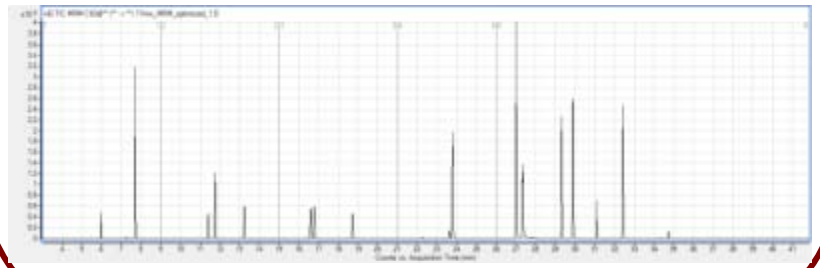
-- "Ready to Go" Analyzer based on the most comprehensive MRM database

Ready to use Fast Track Analyzers

… no on-site break-in needed, ready for injections

At Factory





Plug and Play

At User's Lab

Quick installation and start-up

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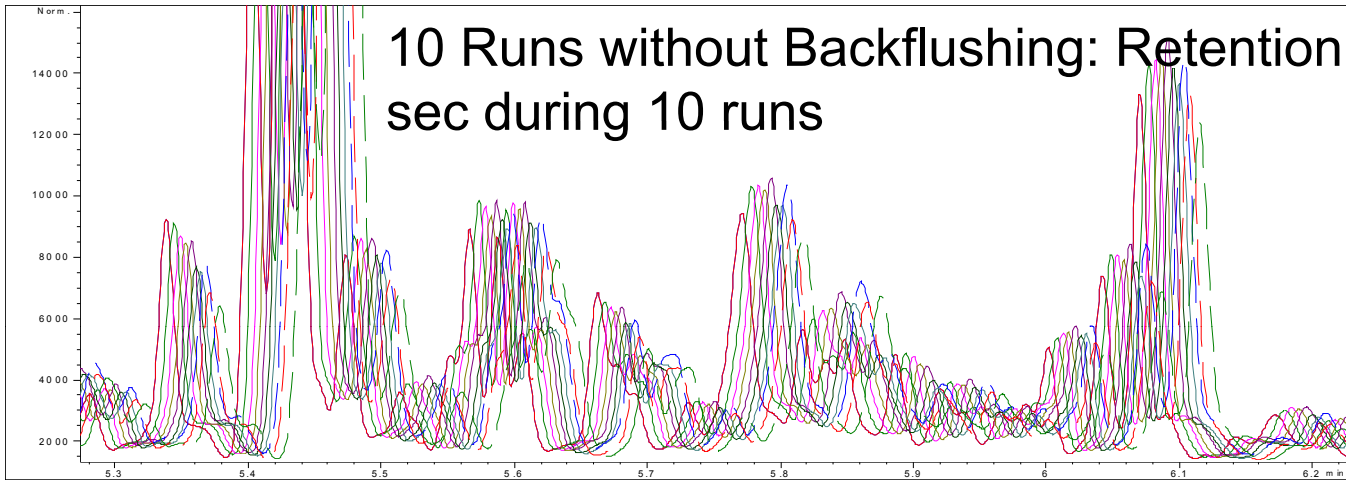
Why Do We Need Backflush?

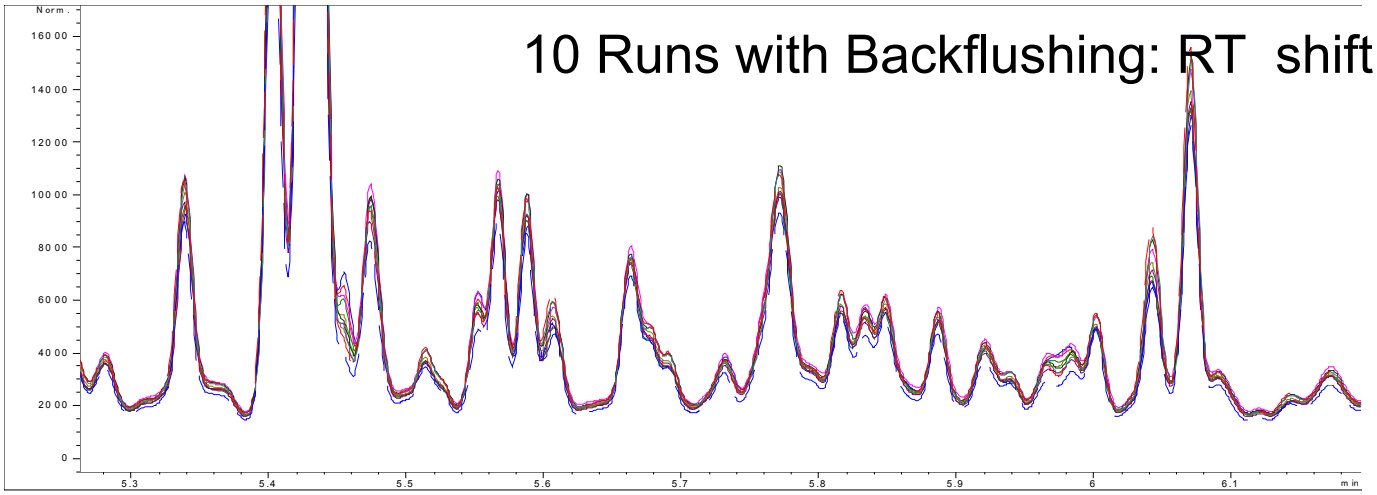
- With the selectivity of MS/MS, **users cannot see "dirty matrix"**
- MS/MS users want the LOWEST detection limits – **inject more** with large volume injection
- Many late eluting peaks are not "chromatographically ideal" and **leave a residue** throughout the column
- Heavy matrix contaminates the source faster --- **performance is LOST!**

Backflush ensures the highest data quality with GC/MS/MS!
The trade-off is 10-20% decrease in sensitivity.

10% Fish Oil In Acetone: Retention Time Shifts Eliminated With Backflushing

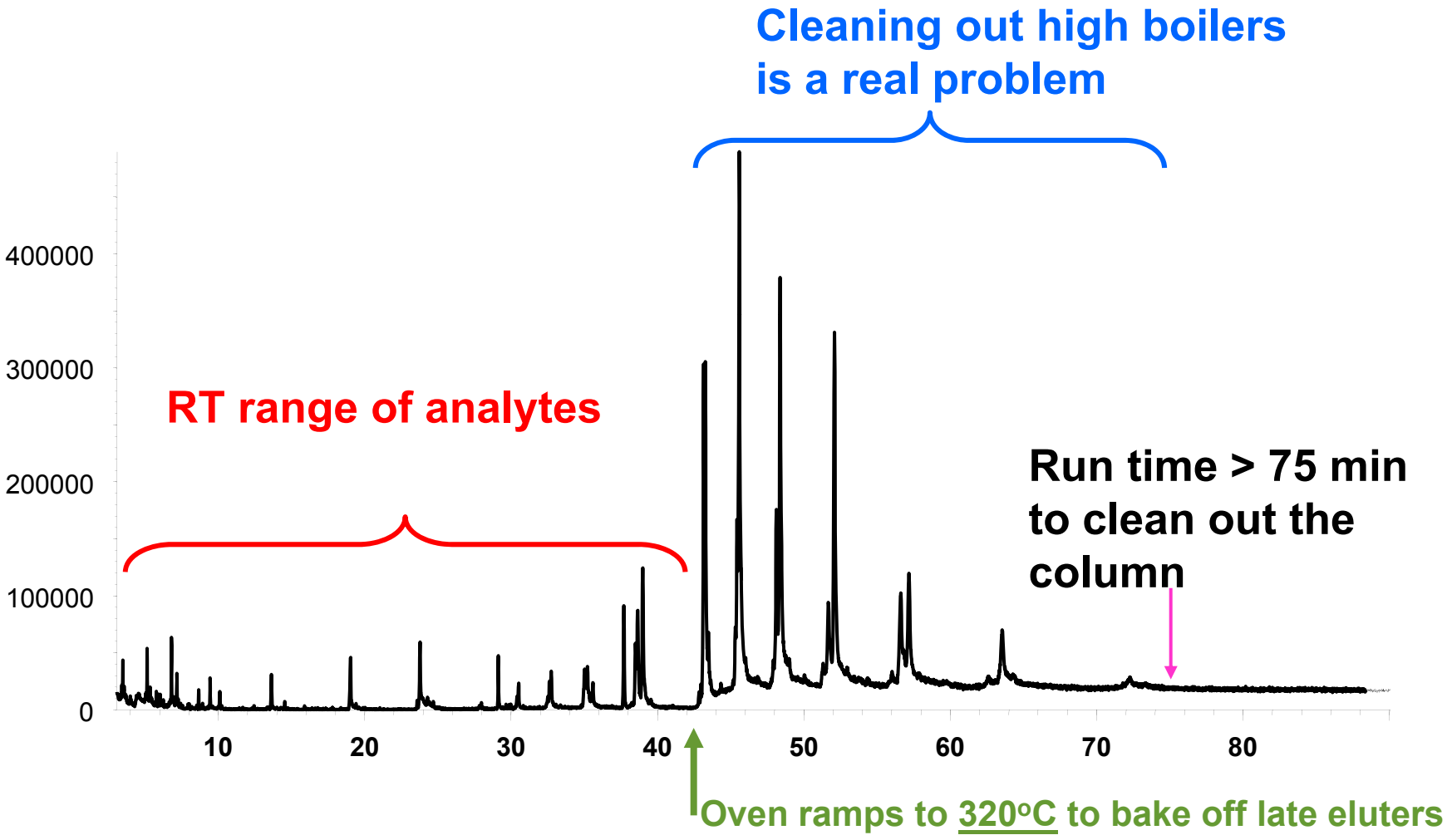


10 Runs without Backflushing: Retention times shift ~4-5 sec during 10 runs



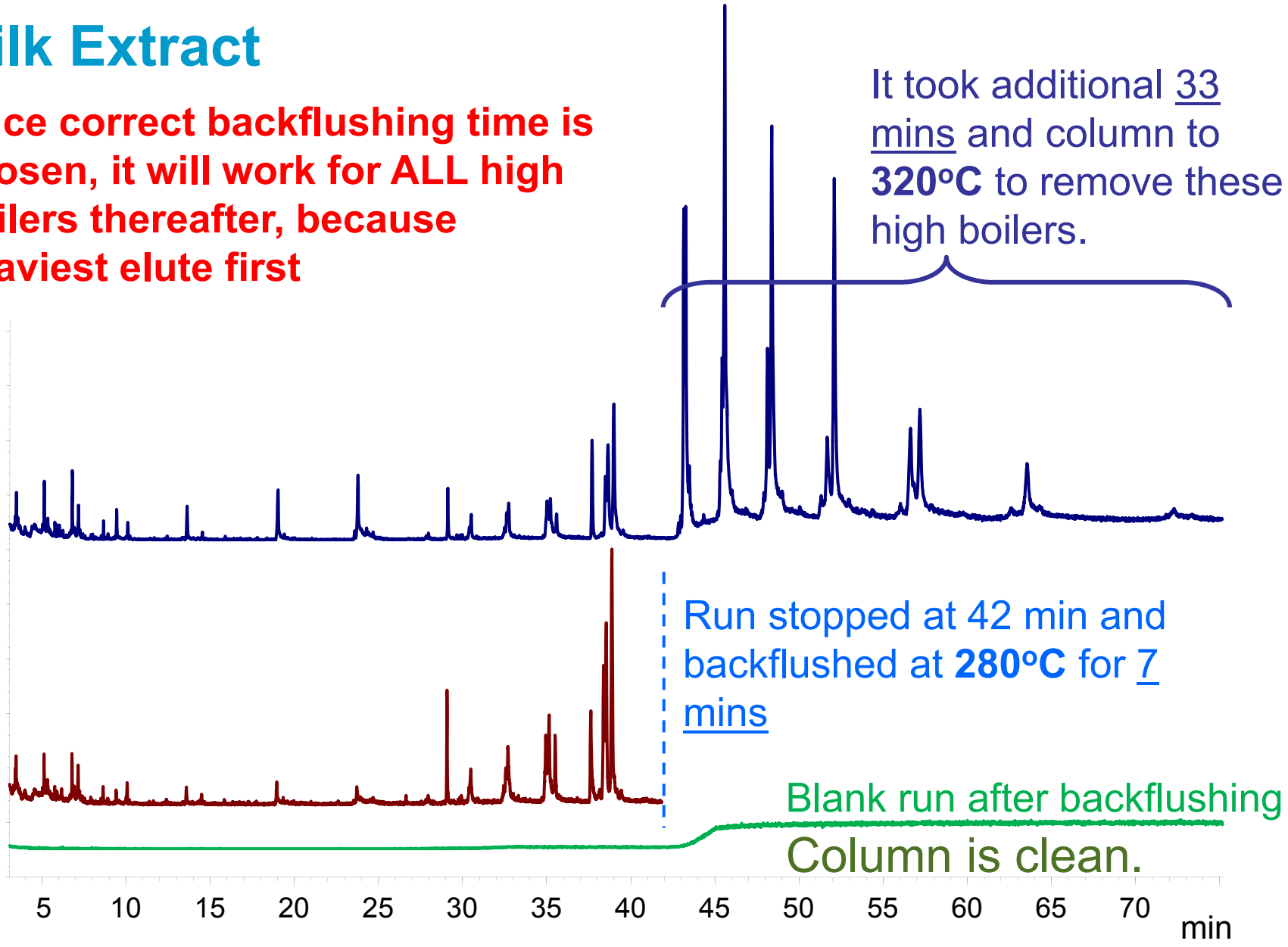
10 Runs with Backflushing: RT shift eliminated

Milk Extract - Using Bakeout To Remove High Boilers



Milk Extract

Once correct backflushing time is chosen, it will work for ALL high boilers thereafter, because heaviest elute first



Backflush: Many Advantages for GC/MS(/MS) Analysis of Complex Samples ('Dirty Matrices')

- Provides **more consistent GC retention times**
- Provides better, **more consistent MS spectra** through sequence
  - **Reduces chemical noise** that due to small carryover of matrix
  - **Higher quality quantitation** without increase in interfering ions
- **Reduces contamination** for the source
- **Reduces analysis time**
- **Increases lifetime of analytical column**

Benefits of Agilent GC/MS/MS Pesticide Analyzer

Retention Time Locking	• **No need to update the time segment RTs** after a column maintenance
Multimode inlet (MMI)	• injector adds flexibility by including standard, cold split/splitless, solvent vent (**LVI**) capabilities.
Capillary Flow Technology (CFT) and backflush	• Shorter analysis time, more consistent retention times and spectra, longer column life, and less frequent source cleaning -- **improve uptime.**
MS/MS MRM Database	• **Optimized and flexible MRM database** of hundreds of compounds
Pre-config. and factory setup analyzer	• **Factory setup and checked out on pesticide mixture -** ready to generate results on Day One

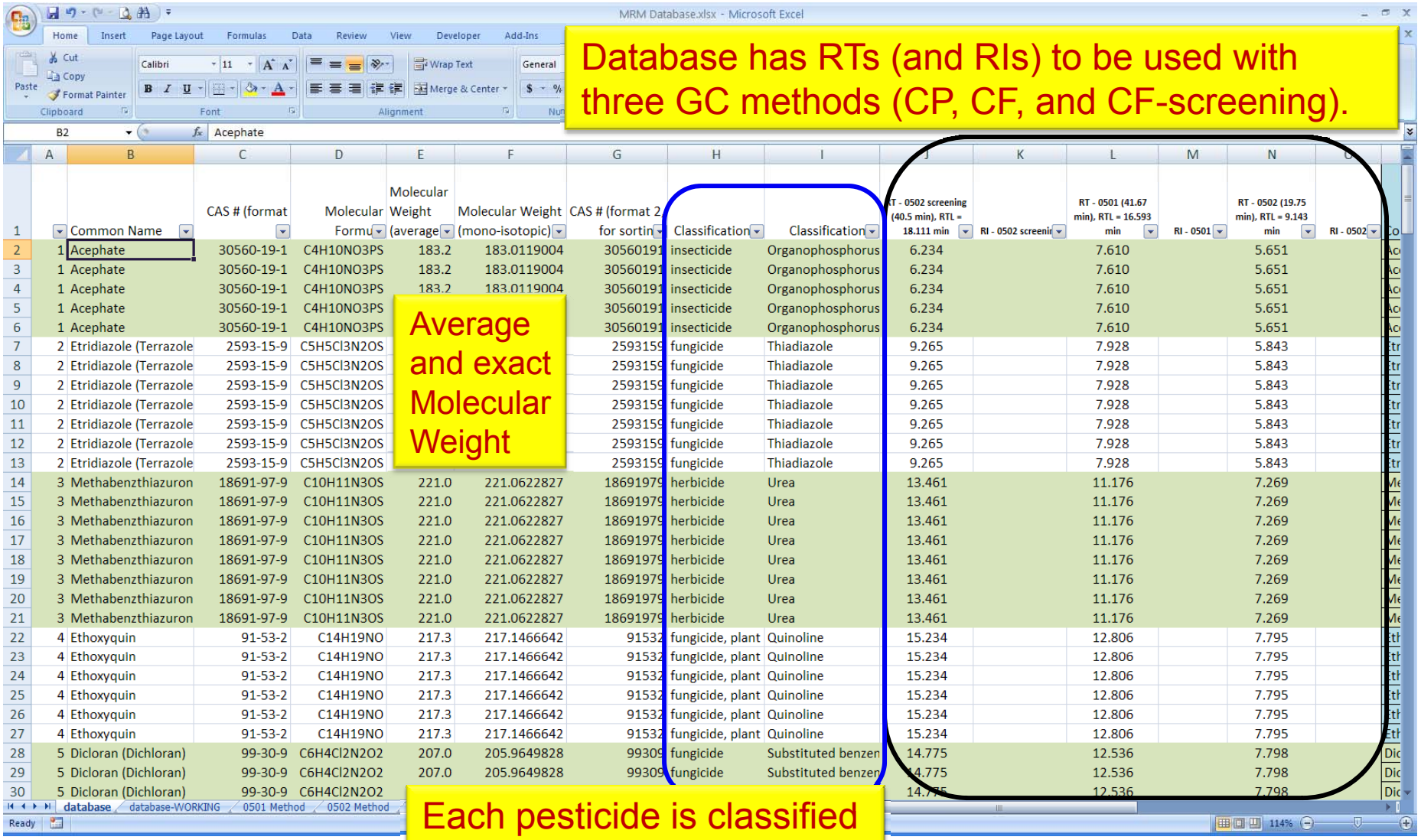
But…

How does the Analyzer work with the list of target pesticides in my lab?

Agilent's New Comprehensive MRM database with Extensive Flexibility

- **Contains 7000 optimized MRMs for 1000 pesticides**
  - -- over 3000 injections on $70,000 worth of **chemical standards**
- **Extensive flexibility allows method optimization**
  - average of 7 MRM transitions with relative intensity for each compound
    - -- provides alternatives to **avoid matrix interference**
  - compound classification, CAS number etc. in excel format
    - -- allows **easy searching and sorting** for method customization
  - three chromatographic methods (constant flow or pressure) with Retention Time and Retention Index
    - -- allows maximum freedom to follow **customer's workflow**
  - absolute intensity for each MRM transition
    - -- allows **semi-quantitation** without standards

The Flexibility: 7 transitions; classifications; 3 RTs and RIs



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1		Common Name	CAS # (format	Molecular Formu	Molecular Weight (average	Molecular Weight (mono-isotopic)	CAS # (format 2 for sortin	Classification	Classification	RT - 0502 screening (40.5 min), RTL = 18.111 min	RI - 0502 screeni	RT - 0501 (41.67 min), RTL = 16.593 min	RI - 0501	RT - 0502 (19.75 min), RTL = 9.143 min	RI - 0502
2	1	Acephate	30560-19-1	C4H10NO3PS	183.2	183.0119004	30560191	insecticide	Organophosphorus	6.234		7.610		5.651	
3	1	Acephate	30560-19-1	C4H10NO3PS	183.2	183.0119004	30560191	insecticide	Organophosphorus	6.234		7.610		5.651	
4	1	Acephate	30560-19-1	C4H10NO3PS	183.2	183.0119004	30560191	insecticide	Organophosphorus	6.234		7.610		5.651	
5	1	Acephate	30560-19-1	C4H10NO3PS			30560191	insecticide	Organophosphorus	6.234		7.610		5.651	
6	1	Acephate	30560-19-1	C4H10NO3PS			30560191	insecticide	Organophosphorus	6.234		7.610		5.651	
7	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
8	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
9	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
10	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
11	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
12	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
13	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS			2593159	fungicide	Thiadiazole	9.265		7.928		5.843	
14	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
15	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
16	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
17	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
18	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
19	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
20	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
21	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	1869197	herbicide	Urea	13.461		11.176		7.269	
22	4	Ethoxyquin	91-53-2	C14H19NO	217.3	217.1466642	91532	fungicide, plant	Quinoline	15.234		12.806		7.795	
23	4	Ethoxyquin	91-53-2	C14H19NO	217.3	217.1466642	91532	fungicide, plant	Quinoline	15.234		12.806		7.795	
24	4	Ethoxyquin	91-53-2	C14H19NO	217.3	217.1466642	91532	fungicide, plant	Quinoline	15.234		12.806		7.795	
25	4	Ethoxyquin	91-53-2	C14H19NO	217.3	217.1466642	91532	fungicide, plant	Quinoline	15.234		12.806		7.795	
26	4	Ethoxyquin	91-53-2	C14H19NO	217.3	217.1466642	91532	fungicide, plant	Quinoline	15.234		12.806		7.795	
27	4	Ethoxyquin	91-53-2	C14H19NO	217.3	217.1466642	91532	fungicide, plant	Quinoline	15.234		12.806		7.795	
28	5	Dicloran (Dichloran)	99-30-9	C6H4Cl2N2O2	207.0	205.9649828	99309	fungicide	Substituted benzen	14.775		12.536		7.798	
29	5	Dicloran (Dichloran)	99-30-9	C6H4Cl2N2O2	207.0	205.9649828	99309	fungicide	Substituted benzen	14.775		12.536		7.798	
30	5	Dicloran (Dichloran)	99-30-9	C6H4Cl2N2O2											

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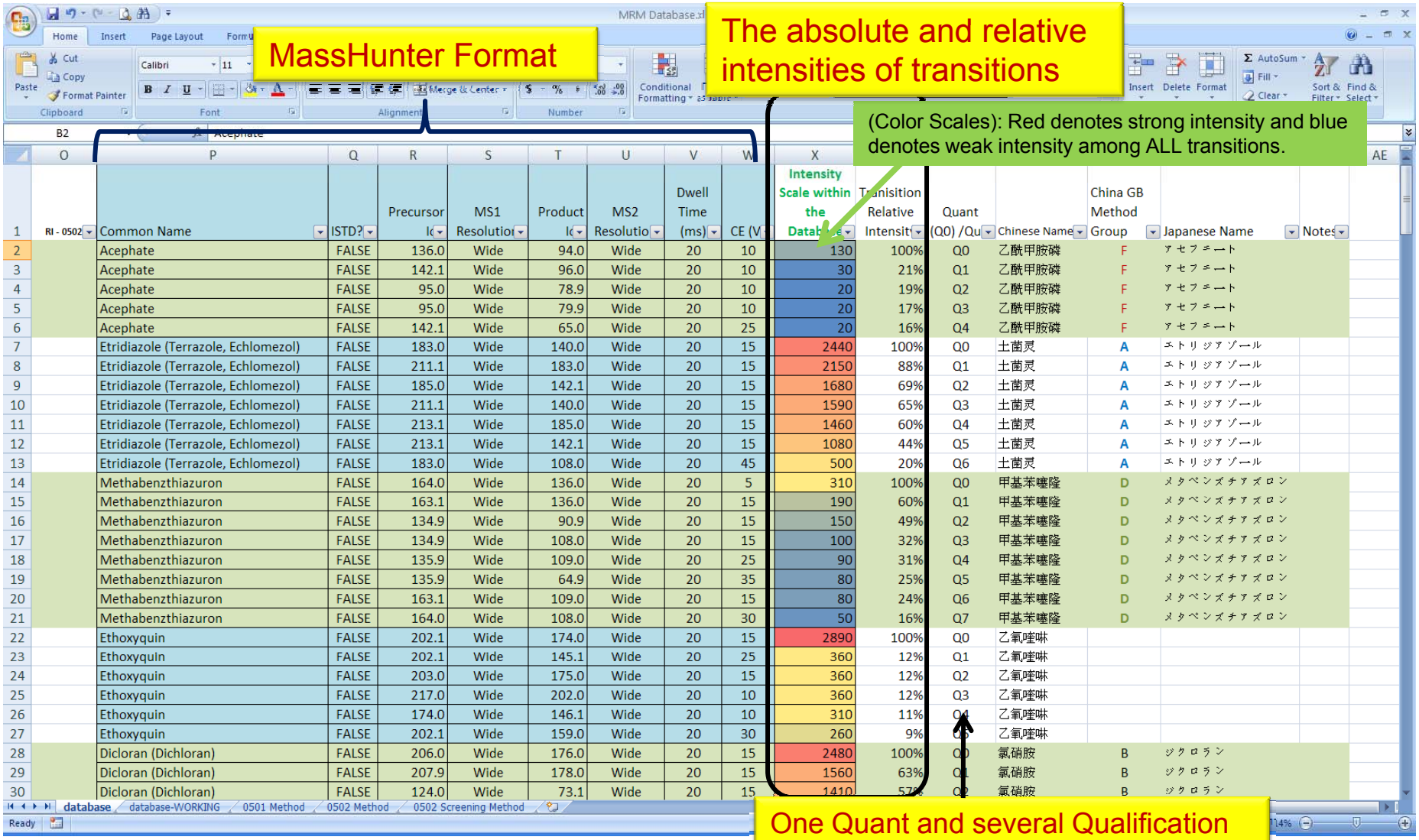
The Flexibility: Excel format, relative and absolute Transition intensity



	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE
1	RI - 0502	Common Name	ISTD?	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell Time (ms)	CE (V)	Intensity Scale within the Database	Transition Relative Intensity	Quant (Q0) /Qu	Chinese Name	China GB Method Group	Japanese Name	Notes	
2		Acephate	FALSE	136.0	Wide	94.0	Wide	20	10	130	100%	Q0	乙酰甲胺磷	F	アセフェート		
3		Acephate	FALSE	142.1	Wide	96.0	Wide	20	10	30	21%	Q1	乙酰甲胺磷	F	アセフェート		
4		Acephate	FALSE	95.0	Wide	78.9	Wide	20	10	20	19%	Q2	乙酰甲胺磷	F	アセフェート		
5		Acephate	FALSE	95.0	Wide	79.9	Wide	20	10	20	17%	Q3	乙酰甲胺磷	F	アセフェート		
6		Acephate	FALSE	142.1	Wide	65.0	Wide	20	25	20	16%	Q4	乙酰甲胺磷	F	アセフェート		
7		Etridiazole (Terrazole, Echlomezol)	FALSE	183.0	Wide	140.0	Wide	20	15	2440	100%	Q0	土菌灵	A	エトリジアゾール		
8		Etridiazole (Terrazole, Echlomezol)	FALSE	211.1	Wide	183.0	Wide	20	15	2150	88%	Q1	土菌灵	A	エトリジアゾール		
9		Etridiazole (Terrazole, Echlomezol)	FALSE	185.0	Wide	142.1	Wide	20	15	1680	69%	Q2	土菌灵	A	エトリジアゾール		
10		Etridiazole (Terrazole, Echlomezol)	FALSE	211.1	Wide	140.0	Wide	20	15	1590	65%	Q3	土菌灵	A	エトリジアゾール		
11		Etridiazole (Terrazole, Echlomezol)	FALSE	213.1	Wide	185.0	Wide	20	15	1460	60%	Q4	土菌灵	A	エトリジアゾール		
12		Etridiazole (Terrazole, Echlomezol)	FALSE	213.1	Wide	142.1	Wide	20	15	1080	44%	Q5	土菌灵	A	エトリジアゾール		
13		Etridiazole (Terrazole, Echlomezol)	FALSE	183.0	Wide	108.0	Wide	20	45	500	20%	Q6	土菌灵	A	エトリジアゾール		
14		Methabenzthiazuron	FALSE	164.0	Wide	136.0	Wide	20	5	310	100%	Q0	甲基苯噻隆	D	メタベンズチアズロン		
15		Methabenzthiazuron	FALSE	163.1	Wide	136.0	Wide	20	15	190	60%	Q1	甲基苯噻隆	D	メタベンズチアズロン		
16		Methabenzthiazuron	FALSE	134.9	Wide	90.9	Wide	20	15	150	49%	Q2	甲基苯噻隆	D	メタベンズチアズロン		
17		Methabenzthiazuron	FALSE	134.9	Wide	108.0	Wide	20	15	100	32%	Q3	甲基苯噻隆	D	メタベンズチアズロン		
18		Methabenzthiazuron	FALSE	135.9	Wide	109.0	Wide	20	25	90	31%	Q4	甲基苯噻隆	D	メタベンズチアズロン		
19		Methabenzthiazuron	FALSE	135.9	Wide	64.9	Wide	20	35	80	25%	Q5	甲基苯噻隆	D	メタベンズチアズロン		
20		Methabenzthiazuron	FALSE	163.1	Wide	109.0	Wide	20	15	80	24%	Q6	甲基苯噻隆	D	メタベンズチアズロン		
21		Methabenzthiazuron	FALSE	164.0	Wide	108.0	Wide	20	30	50	16%	Q7	甲基苯噻隆	D	メタベンズチアズロン		
22		Ethoxyquin	FALSE	202.1	Wide	174.0	Wide	20	15	2890	100%	Q0	乙氧喹啉				
23		Ethoxyquin	FALSE	202.1	Wide	145.1	Wide	20	25	360	12%	Q1	乙氧喹啉				
24		Ethoxyquin	FALSE	203.0	Wide	175.0	Wide	20	15	360	12%	Q2	乙氧喹啉				
25		Ethoxyquin	FALSE	217.0	Wide	202.0	Wide	20	10	360	12%	Q3	乙氧喹啉				
26		Ethoxyquin	FALSE	174.0	Wide	146.1	Wide	20	10	310	11%	Q4	乙氧喹啉				
27		Ethoxyquin	FALSE	202.1	Wide	159.0	Wide	20	30	260	9%	Q5	乙氧喹啉				
28		Dicloran (Dichloran)	FALSE	206.0	Wide	176.0	Wide	20	15	2480	100%	Q0	氯硝胺	B	ジクロラン		
29		Dicloran (Dichloran)	FALSE	207.9	Wide	178.0	Wide	20	15	1560	63%	Q1	氯硝胺	B	ジクロラン		
30		Dicloran (Dichloran)	FALSE	124.0	Wide	73.1	Wide	20	15	1410	57%	Q2	氯硝胺	B	ジクロラン		

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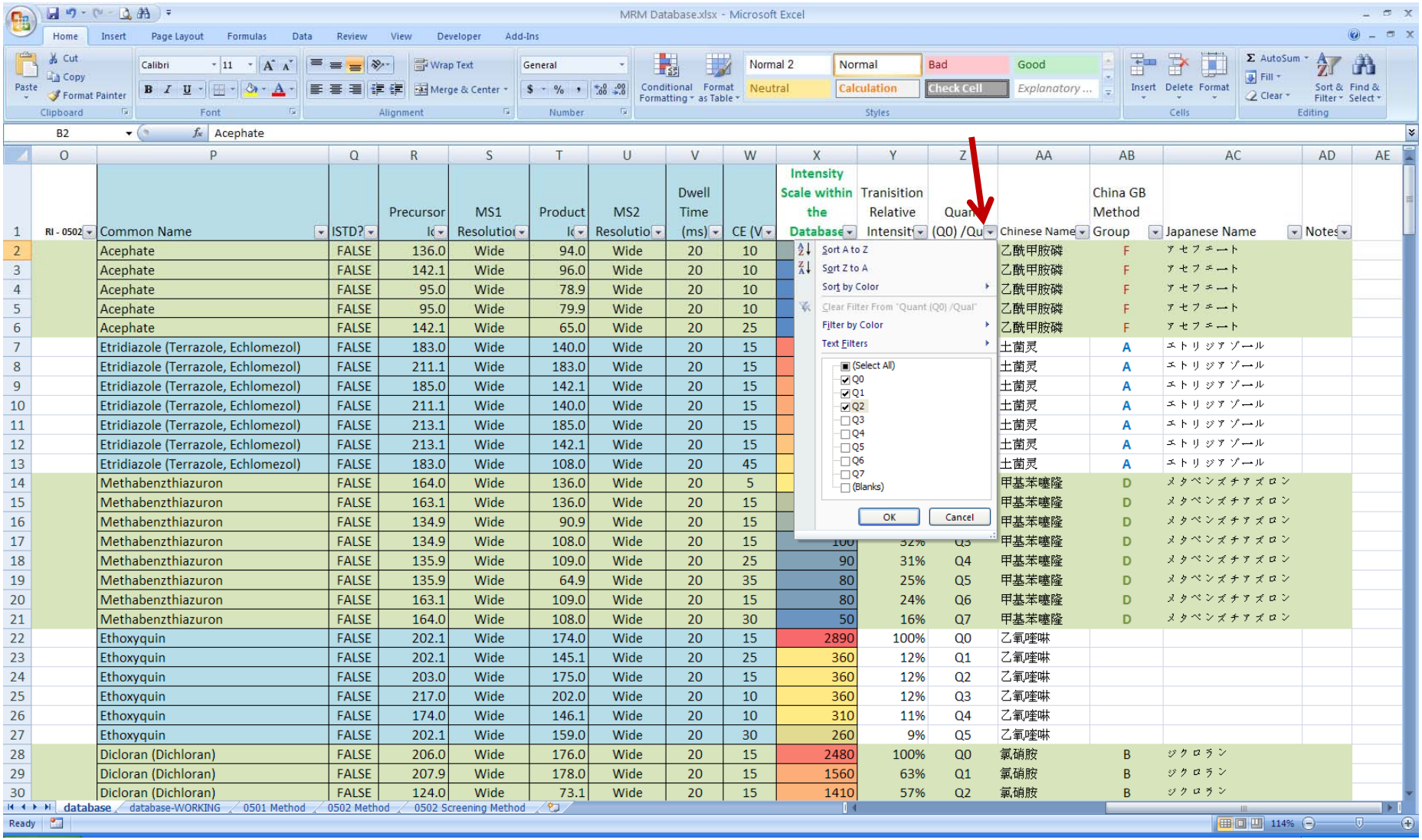
Click on the sorting button to show/hide Quant and Qualifier Ions



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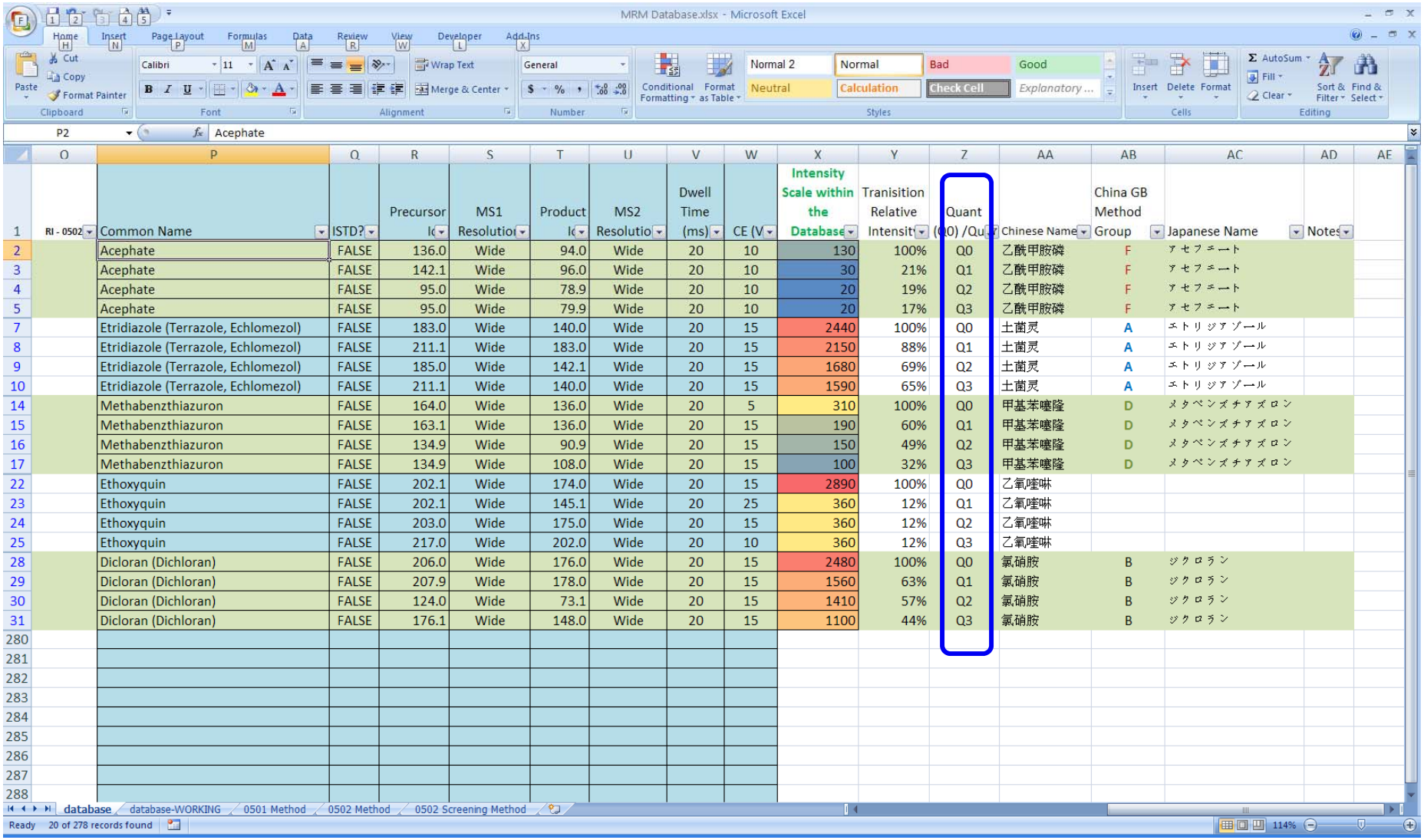
Use the sorting function to quickly select a Quant (Q0) and top three Qualifier ions (to build a method)!



MRM Database.xlsx - Microsoft Excel

	Common Name	ISTD?	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell Time (ms)	CE (V	Intensity Scale within the Database	Tranisition Relative Intensity	Quant (Q0) /Qu	Chinese Name	China GB Method Group	Japanese Name	Notes
2	Acephate	FALSE	136.0	Wide	94.0	Wide	20	10	130	100%	Q0	乙酰甲胺磷	F	アセフェート	
3	Acephate	FALSE	142.1	Wide	96.0	Wide	20	10	30	21%	Q1	乙酰甲胺磷	F	アセフェート	
4	Acephate	FALSE	95.0	Wide	78.9	Wide	20	10	20	19%	Q2	乙酰甲胺磷	F	アセフェート	
5	Acephate	FALSE	95.0	Wide	79.9	Wide	20	10	20	17%	Q3	乙酰甲胺磷	F	アセフェート	
7	Etridiazole (Terrazole, Echlomezol)	FALSE	183.0	Wide	140.0	Wide	20	15	2440	100%	Q0	土菌灵	A	エトリジアゾール	
8	Etridiazole (Terrazole, Echlomezol)	FALSE	211.1	Wide	183.0	Wide	20	15	2150	88%	Q1	土菌灵	A	エトリジアゾール	
9	Etridiazole (Terrazole, Echlomezol)	FALSE	185.0	Wide	142.1	Wide	20	15	1680	69%	Q2	土菌灵	A	エトリジアゾール	
10	Etridiazole (Terrazole, Echlomezol)	FALSE	211.1	Wide	140.0	Wide	20	15	1590	65%	Q3	土菌灵	A	エトリジアゾール	
14	Methabenzthiazuron	FALSE	164.0	Wide	136.0	Wide	20	5	310	100%	Q0	甲基苯噻隆	D	メタベンズチアズロン	
15	Methabenzthiazuron	FALSE	163.1	Wide	136.0	Wide	20	15	190	60%	Q1	甲基苯噻隆	D	メタベンズチアズロン	
16	Methabenzthiazuron	FALSE	134.9	Wide	90.9	Wide	20	15	150	49%	Q2	甲基苯噻隆	D	メタベンズチアズロン	
17	Methabenzthiazuron	FALSE	134.9	Wide	108.0	Wide	20	15	100	32%	Q3	甲基苯噻隆	D	メタベンズチアズロン	
22	Ethoxyquin	FALSE	202.1	Wide	174.0	Wide	20	15	2890	100%	Q0	乙氧喹啉			
23	Ethoxyquin	FALSE	202.1	Wide	145.1	Wide	20	25	360	12%	Q1	乙氧喹啉			
24	Ethoxyquin	FALSE	203.0	Wide	175.0	Wide	20	15	360	12%	Q2	乙氧喹啉			
25	Ethoxyquin	FALSE	217.0	Wide	202.0	Wide	20	10	360	12%	Q3	乙氧喹啉			
28	Dicloran (Dichloran)	FALSE	206.0	Wide	176.0	Wide	20	15	2480	100%	Q0	氯硝胺	B	ジクロラン	
29	Dicloran (Dichloran)	FALSE	207.9	Wide	178.0	Wide	20	15	1560	63%	Q1	氯硝胺	B	ジクロラン	
30	Dicloran (Dichloran)	FALSE	124.0	Wide	73.1	Wide	20	15	1410	57%	Q2	氯硝胺	B	ジクロラン	
31	Dicloran (Dichloran)	FALSE	176.1	Wide	148.0	Wide	20	15	1100	44%	Q3	氯硝胺	B	ジクロラン	

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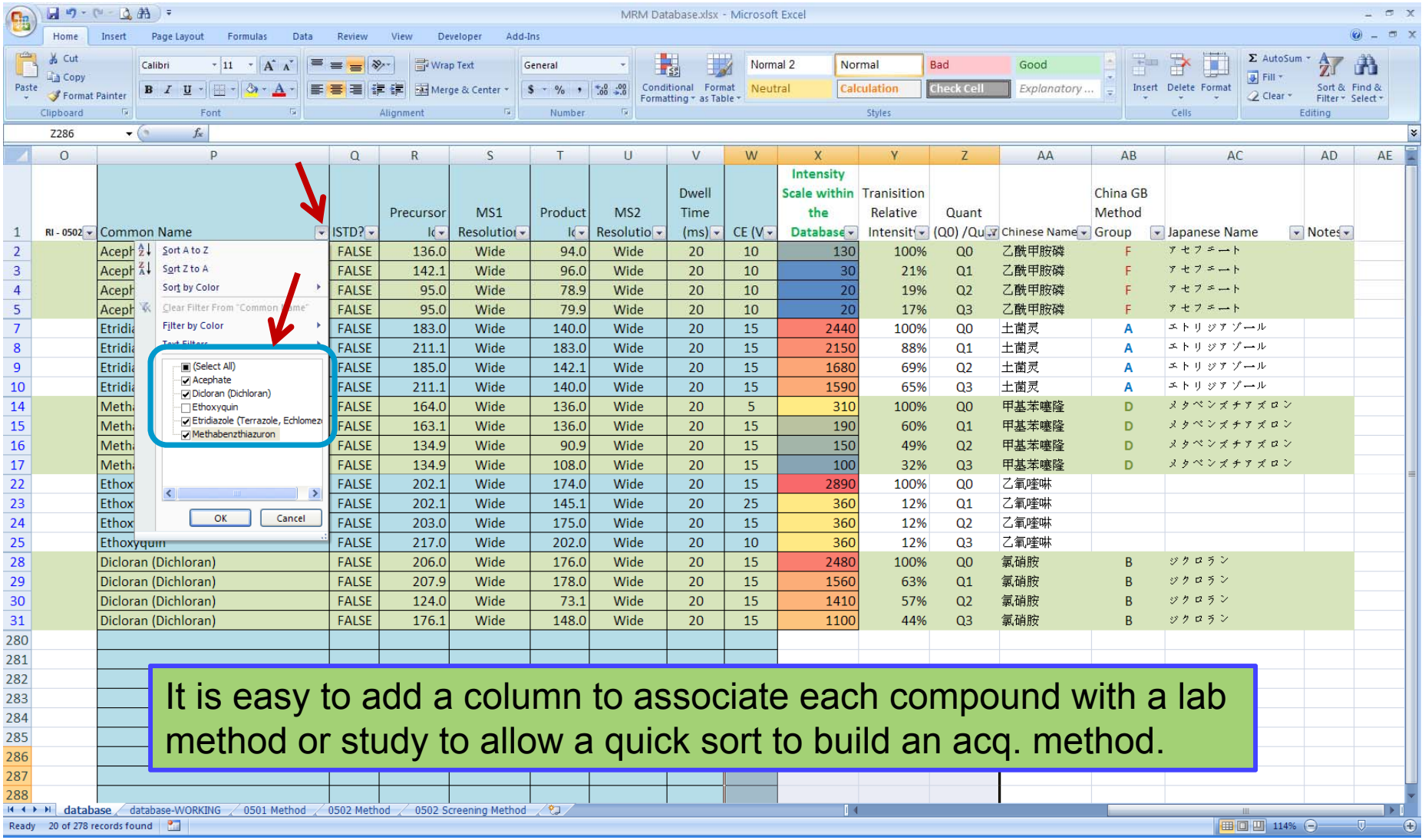
Click on the sorting button to select/show the compounds to be added into the acquisition method



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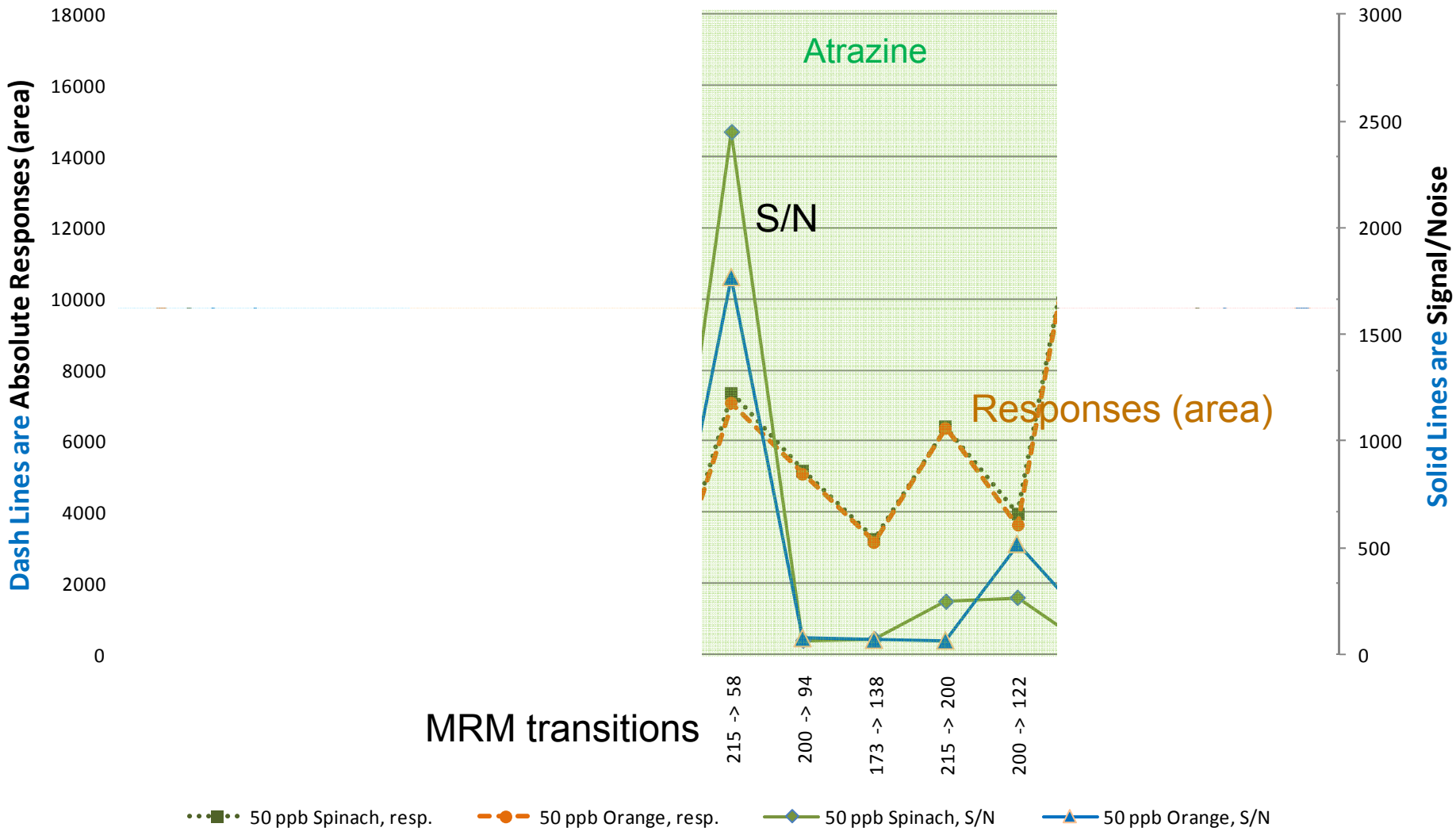
Why Do We Need More than 2 MRM Transitions?



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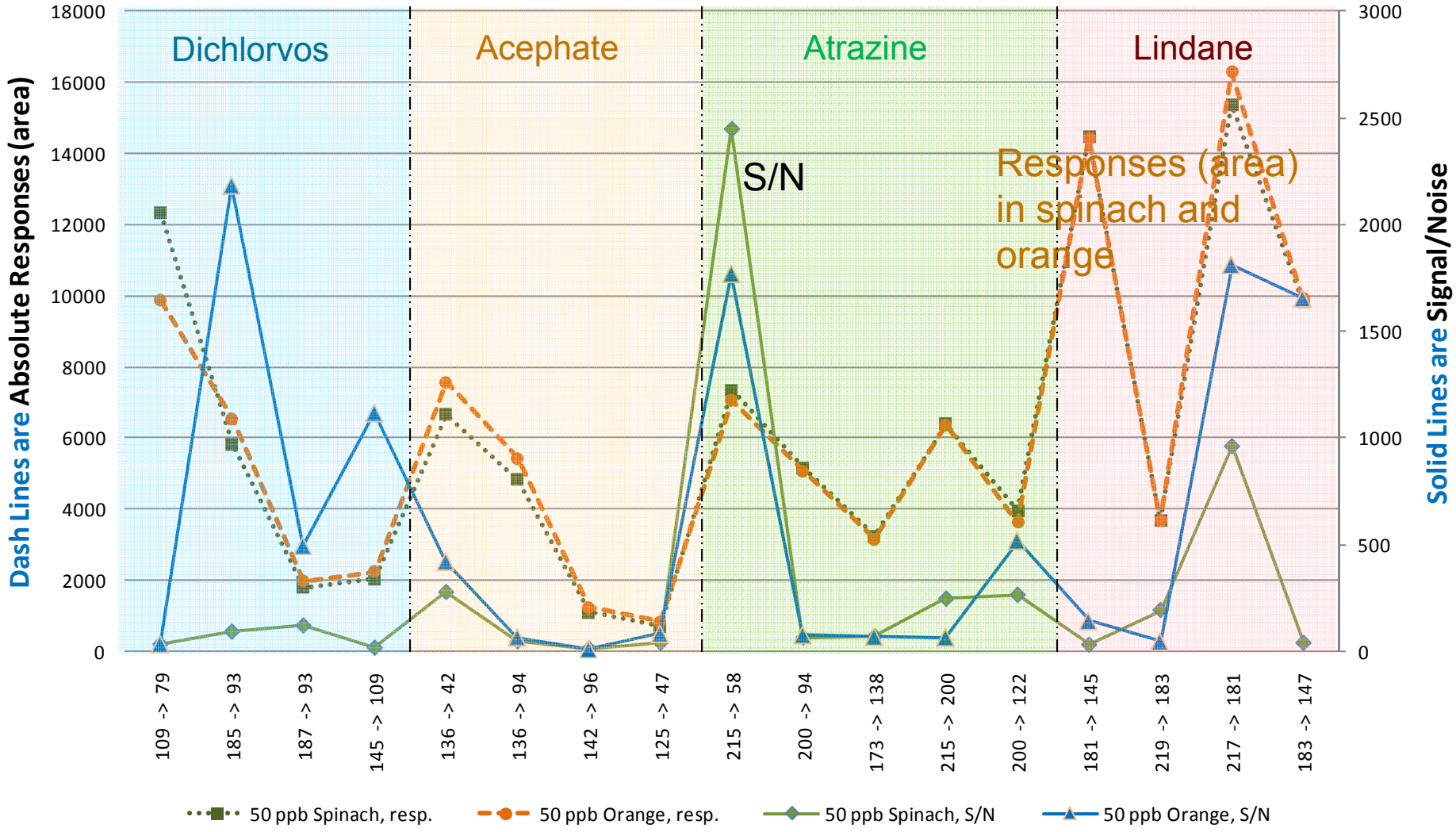
MRM Transitions are not Universal, Should Choose them According to Matrices



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Summary: Pesticide GC/MS/MS Analyzer

The Pesticide GC/MS/MS Analyzer is **tested as a unit** in the factory to ensure a quick and successful installation

New **flexible and comprehensive** Pesticide MRM Database expands the target compound list to 1000 to meet users' need

The MRM Database

- allows users to build acquisition methods without acquiring expensive or hard-to-get pesticide standards (saves time and money)
- applies to either constant flow or constant pressure method (adapts to user's preference or analytical method)
- has multiple MRM transitions (average 7) for each compound (helps to provide alternatives to work around matrix interference)
- shows relative intensity of each MRM transition (facilitates transition selection and acquisition method creation)

ASMS 2011 Introduction:
7200 High Resolution, Accurate Mass GC/Q-TOF

Many ASMS Conferees Asked:
How Would a GC/Q-TOF Benefit My Lab?

Other ASMS Conferees Asked:
Why Q-TOF and Not Just TOF?

For This e-Seminar, You Might Ask:
How Can a Q-TOF Extract More from Complex Samples?

Fundamental Benefits (Agilent 7200 Q-TOF)

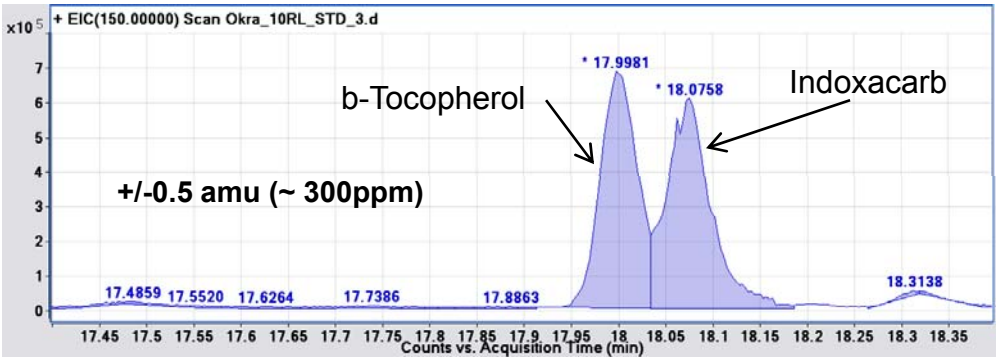
- High resolution (> 10K, typically > 13K FWHM)
  - Increased detector selectivity (few interferences)

TOF Accurate Mass to Eliminate Matrix Interferants

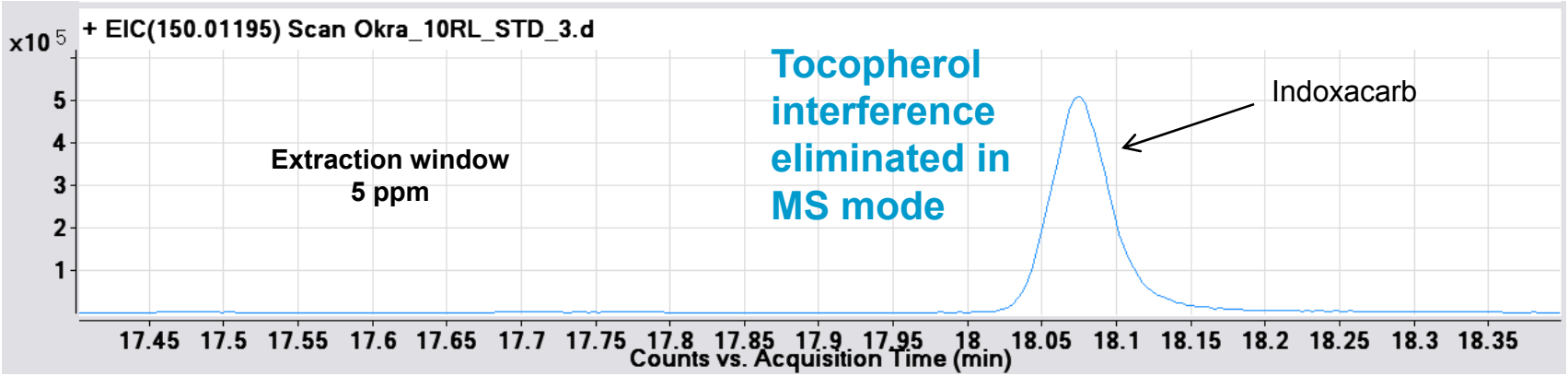
Okra QuEChERS Extract
Matrix interferant ion (b-Tocopherol)
150.06839 Da
Analyte Indoxacarb ion (100pg)
150.01195 Da (fragment ion)

Δm = 0.0564 Da.

'MSD' resolution



TOF high resolution



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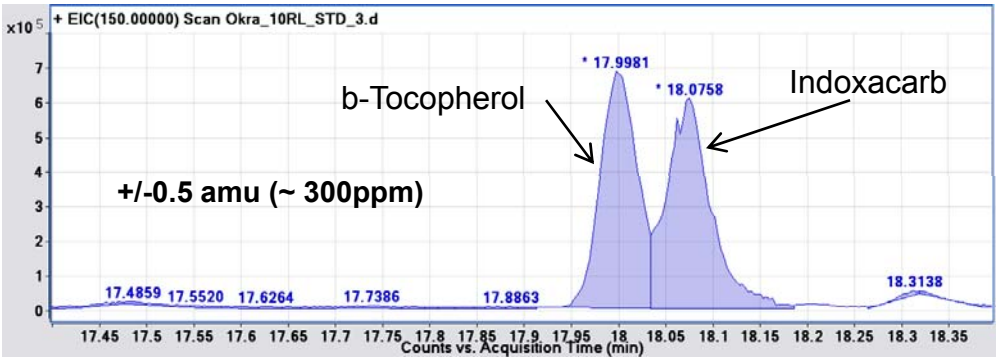

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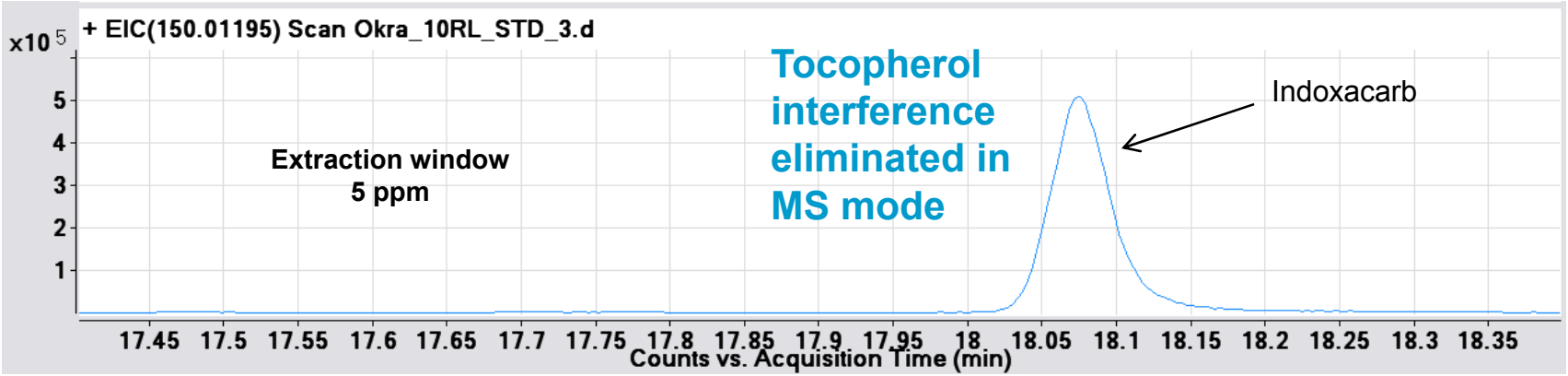
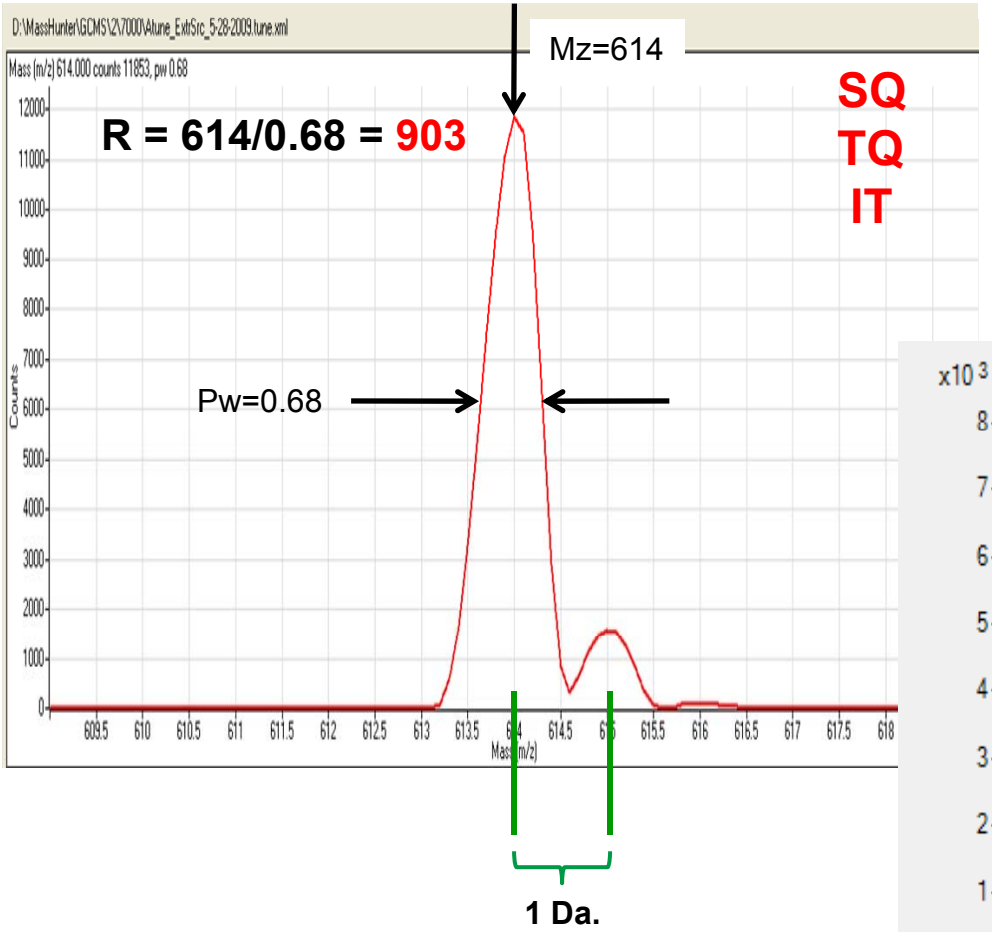


If even more selectivity is needed, option of MS/MS
MS/MS with high resolution and accurate mass!

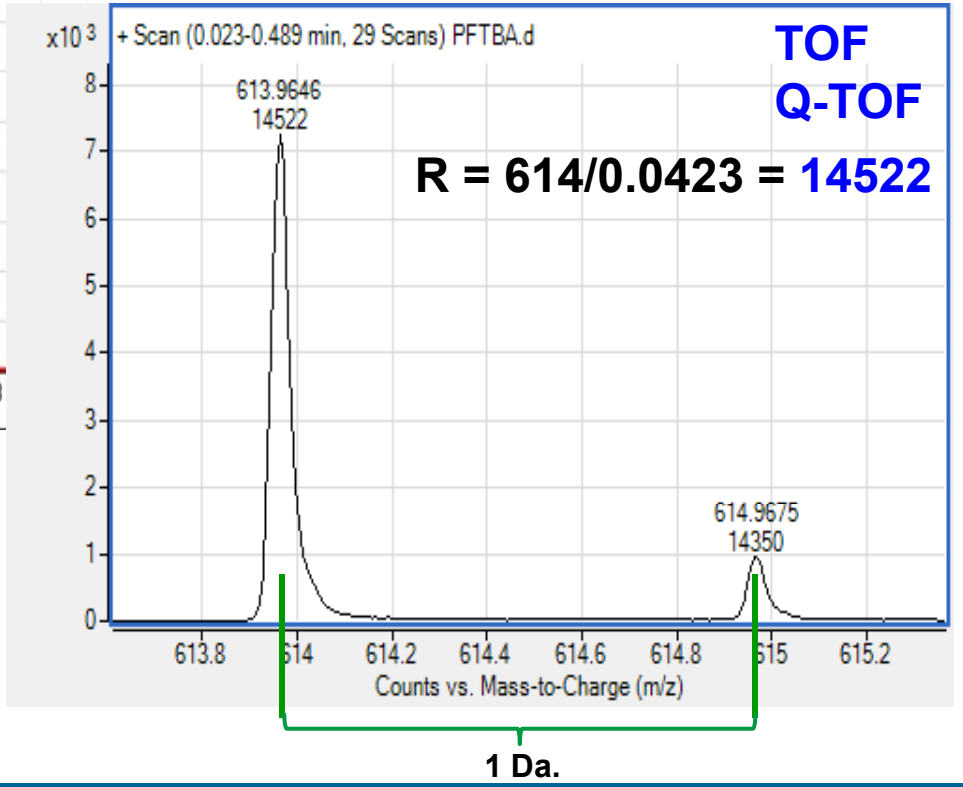
Resolving Power



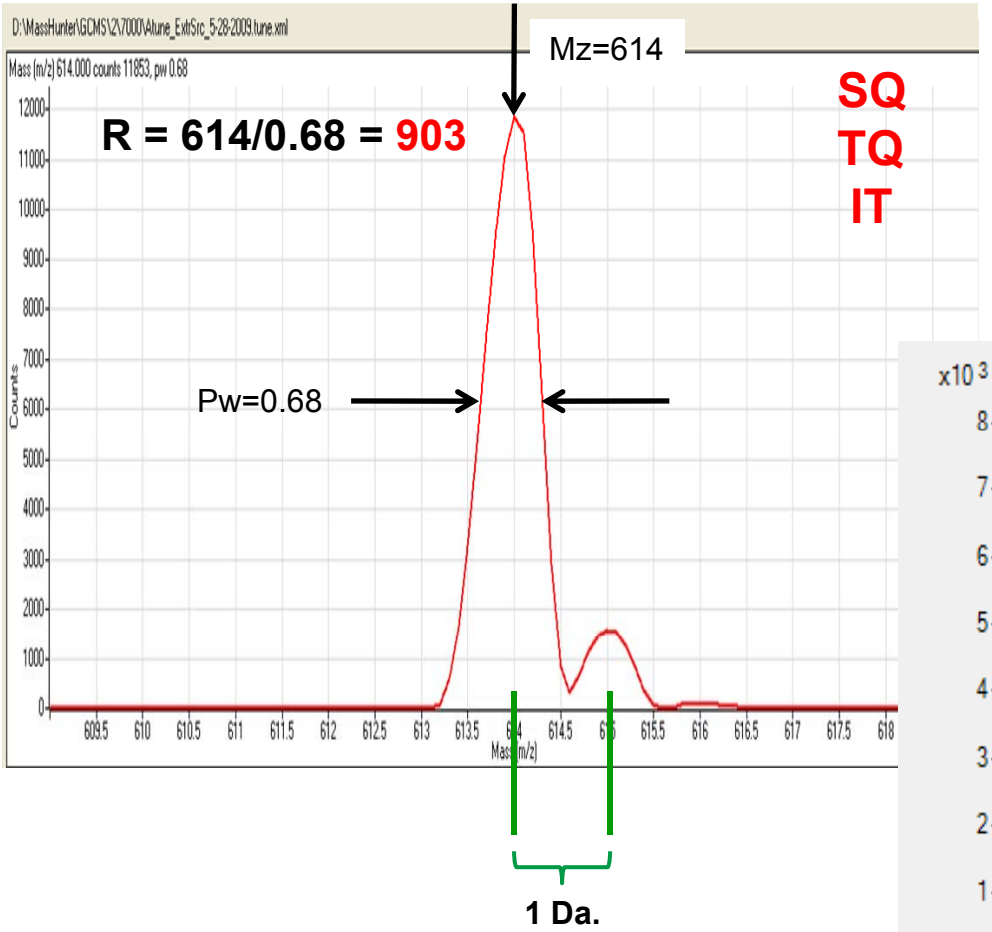
Resolving Power:
R=mz/FWHM

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

PFTBA mass 614
C12F24N=613.964203



Resolving Power



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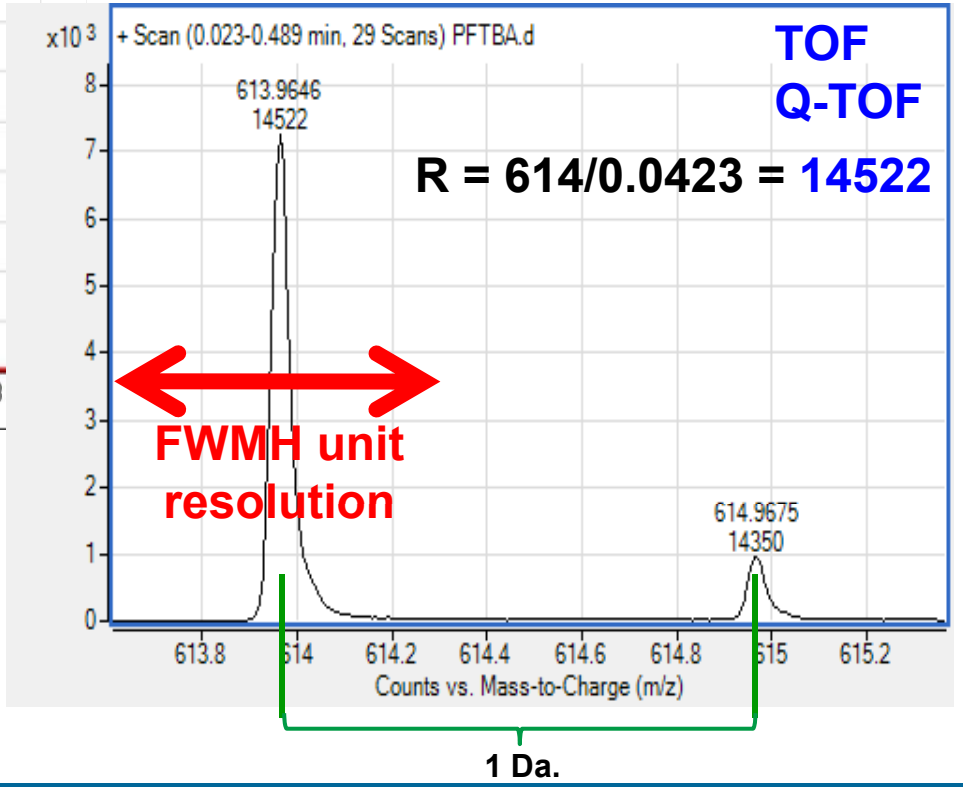
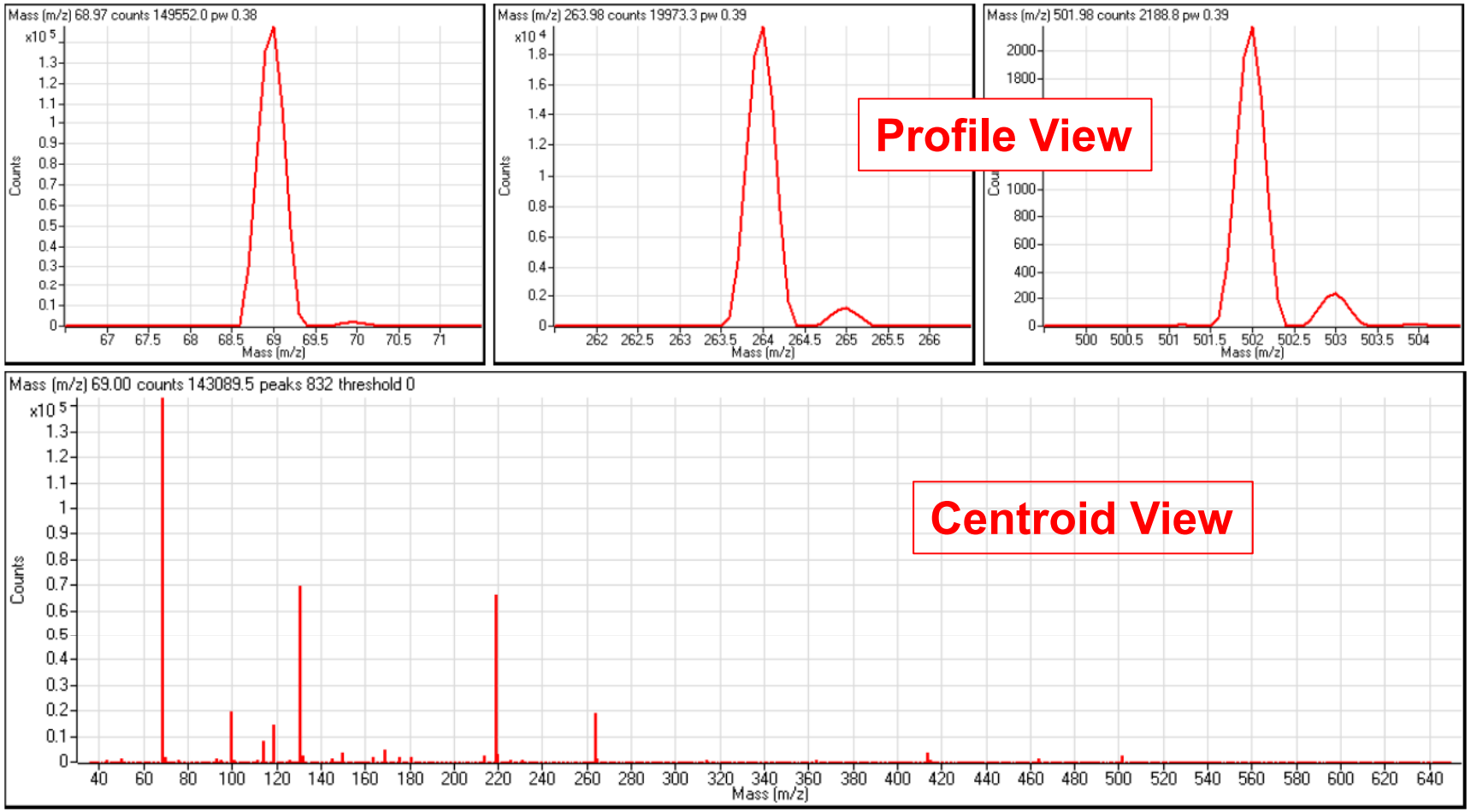
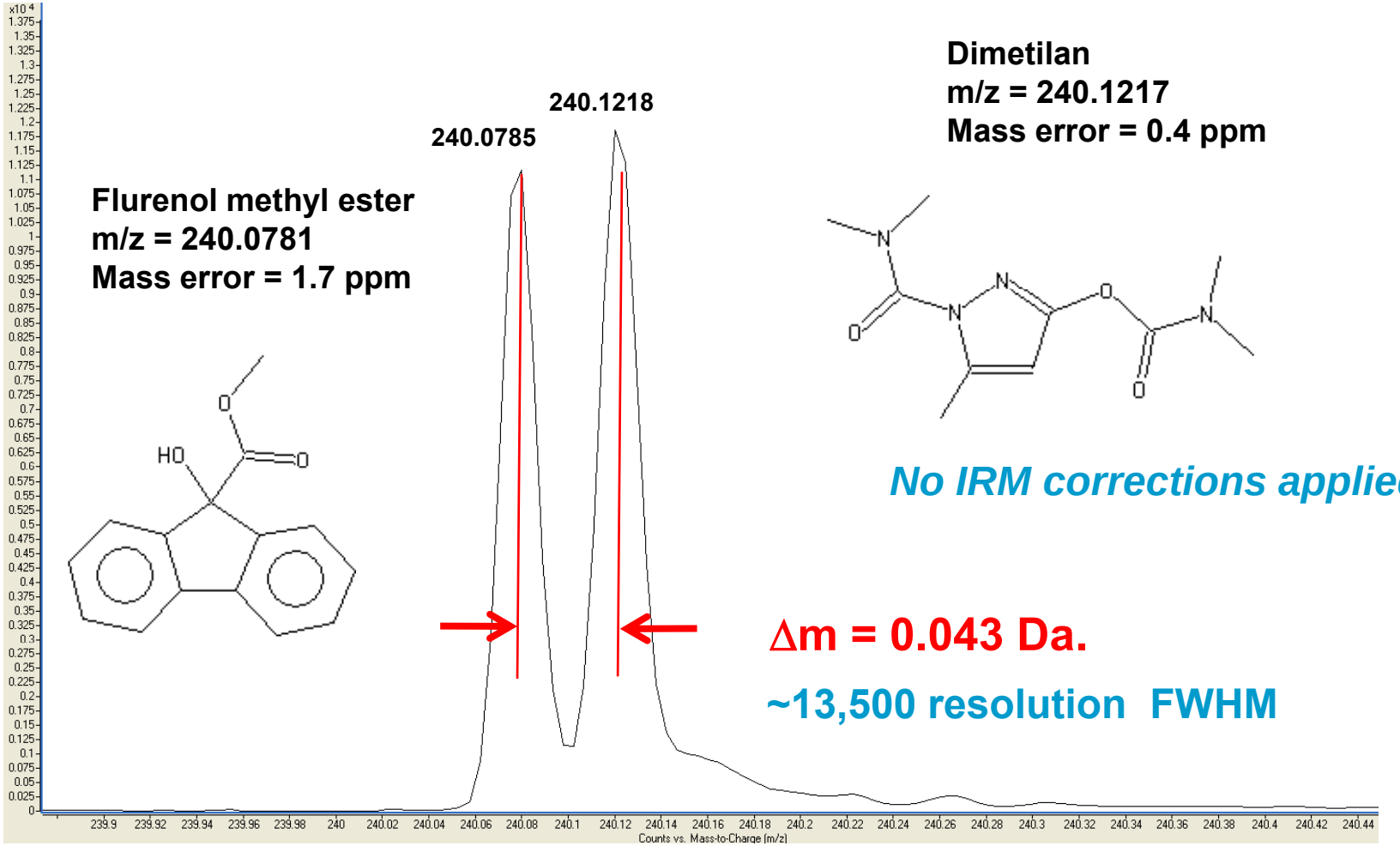


Spectral Presentation (Tune File)

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



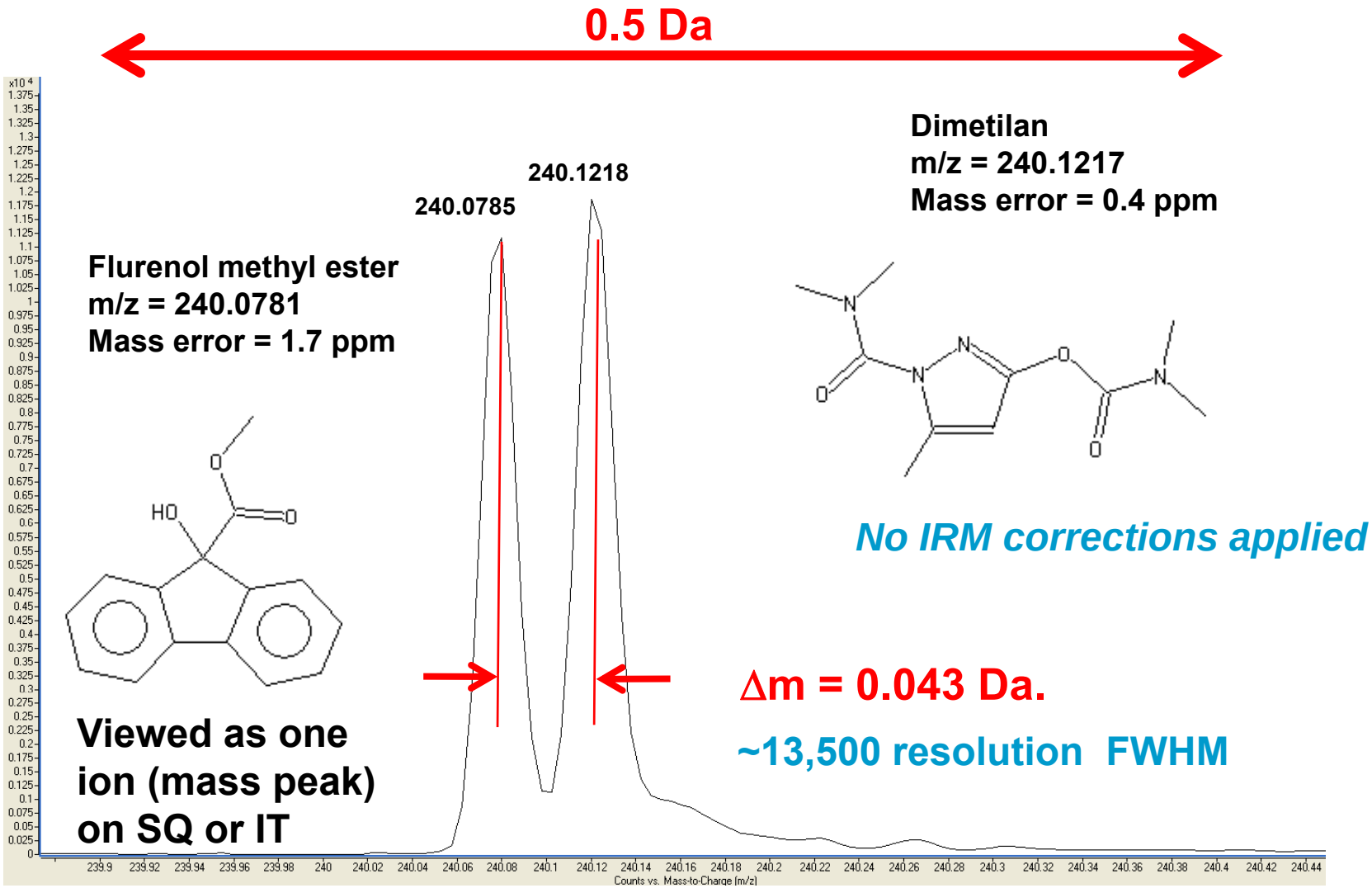
Selectivity for Isobaric Ions



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

Selectivity for Isobaric Ions



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- Accurate mass measurements (low to sub-ppm)
  - < 5 ppm in TOF (typically < 2 ppm)
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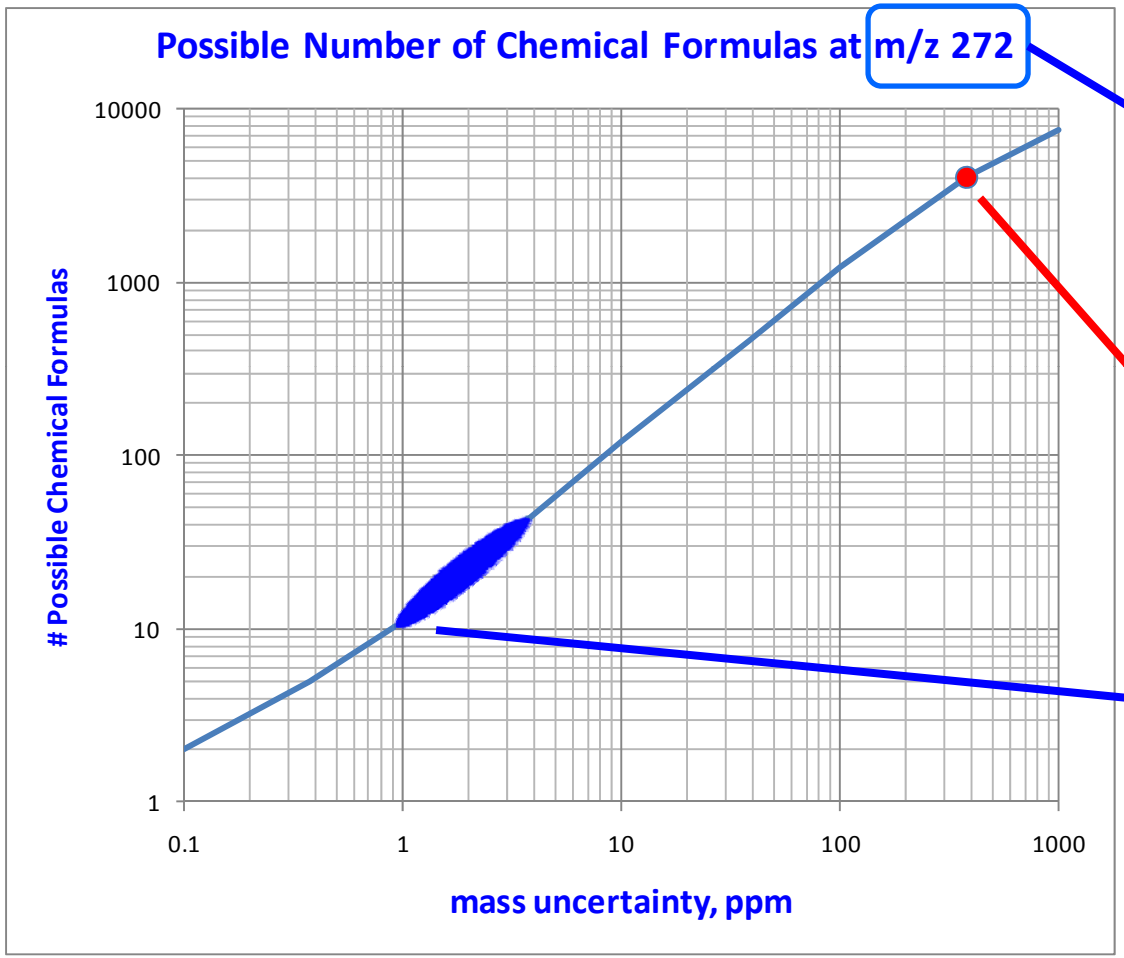
  - Valuable qualitative information about each ion

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

Fragment ion mass with high mass accuracy

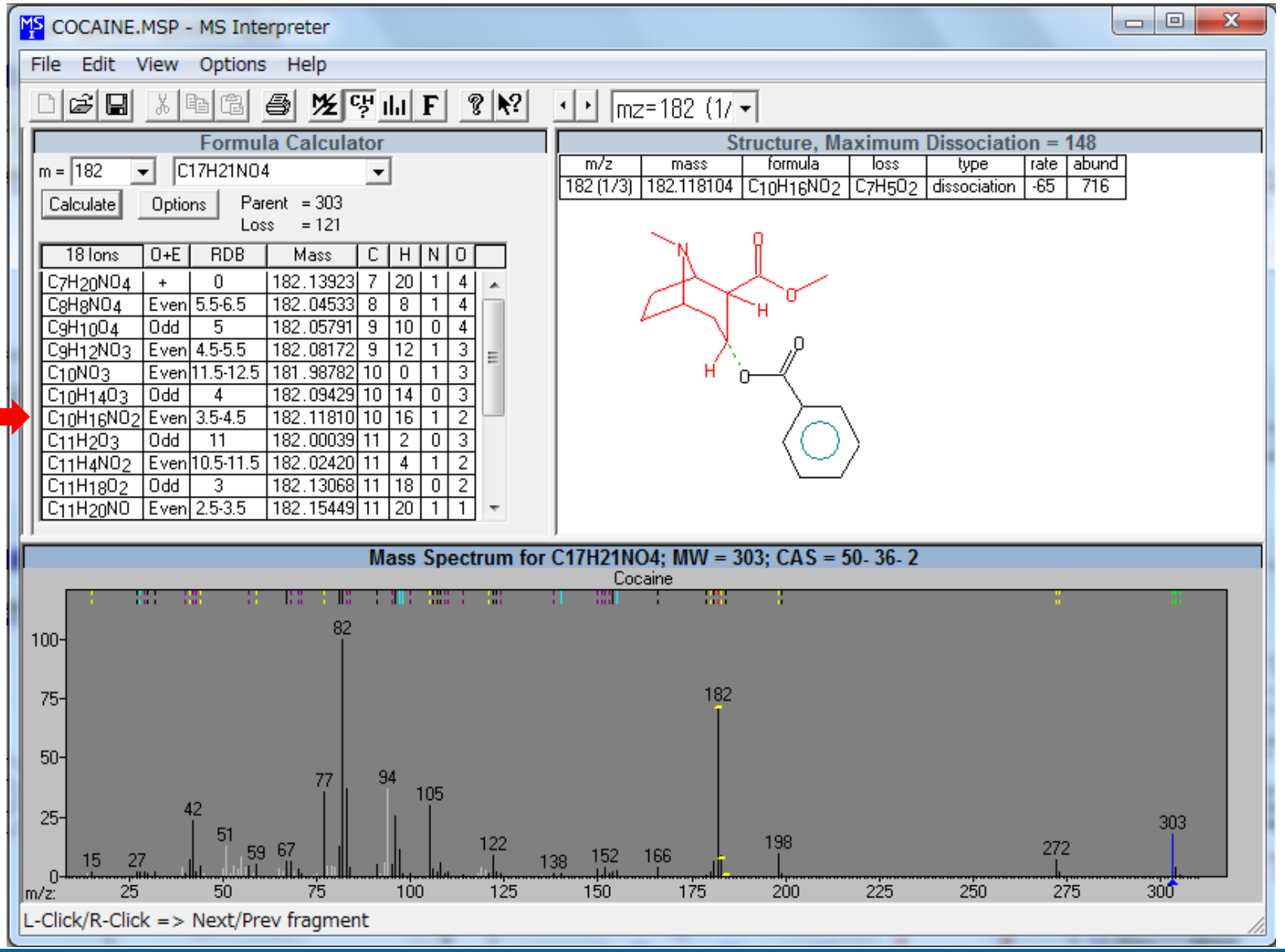
Helps unambiguously identify corresponding formula and hence exact mass of a fragment

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

NIST 2011 MS Interpreter with Accurate Mass



Agilent Technologies

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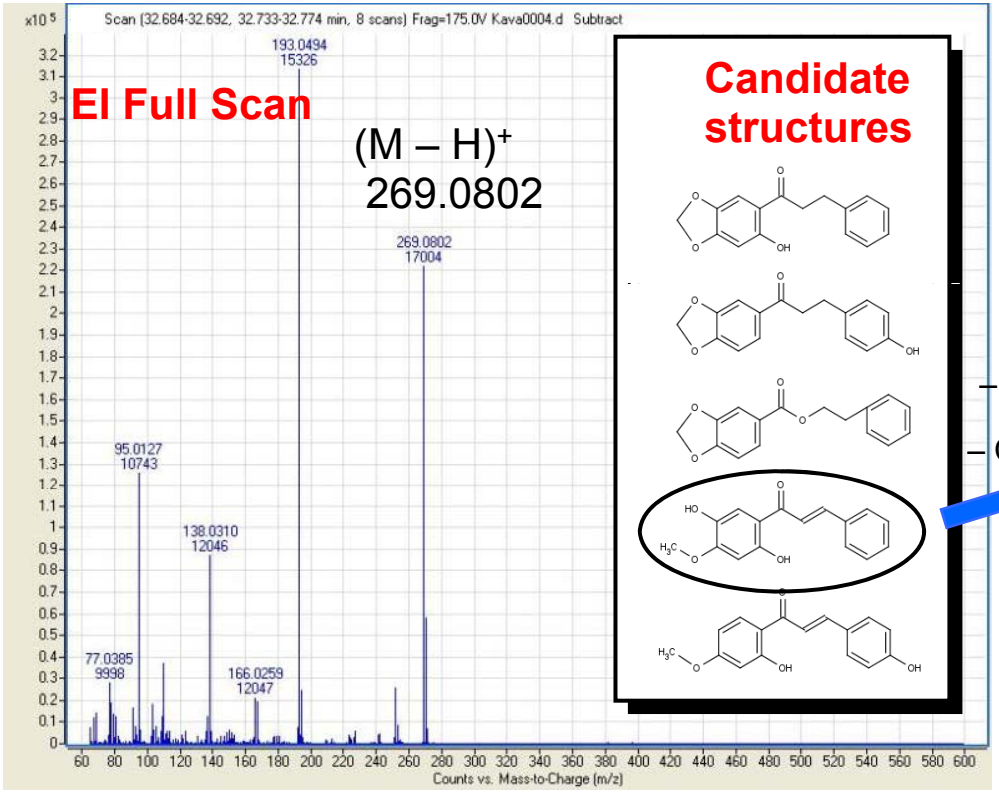
- Structural elucidation with *Accurate Mass* MS/MS studies
  - High sensitivity tool to complement NMR

The Problem – Confirm Most Likely Structure

Kava Extract - Compound "B", $C_{16}H_{14}O_4$ (Rings + Double Bonds = 10)



– H

– C_6H_5

– $CH=CH–C_6H_5$

– $CH_2=CH–C_6H_5$

– CO

– CO

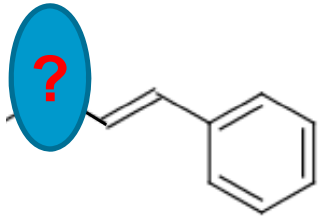
– CH_3

Experimental measurements

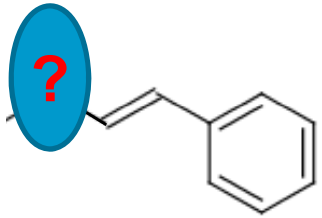
m/z (experimental)	Formula	Error (ppm)	Score
269.0802	**$C_{16}H_{13}O_4$**	**2.2**	**80.7**
193.0494	**$C_{10}H_9O_4$**	**0.6**	**96.7**
167.0334	**$C_8H_7O_4$**	**3.0**	**N/A**
166.0259	**$C_8H_6O_4$**	**0.6**	**N/A**
138.0310	**$C_7H_6O_3$**	**1.1**	**98.1**
110.0359	**$C_6H_6O_2$**	**3.0**	**N/A**
95.0127	**$C_5H_3O_2$**	**0.9**	**99.5**

For the 5 candidate structures, only one fit the losses identified by CID experiments on multiple precursor ions

Problem – confirm most likely structure

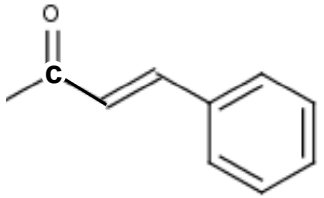


Problem – confirm most likely structure



Mass at 138 is consistent with loss of **COCH**=CH-C_6H_5 (131.04969)
or
C_2H_4CH=CH-C_6H_5 (131.086075) from 269.08020.

Problem – confirm most likely structure



Mass at 138 is consistent with loss of **COCH**=CH-C_6H_5 (131.04969)
or
C_2H_2CH=CH-C_6H_5 (131.086075) from 269.0802.

However, measured value of 269.0802 - 138.0310 = 131.04920 is consistent only with **COCH**=CH- C_6H_5.

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  - High sensitivity tool to complement NMR
- "Fast", full spectra acquisition with excellent sensitivity

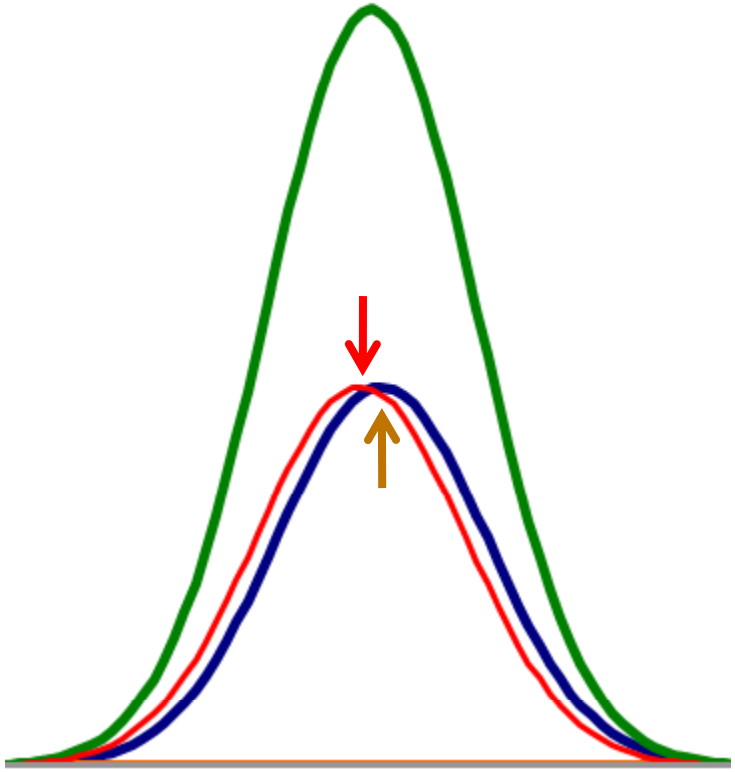
What about TOF *SPEED?*

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

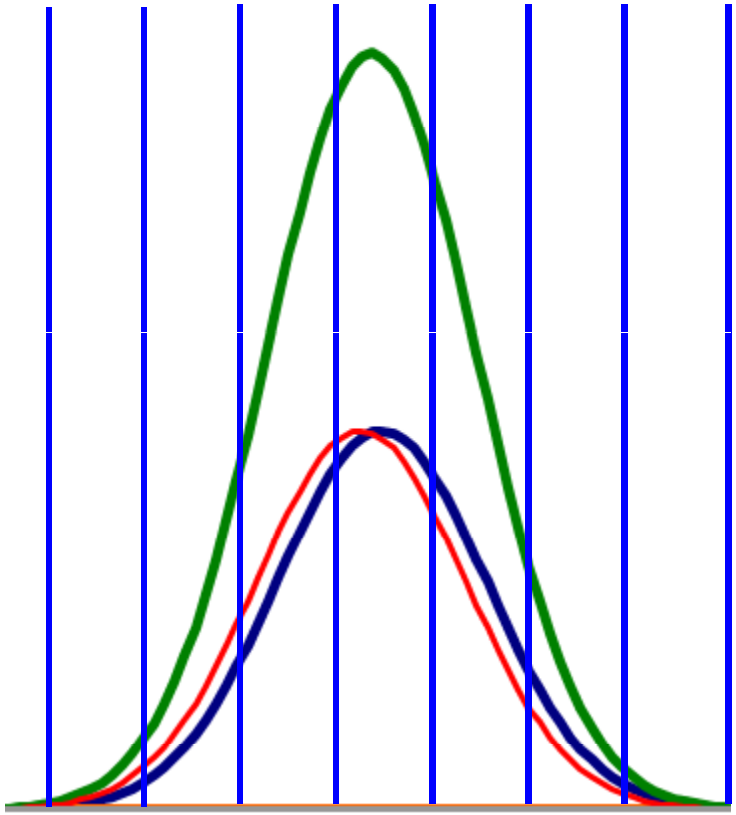
"*Speed*" Enhances Deconvolution

Deconvolution Requires Time Offset



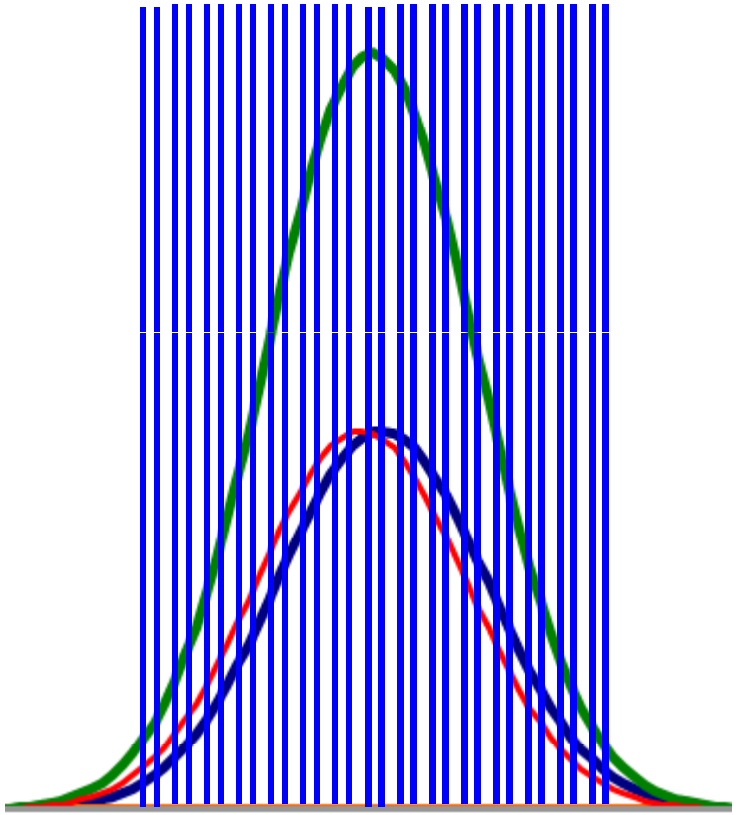
Time

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

Successful GC/MS Applications Require
the Correct Combination of:

GC Resolution

+

MS Resolving Power

Successful GC/MS Applications Require
the Correct Combination of:

GC Resolution

+

MS Resolving Power

+

ΔMass Defect (Mother Nature)

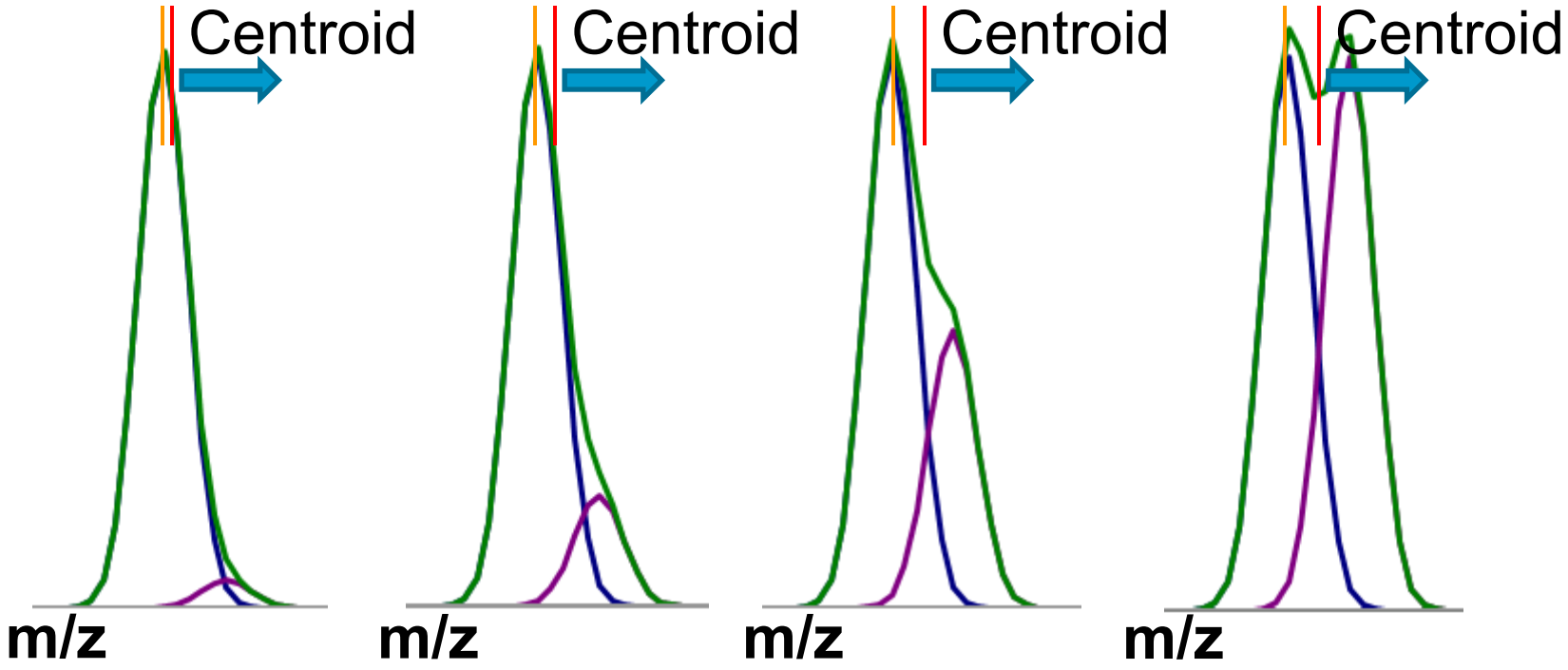
+

Relative Ion Intensities (Sample)

There is more to learn about these new apps

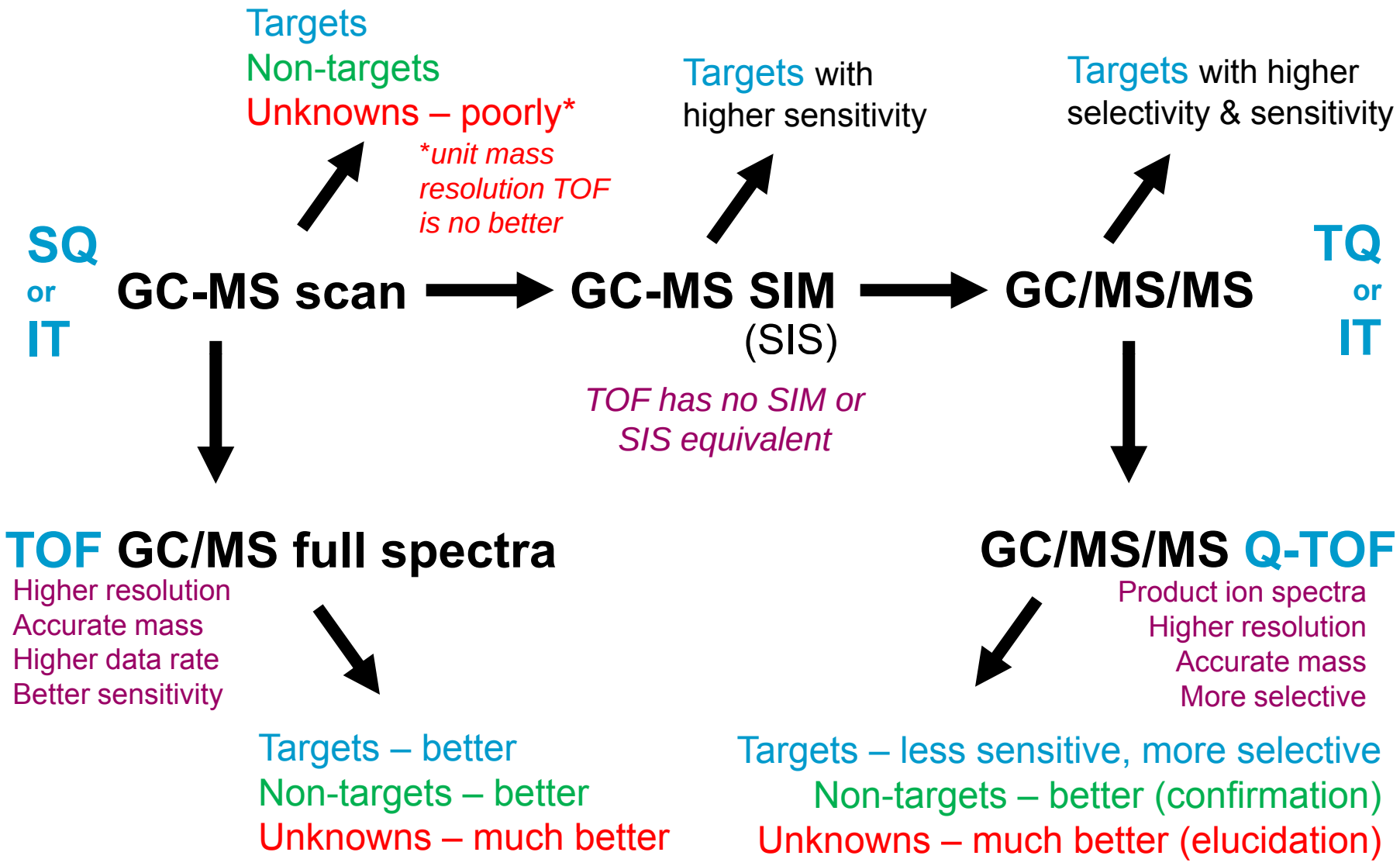
GC or MS:
Relative intensity affects the result

Profile view of mass peaks



Centroid view of mass peaks obscures this fact

What Are the Application Drivers for Q-TOF?



Thank You
For Joining Us Today

Time For
Q&A