Expanding Lab Capability using Agilent's GC/QQQ Analyzer with a New Versatile 1000-compound Pesticide MRM Database

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

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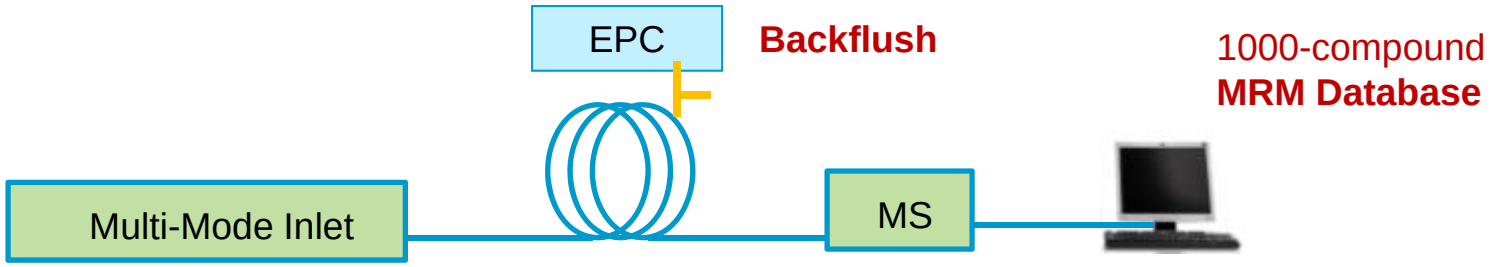
What is a Pesticide GC/MS/MS Analyzer?

A pre-configured and chemically tested GC/TQ system loaded with methods and a 1000-compound Pesticide MRM database for quick installation and start-up.

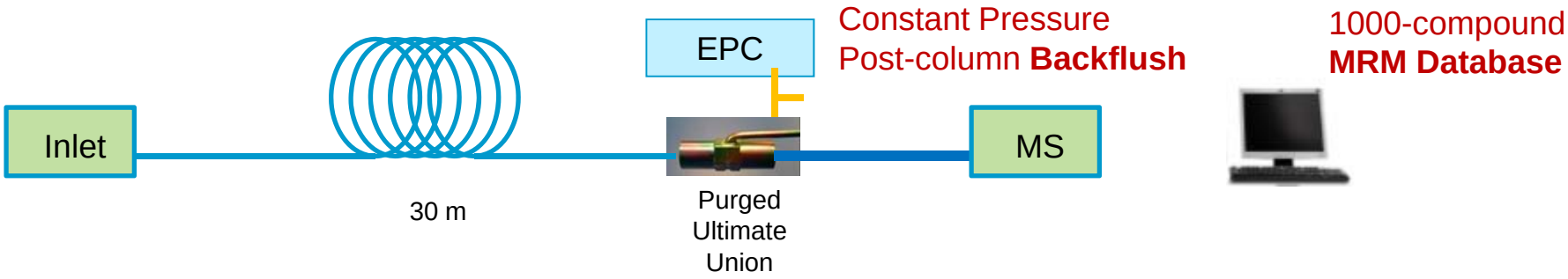


Hot split/splitless
Cold splitless
Solvent vent (LVI)

Backflush: reversing the column flow

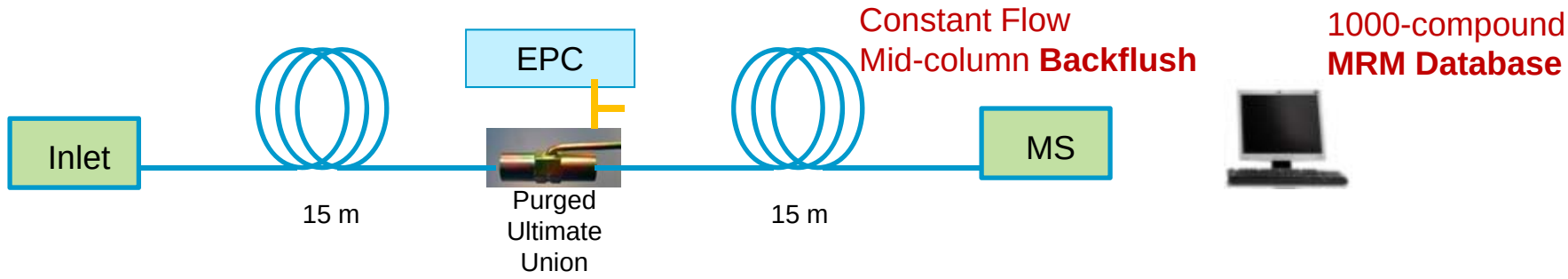
Pesticide Analyzer System Configuration

SP1 7890-0501 Setup



Flexible to add GC detectors and easily scaled for shorter runtime

SP1 7890-0502 Setup



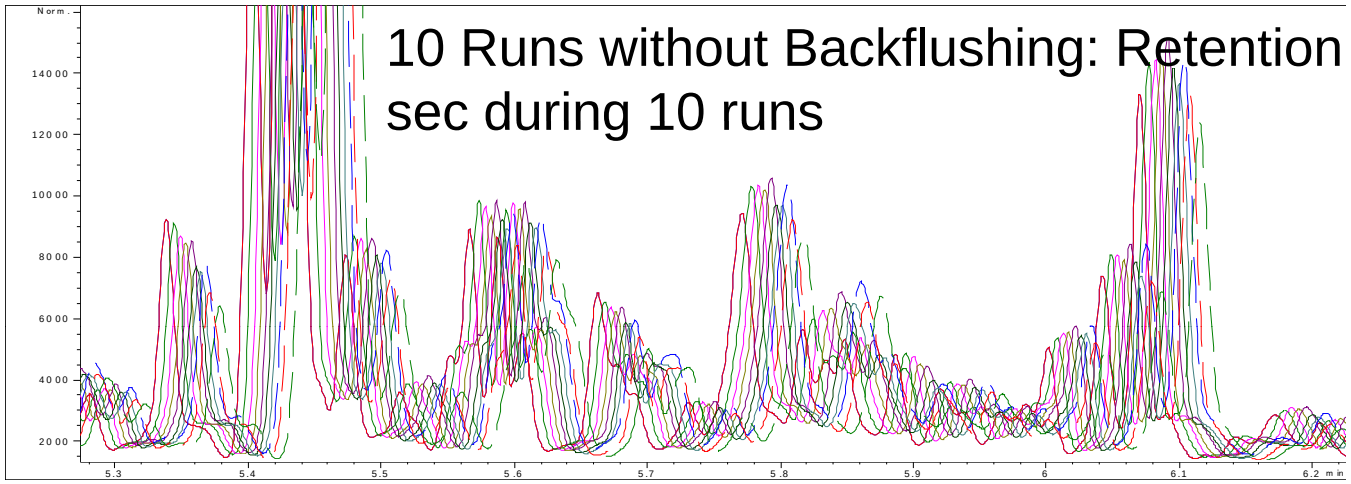
Provides ultimate performance and shortest cycle time

Why Do We Need Backflush?

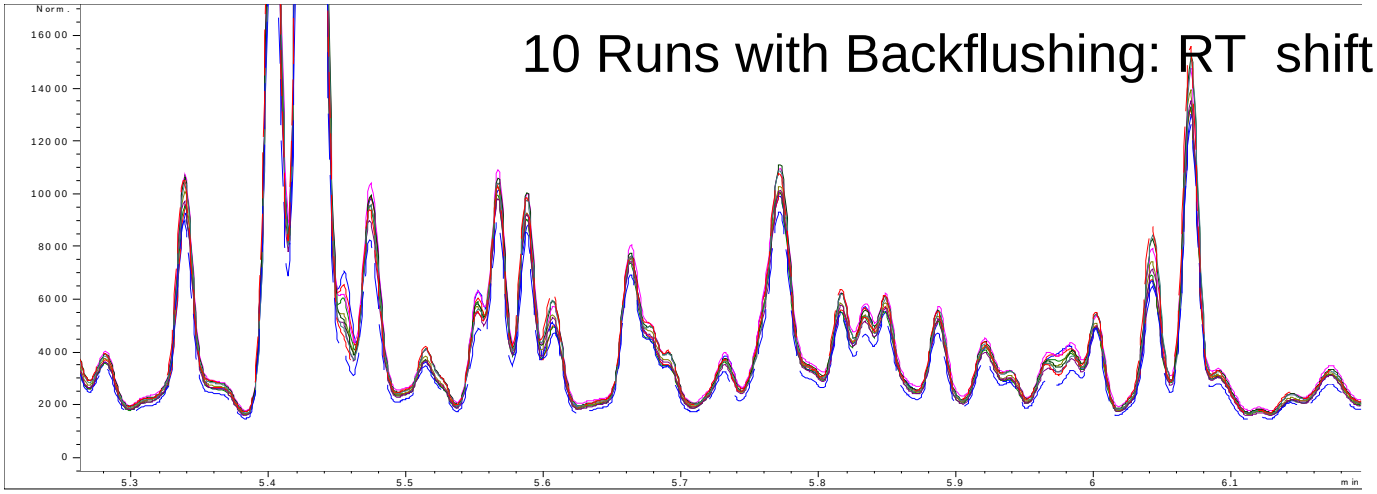
- With the selectivity of MS/MS, **users cannot see "dirty matrix"**
- MS/MS users want the LOWEST detection limits – **inject more** with large volume injection
- Many late eluting peaks are not "chromatographically ideal" and **leave a residue** throughout the column
- Heavy matrix contaminates the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

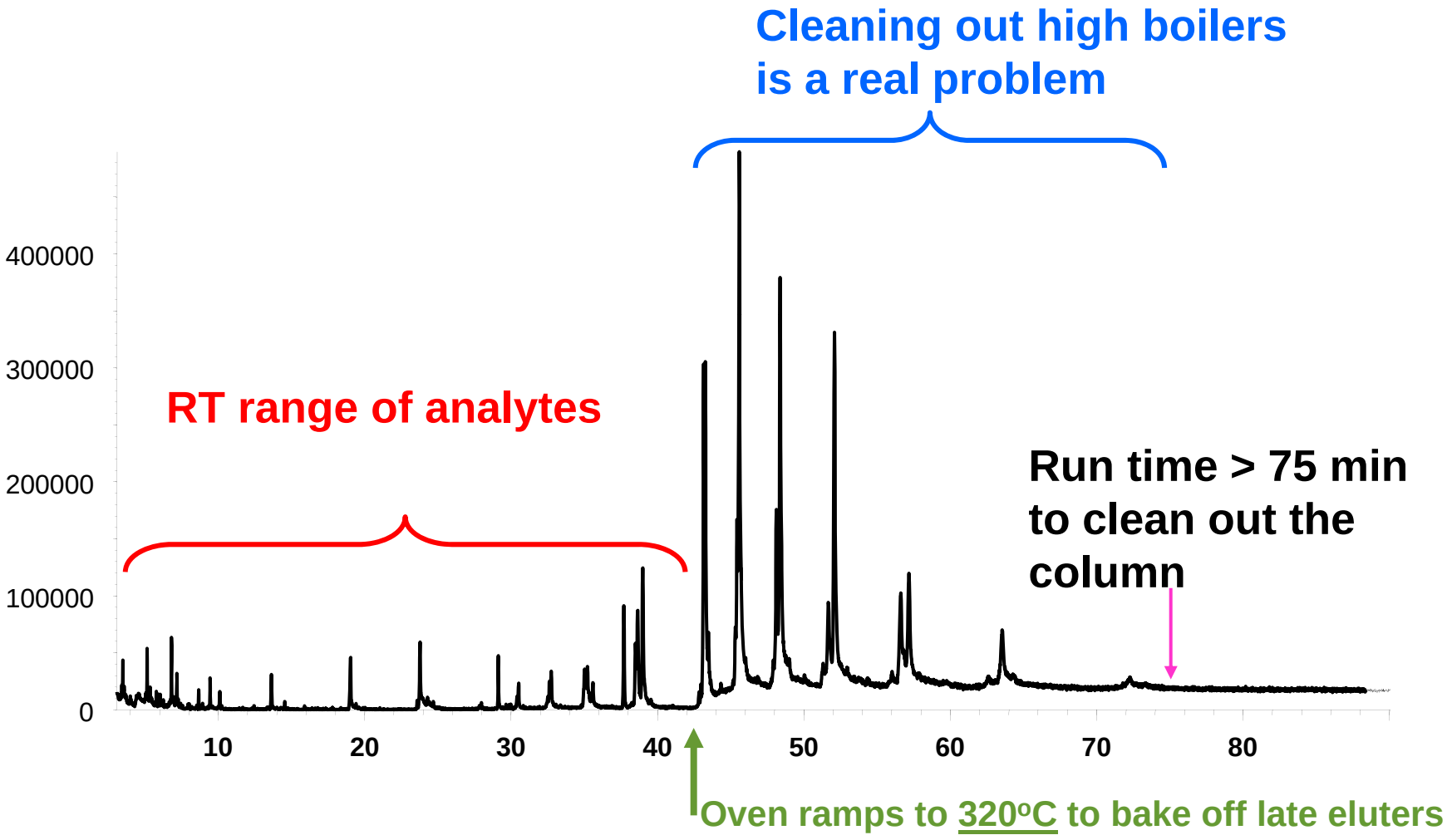


10 Runs without Backflushing: Retention times shift ~4-5 sec during 10 runs

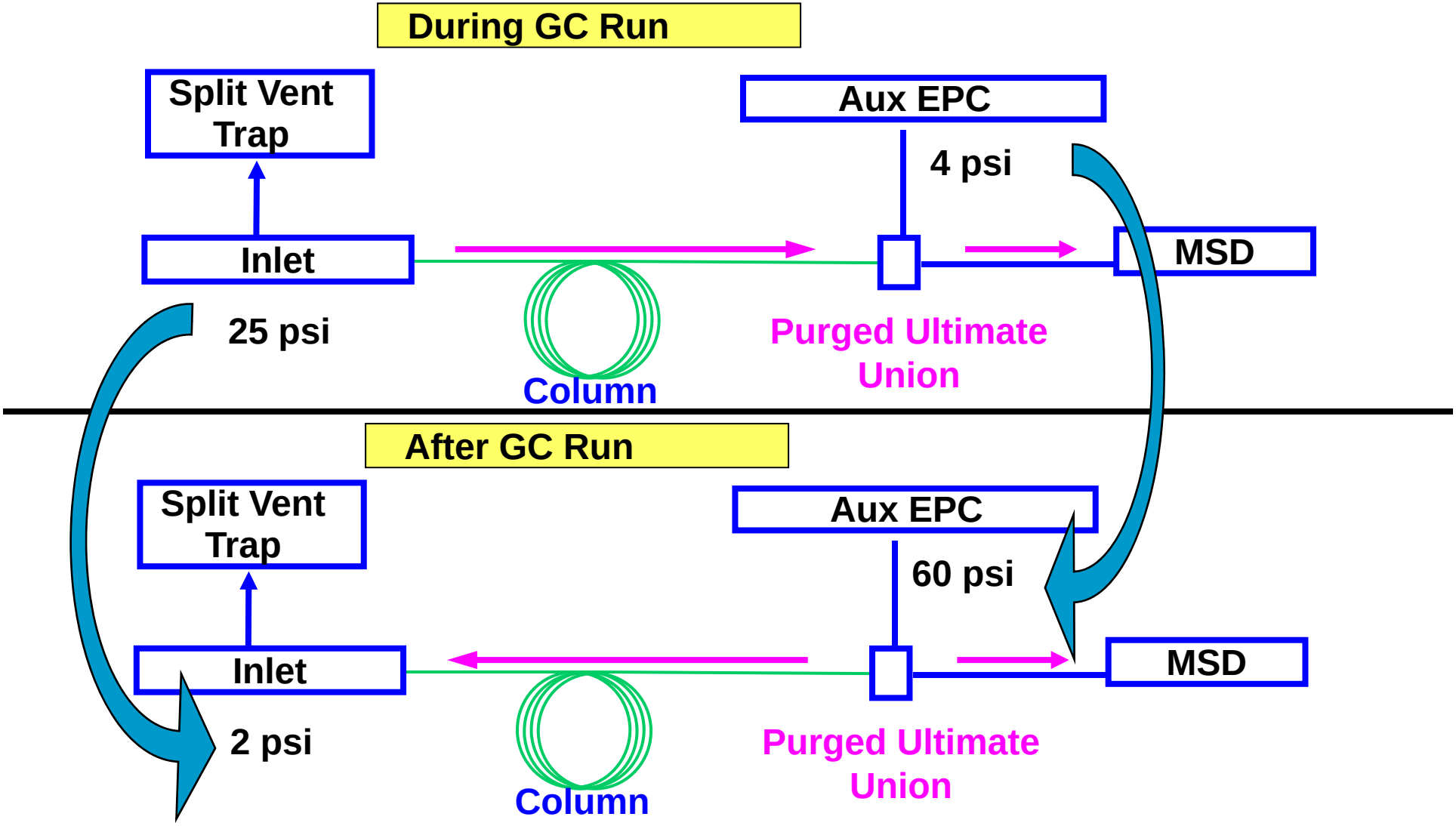


10 Runs with Backflushing: RT shift eliminated

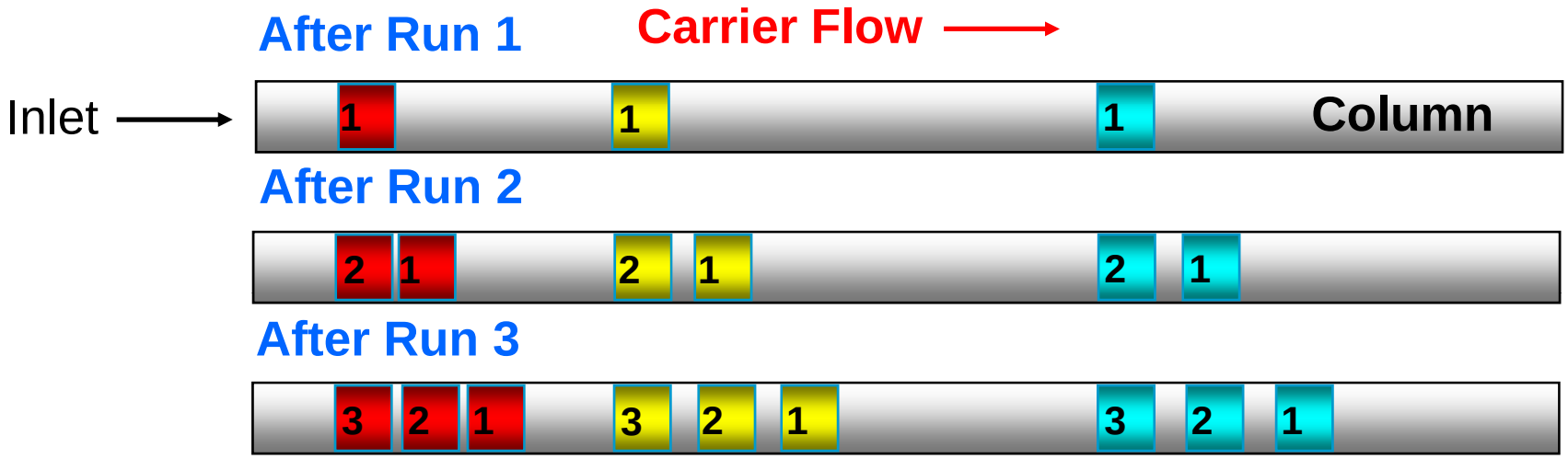
Milk Extract - Using Bakeout To Remove High Boilers



Backflush


During GC Run
Split Vent Trap
Aux EPC
4 psi
Inlet
MSD
25 psi
Column
Purged Ultimate Union
After GC Run
Split Vent Trap
Aux EPC
60 psi
Inlet
MSD
2 psi
Column
Purged Ultimate Union

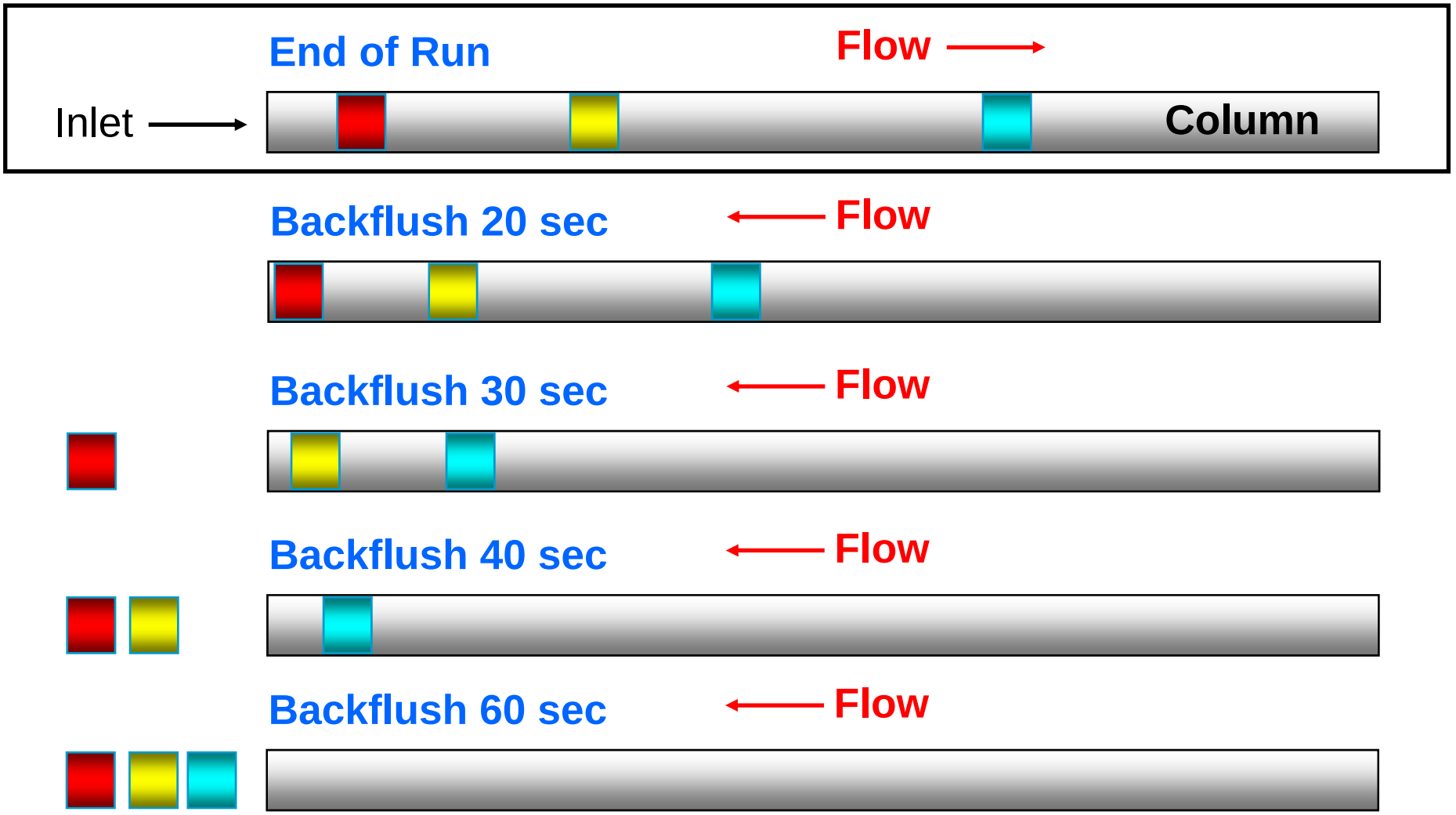
Heavy Compounds May Be Left in Head of Column After Each Injection



These heavy materials build up and travel further into the column with each injection.

This buildup of heavy materials causes retention time shifts, peak distortion, higher bleed, and loss of sensitivity

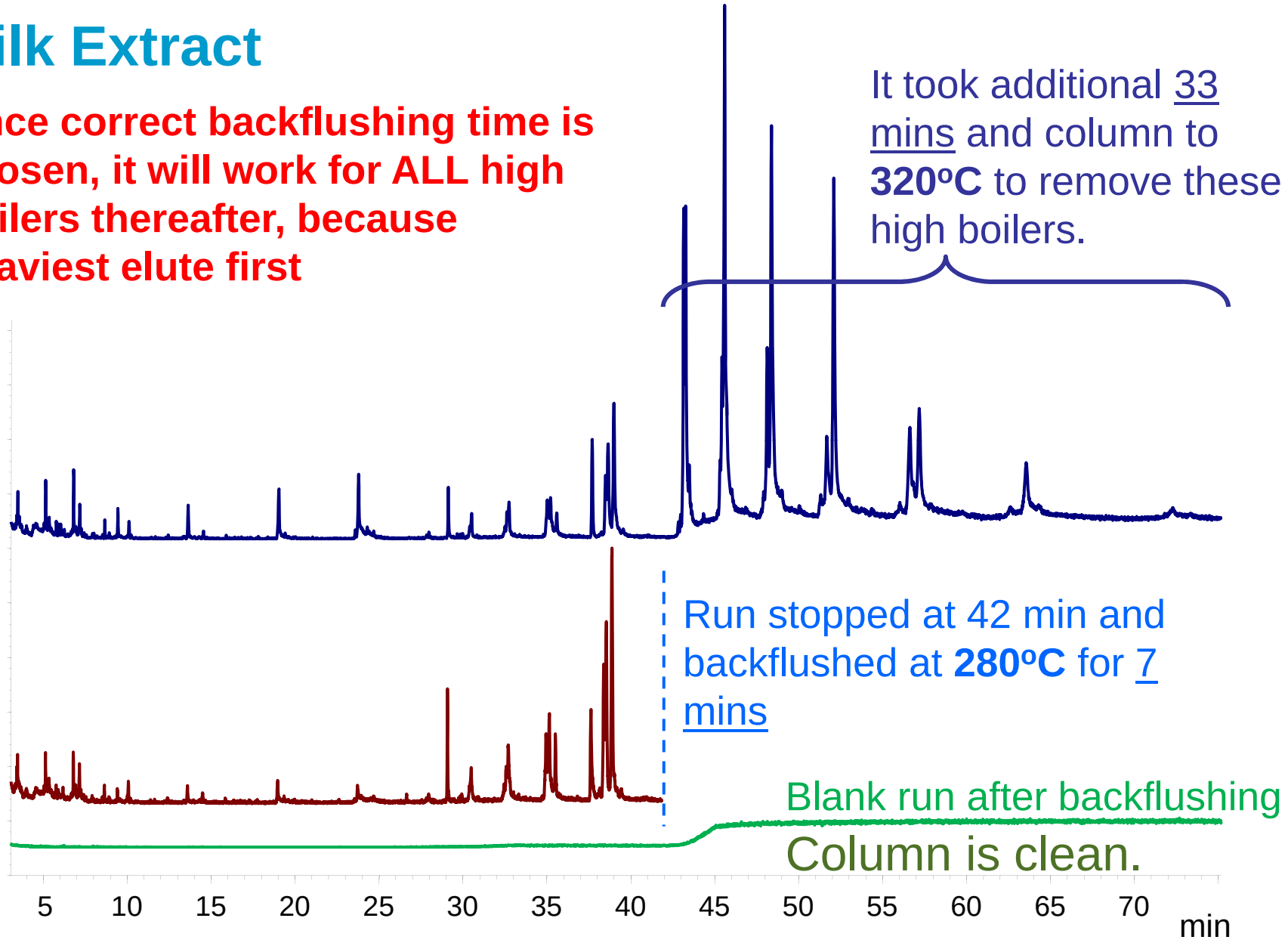
Backflushing After Each Injection



Backflushing removes heavy materials after each injection.

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

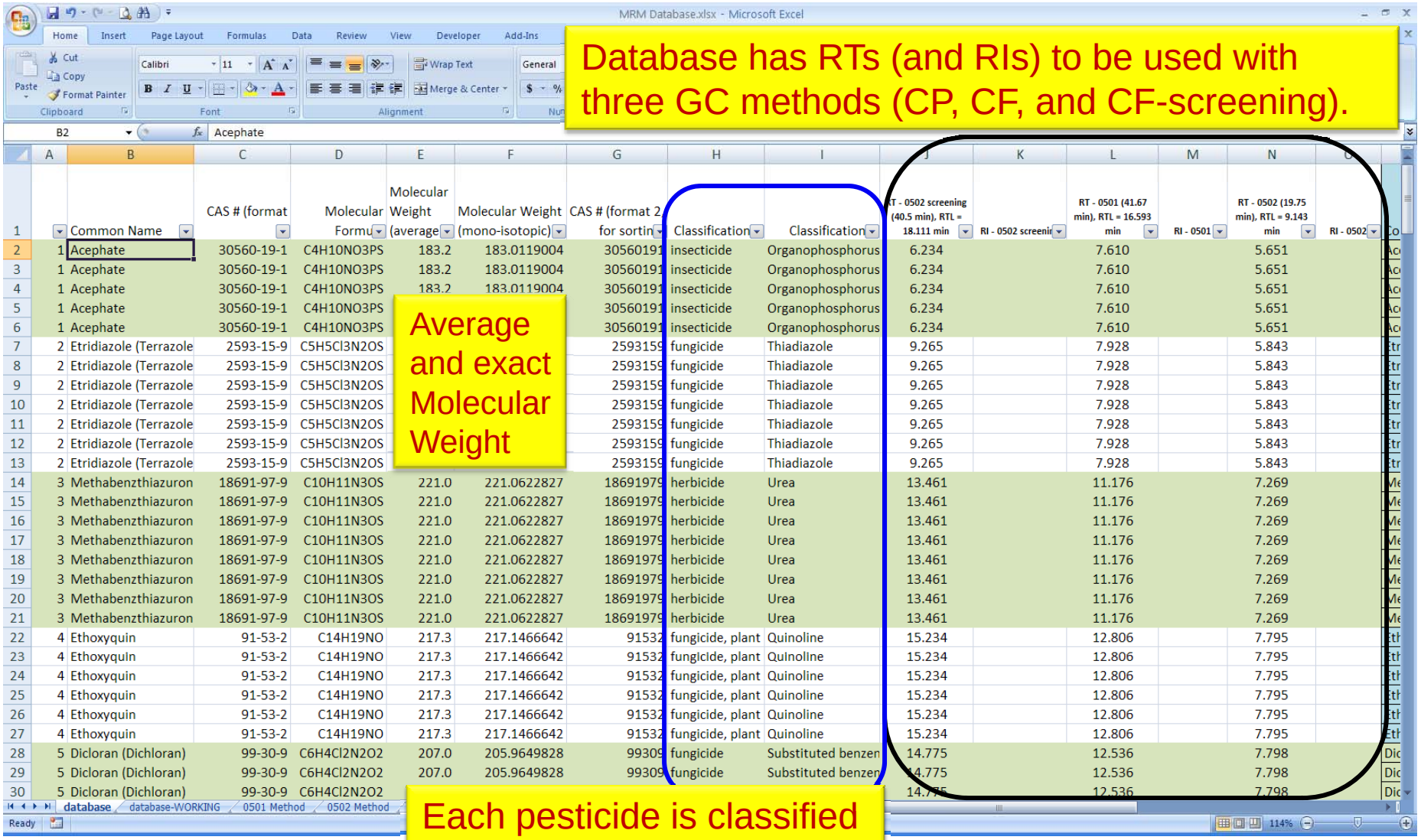
❖ Contains 7000 optimized MRMs for 1000 pesticides

-- 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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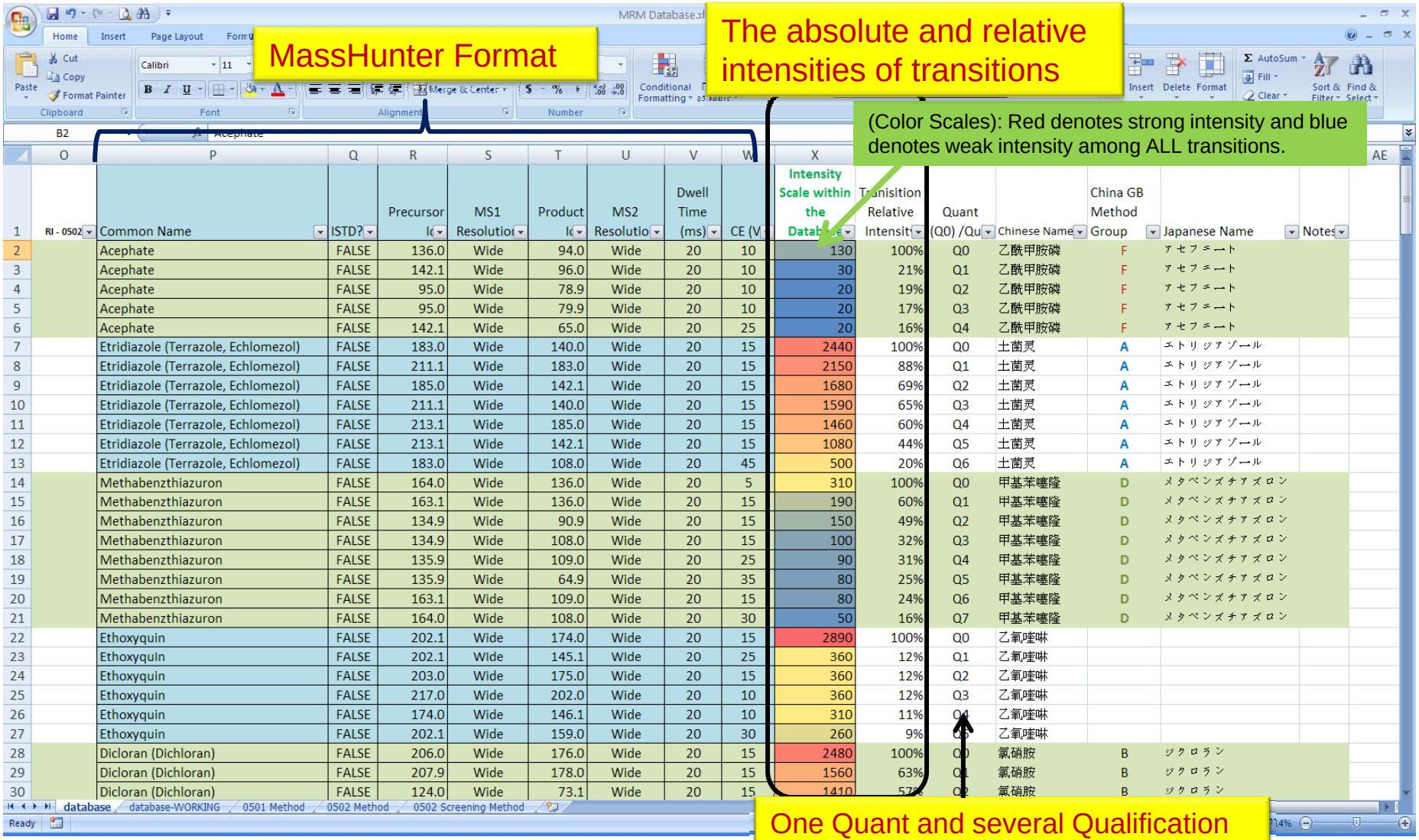
The Flexibility: Excel format, relative and absolute Transition intensity



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) /Qual	Chinese Name	China GB Method Group	Japanese Name	Notes
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	Ethoxyquin	FALSE	202.1	Wide	174.0	Wide	20	15	2890	100%	Q0	乙氧喹啉			
	Ethoxyquin	FALSE	202.1	Wide	145.1	Wide	20	25	360	12%	Q1	乙氧喹啉			
	Ethoxyquin	FALSE	203.0	Wide	175.0	Wide	20	15	360	12%	Q2	乙氧喹啉			
	Ethoxyquin	FALSE	217.0	Wide	202.0	Wide	20	10	360	12%	Q3	乙氧喹啉			
	Ethoxyquin	FALSE	174.0	Wide	146.1	Wide	20	10	310	11%	Q4	乙氧喹啉			
	Ethoxyquin	FALSE	202.1	Wide	159.0	Wide	20	30	260	9%	Q5	乙氧喹啉			
	Dicloran (Dichloran)	FALSE	206.0	Wide	176.0	Wide	20	15	2480	100%	Q0	氯硝胺	B	ジクロラン	
	Dicloran (Dichloran)	FALSE	207.9	Wide	178.0	Wide	20	15	1560	63%	Q1	氯硝胺	B	ジクロラン	
	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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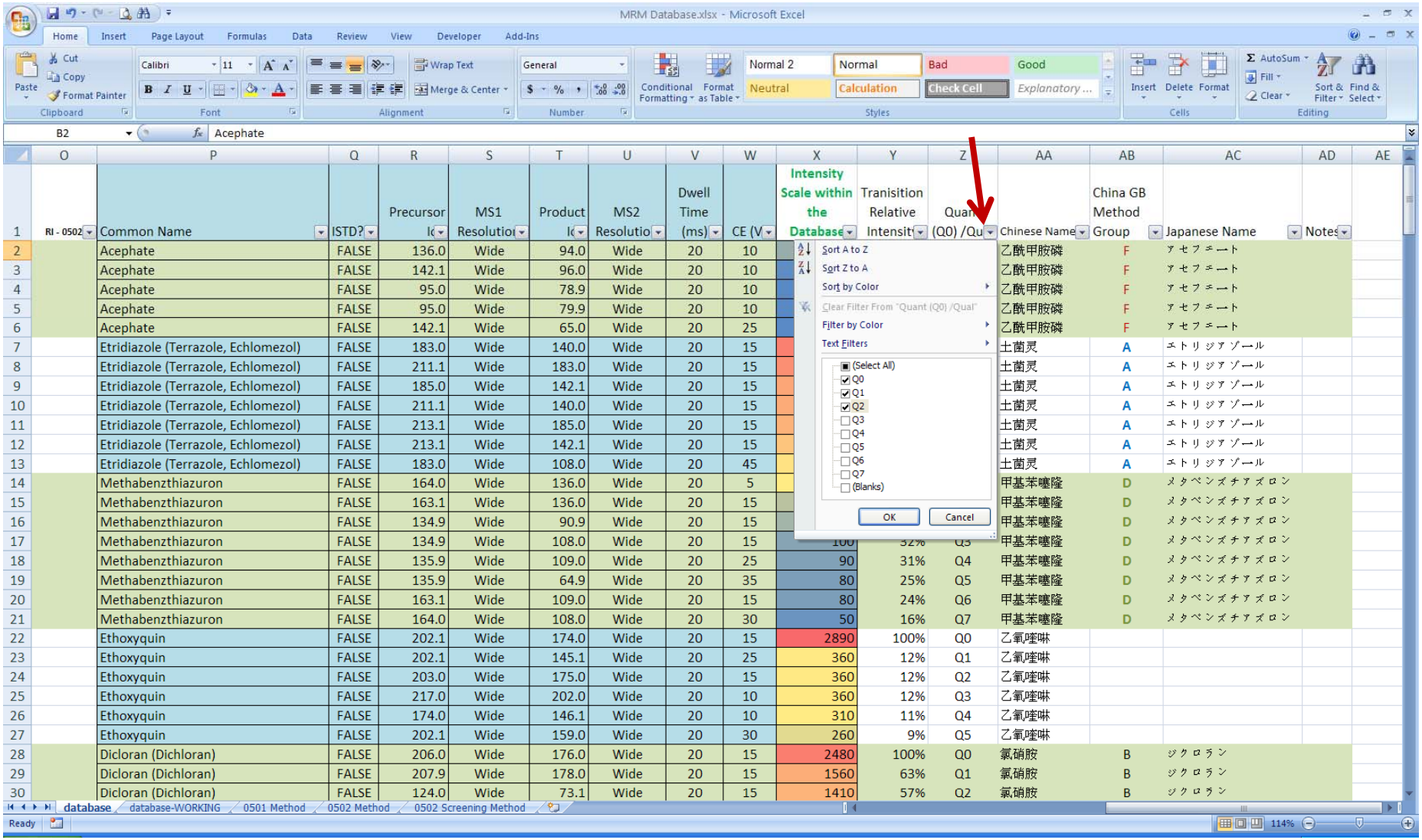
Click on the sorting button to show/hide Quant and Qualifier Ions



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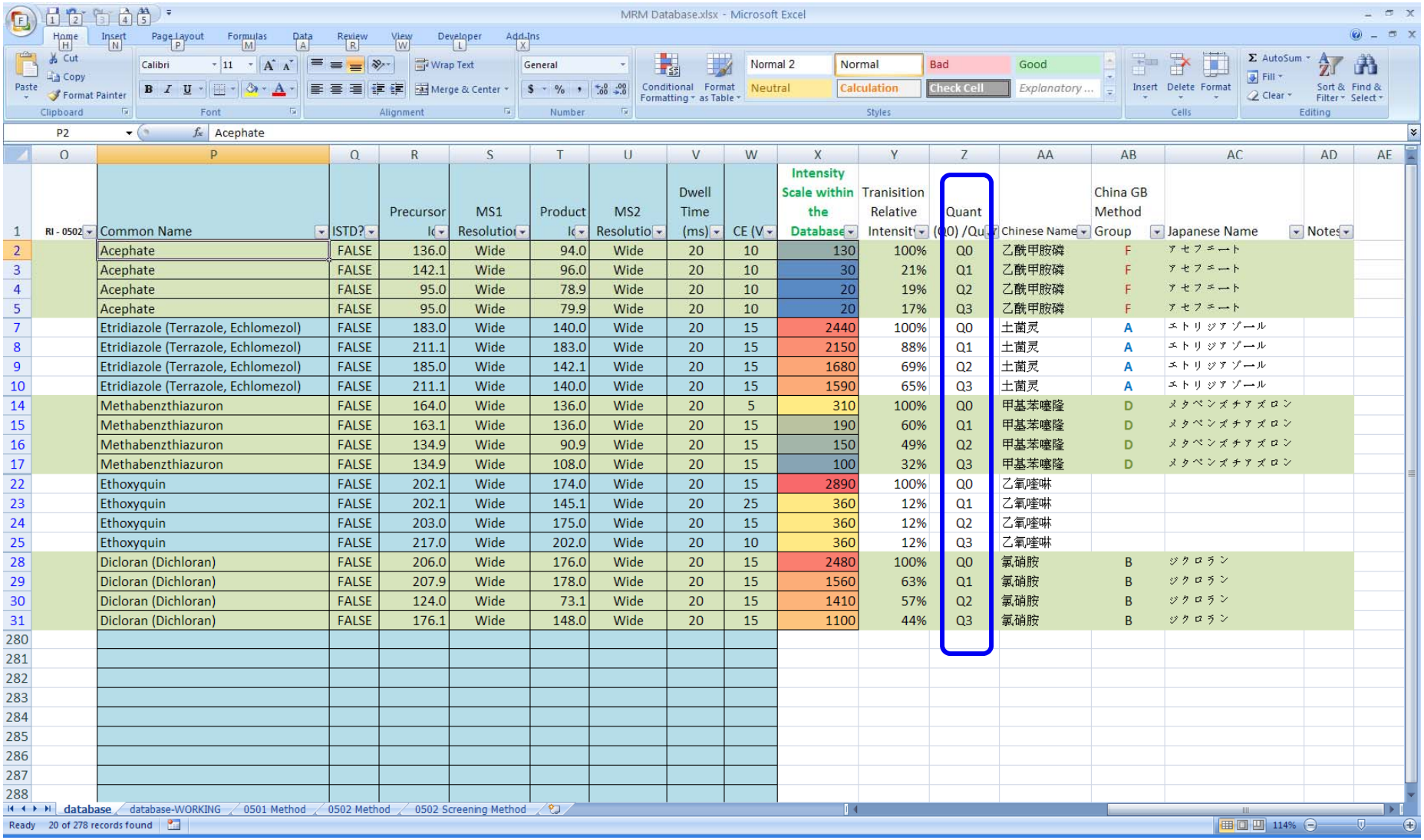
Use the sorting function to quickly select a Quant (Q0) and top three Qualifier ions (to build a method)!



RI - 0502	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) /Qual	Chinese Name	China GB Method Group	Japanese Name	Notes
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	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	
	Ethoxyquin	FALSE	202.1	Wide	174.0	Wide	20	15	2890	100%	Q0	乙氧喹啉			
	Ethoxyquin	FALSE	202.1	Wide	145.1	Wide	20	25	360	12%	Q1	乙氧喹啉			
	Ethoxyquin	FALSE	203.0	Wide	175.0	Wide	20	15	360	12%	Q2	乙氧喹啉			
	Ethoxyquin	FALSE	217.0	Wide	202.0	Wide	20	10	360	12%	Q3	乙氧喹啉			
	Dicloran (Dichloran)	FALSE	206.0	Wide	176.0	Wide	20	15	2480	100%	Q0	氯硝胺	B	ジクロラン	
	Dicloran (Dichloran)	FALSE	207.9	Wide	178.0	Wide	20	15	1560	63%	Q1	氯硝胺	B	ジクロラン	
	Dicloran (Dichloran)	FALSE	124.0	Wide	73.1	Wide	20	15	1410	57%	Q2	氯硝胺	B	ジクロラン	
	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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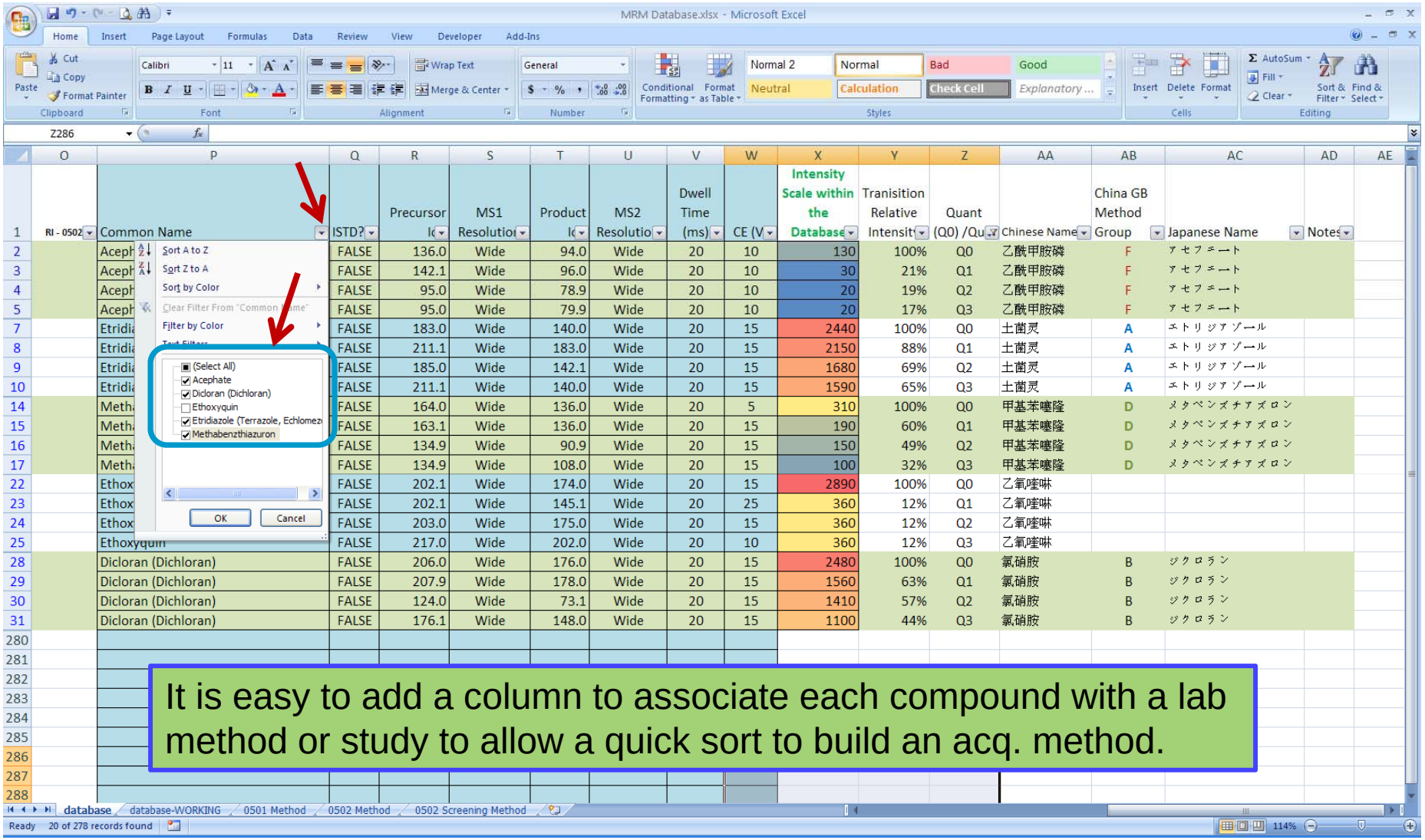
Click on the sorting button to select/show the compounds to be added into the acquisition method



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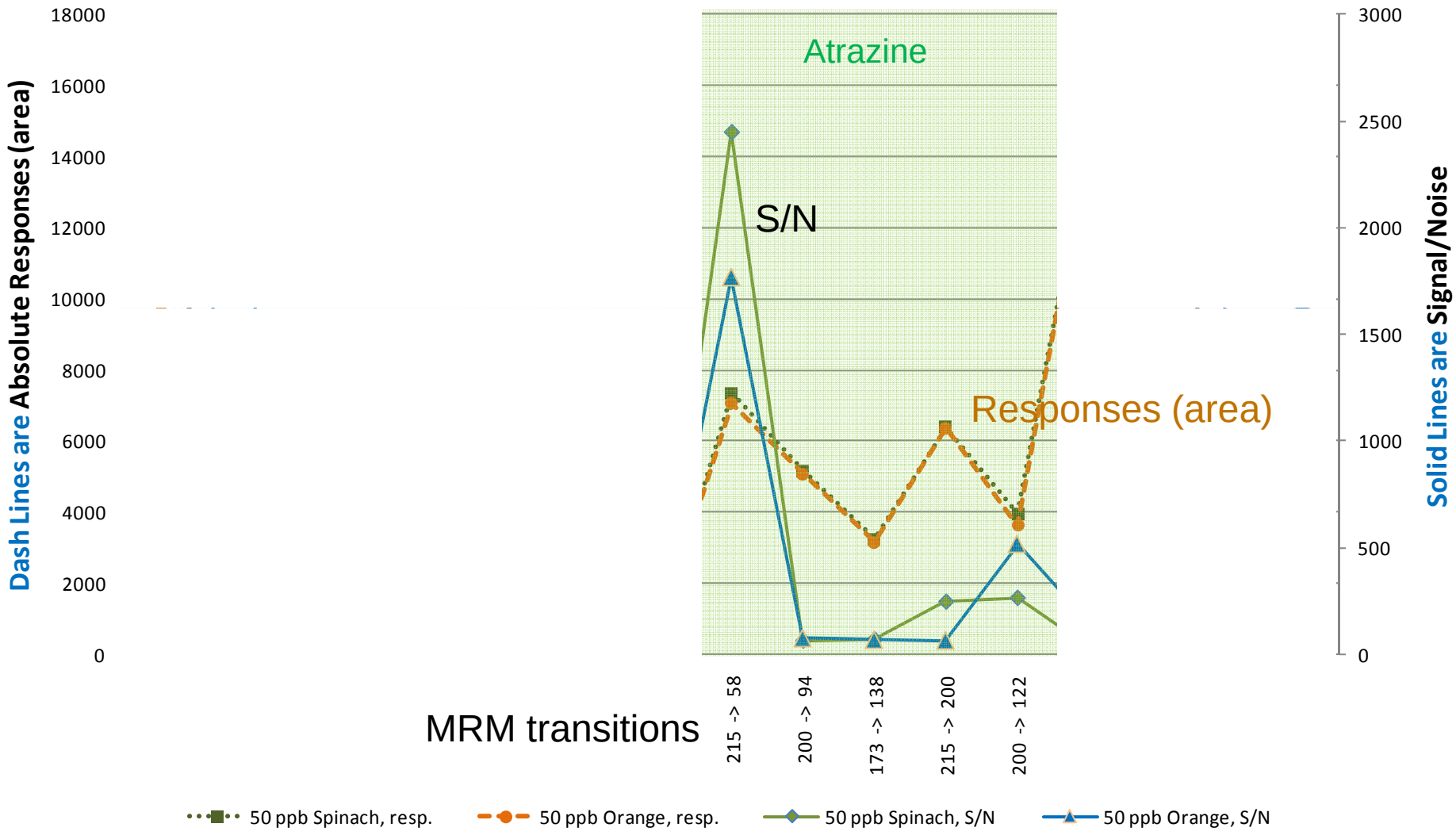
Why Do We Need More than 2 MRM Transitions?



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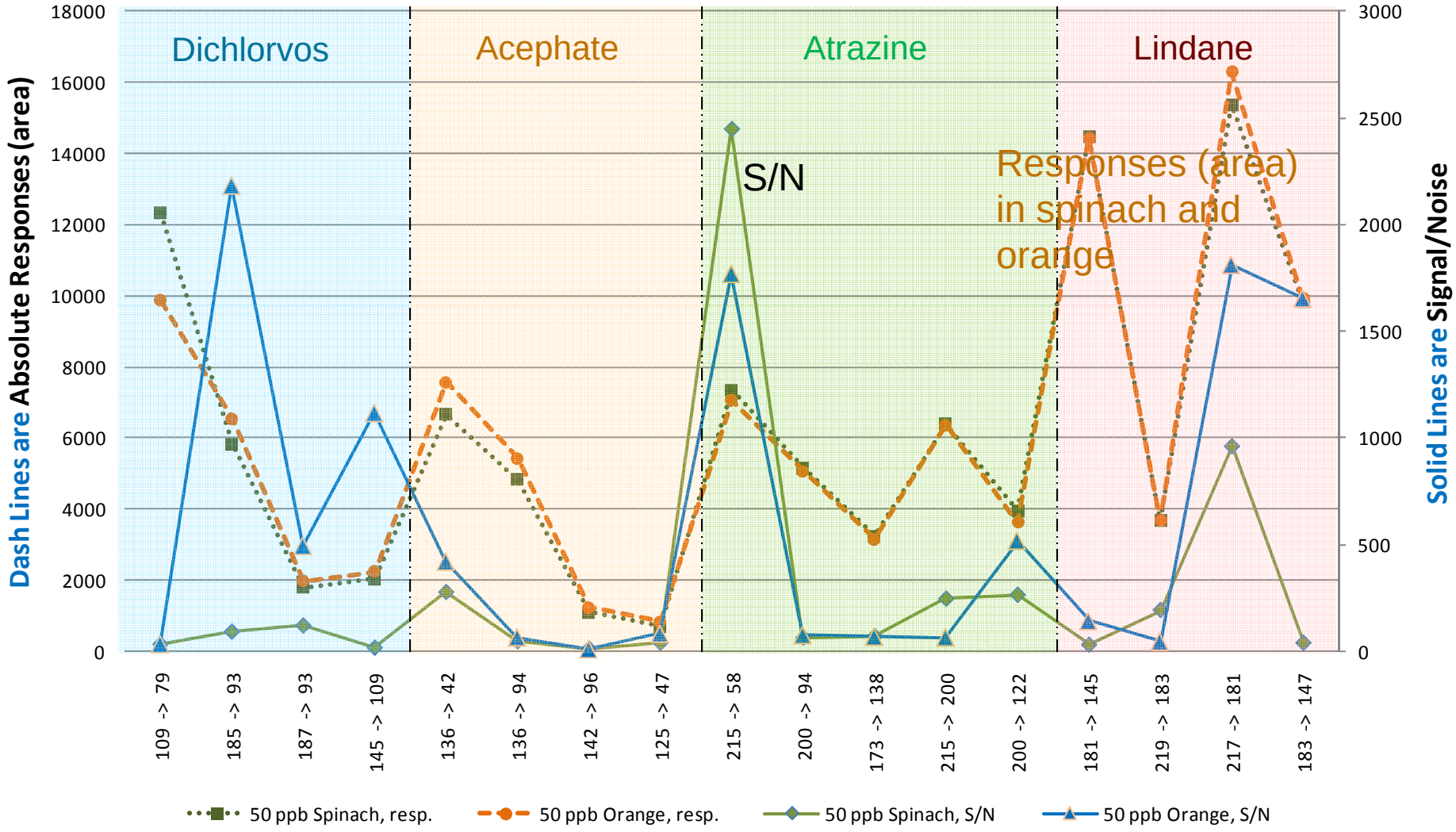
MRM Transitions are not Universal, Should Choose them According to Matrices



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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)