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

> GC/TQ (Triple Quad): Chin-Kai (Kai) Meng, PhD Senior Application Chemist

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

Terry L. Sheehan, PhD GC/MS Marketing Manager





Agilent Technologies

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 <u>break-in</u> needed, ready for injections





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 <u>not</u> "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







Milk Extract - Using Bakeout To Remove High Boilers









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
- <u>Reduces analysis time</u>
- Increases lifetime of analytical column



Benefits of Agilent GC/MS/MS Pesticide Analyzer

Retention Time	 No need to update the time segment RTs after a
Locking	column maintenance
Multimode inlet (MMI)	 injector adds flexibility by including standard, cold split/splitless, solvent vent (LVI) capabilities.
Capillary Flow	 Shorter analysis time, more consistent retention
Technology (CFT) and	times and spectra, longer column life, and less
backflush	frequent source cleaning improve uptime.
MS/MS MRM	 Optimized and flexible MRM database of
Database	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

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3	1	Acephate	30560-19-1	C4H10NO3PS	183.2	183.0119004	30560191	insecticide	Organophosphorus	6.234		7.610		5.651	Aci
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6	1	Acephate	30560-19-1	C4H10NO3PS		erage	30560191	insecticide	Organophosphorus	6.234		7.610		5.651	Aci
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13	2	Etridiazole (Terrazole	2593-15-9	C5H5Cl3N2OS		–	2593159	fungicide	Thiadiazole	9.265		7.928		5.843	itr
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15	3	Methabenzthiazuron	18691-97-9	C10H11N3OS	221.0	221.0622827	18691979	herbicide	Urea	13.461		11.176		7.269	VIE
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29	5	Dicloran (Dichloran)	99-30-9	C6H4Cl2N2O2	207.0	205.9649828	99309	fungicide	Substituted benzen	4.775		12.536		7,798	Dic
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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%	QO	氯硝胺	В	ジクロラン			
29		Dicloran (Dichloran)	FALSE	207.9	Wide	178.0	Wide	20	15		1560	63%	Q1	氯硝胺	В	ジクロラン			
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9 Endiazole (Terrazole, Echlomezol) FALSE 135.0 135 1360 66% 0.2 ± μ̄ 𝔅 A × h y 0 7 7 - μ I 14 Methabenzhiazuron FALSE 121.1 Wide 140.0 Wide 20 5 150 65% 0.3 ± μ̄ 𝔅 A × h y 0 7 7 - μ I 15 Methabenzhiazuron FALSE 164.0 Wide 136.0 Wide 20 15 190 66% 0.1 甲基苯噻酸 D × J * * V × X * J × X * X * J × X * X * Z * X * X * Z * X * X * Z * X * X	8		Etridiazole (Terrazole, Echlomezol)	FALSE	211.1	Wide	183.0	Wide	20	15	2150	88%	Q1	土菌灵	Α	エトリジアゾー	- JL			
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Click on the sorting button to select/show the compounds to be added into the acquisition method

	MRM Database.xlsx - Microsoft Excel																	
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23		Ethox	FALSE	202.1	Wide	145.1	Wide	20	25	360	12%	01	乙氧喹啉					
24		Ethox OK Cancel	FALSE	203.0	Wide	175.0	Wide	20	15	360	12%	Q2	乙氧喹啉					
25		Ethoxygum .::	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%	QO	氯硝胺	В	ジクロラン			
29		Dicloran (Dichloran)	FALSE	207.9	Wide	178.0	Wide	20	15	1560	63%	Q1	氯硝胺	В	ジクロラン			
30		Dicloran (Dichloran)	FALSE	124.0	Wide	73.1	Wide	20	15	1410	57%	Q2	氯硝胺	В	ジクロラン			
31		Dicloran (Dichloran)	FALSE	176.1	Wide	148.0	Wide	20	15	1100	44%	Q3	氯硝胺	В	ジクロラン			
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Why Do We Need More than 2 MRM Transitions?





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



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 <u>flexible and comprehensive</u> 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 (<u>adapts to</u> <u>user's preference</u> or analytical method)
- has multiple MRM transitions (average 7) for each compound (<u>helps to</u> provide alternatives to work around matrix interference)
- shows relative intensity of each MRM transition (<u>facilitates transition</u> <u>selection and acquisition method creation</u>)



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

'MSD' resolution + EIC(150.00000) Scan Okra 10RL STD 3.d x10 **Okra QuEChERS Extract** 17,9981 Matrix interferant ion (b-Tocopherol) Indoxacarb * 18,0758 b-Tocopherol 150.06839 Da Analyte Indoxacarb ion (100pg) +/-0.5 amu (~ 300ppm) 3 150.01195 Da (fragment ion) 2 18.3138 17.4859 17.5520 17.6264 17,7386 17,8863 ∆m = 0.0564 Da. 17.45 17.5 17.55 17.6 17.65 17.7 17.75 17.8 17.85 17.9 17.95 18 18.05 18.1 18.15 18.2 18.25 18.3 18.35

TOF high resolution





TOF Accurate Mass to Eliminate Matrix Interferants



TOF high resolution



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



Resolving Power





Resolving Power





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

			Integer	Exact		X+1	X+2	Mass
Туре	Element	Symbol	Mass	Mass	Abundance	Factor	Factor	Defect
Х	Hydrogen	Н	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 0	17	16.9991	0.04	0.04n ₀		-0.0009
		¹⁸ O	18	17.9992	0.2		0.20n ₀	-0.0008
Х	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
Х	Phosphorus	Р	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
Х	lodine		127	126.9045	100			-0.0955



Selectivity for Isobaric Ions





Fundamental Benefits (Agilent 7200 Q-TOF)

- High resolution (> 10K, typically > 13K FWHM)
 - Increased detector selectivity (few interferences)
- Accurate mass measurements (low to sub-ppm)
 - < 5 ppm in TOF (typically < 2 ppm)</p>
 - < 10 ppm in Q-TOF (typically < 5 ppm)</p>
 - Valuable qualitative information about each ion



Many possible formulas with an MSD or IT But only a few with TOF



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

	Mol	ocularion		Fragment lons												
	IVIOI			1		2		3		4						
Pesticide	m/z	Formula	∆ ppm	Formula	∆ ppm	Formula	∆ ppm	Formula	∆ ppm	Formula						
Chlorpyrifos	320.8944	C7H7Cl3NO3PS	-0.7	C7 H7 CI [³⁷ CI] N O3 P S	0.0	C7 H7 Cl2 N O3 P S	0.0	C2 H6 O2 P S								
-meunyi			215.4	C6 H2 CI3 N O2 P S												
Dichlorvos	219 9454	C4H7Cl2O4P	1.6	C4H7CIO4P	-0.9	C2H6O3P	3.7	C4 H7[³⁷ Cl] O4 P								
Dicition vos							336.5	C3 H2 Cl2 O3 P								
Endosulfan	419 8112		-2.1	C9 H6 Cl4[³⁷ Cl] O4 S	-0.7	C5 CI5[³⁷ CI]	0.0	C5 Cl4[³⁷ Cl]2								
sulfate	410.0112						-220.9	C8 H3 CI5								
Propachlor	211 0758	C11 H14 CLN O	-1.0	C10 H11 CI N O	1.1	C11 H14 N O	1.8	C8 H8 CI N O	-3.9	C6 H5						
Порасню	211.0700								771.6	C2 H2 CI O						
Fluazifop-p-	383 1330	C10 H20 E3 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						
butyl	505.1555	0131120131004							-494.2	C7 H14 O3						
Triazonhos	313 0645	C12 H16 N3 O3 P	-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						
	010.00+0	S	-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





Fundamental Benefits (Agilent 7200 Q-TOF)

- High resolution (> 10K, typically > 13K FWHM)
 - Increased detector selectivity (few interferences)
- Accurate mass measurements (low to sub-ppm)
 - < 5 ppm in TOF (typically < 2 ppm)</p>
 - < 10 ppm in Q-TOF (typically < 5 ppm)</p>
 - Valuable qualitative information about each ion
- Structural elucidation with <u>Accurate Mass</u>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)



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-C₆H₅ (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-C₆H₅ (131.04969) or C_2H_2CH =CH-C₆H₅ (131.086075) from 269.0802.

However, measured value of 269.0802 - 138.0310 = $\underline{131.04920}$ is consistent only with **COCH**=CH- C₆H₅.



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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





High Data Rate = Better Deconvolution





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 + AMass Defect (Mother Nature) + Relative Ion Intensities (Sample)

There is more to learn about these new apps



GC or MS: Relative intensity affects the result



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

