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Excellence in Science

Approccio analitico alla sicurezza in campo ambientale e alimentare: potenzialità della LCMS Shimadzu

Pisa, 28 Giugno 2016

Veronica Mainini
LCMS Application Support, Shimadzu Italy
vmainini@shimadzu.it

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Overview

- Method package for pesticides analysis
- Polar pesticides: how to approach them
- Water monitoring: Decisione di esecuzione (UE) 2015/495

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- Water monitoring: Decisione di esecuzione (UE) 2015/495
- LCMS Solutions

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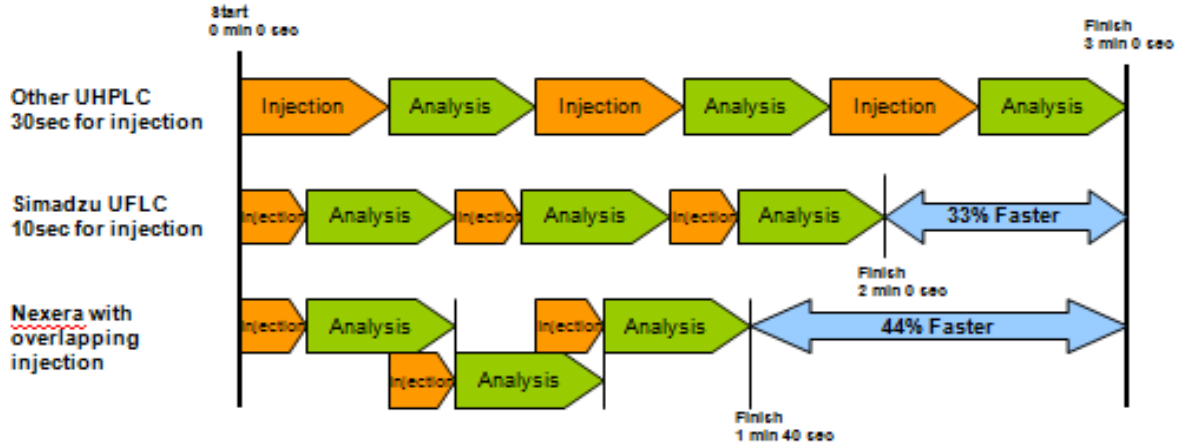
The Need for Speed

A powerful solution combines good performance on the front end as well as on the mass spectrometry side:

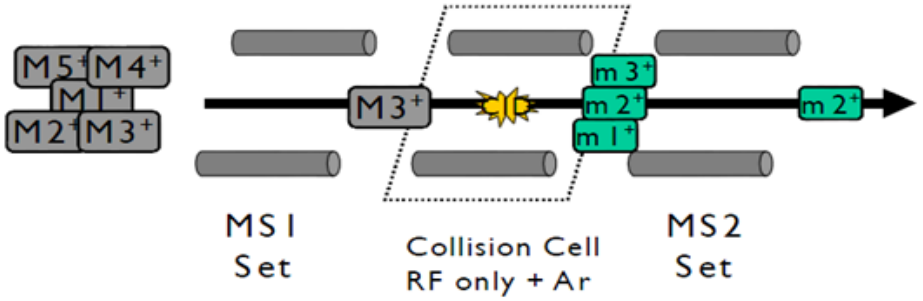
Flexible HPLC front end

- flexibility in the pressure range
- speed and resolution
- reproducibility / precision
- robust
- low carry over
- throughput
- cost saving and easy to use and to maintain UHPLC



Mass spectrometer

- fast polarity switching
- fast scan speed
- high number of MRM transition
- robust
- no cross talk
- cost saving and easy to use and to maintain



Fusion of UF-Technologies

UF-Scanning

UF-Switching

UF-MRM

UF-Scanning : high-speed scanning rate for high-quality mass spectra

UF-MRM : maintain data quality and sensitivity

UF-Switching : high-speed polarity switching

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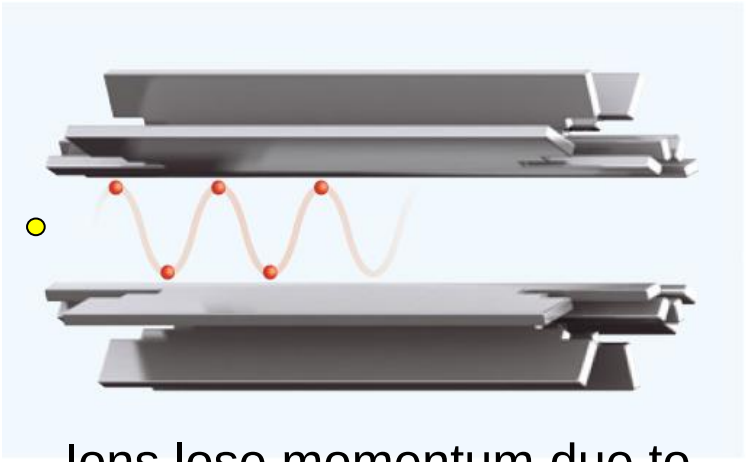
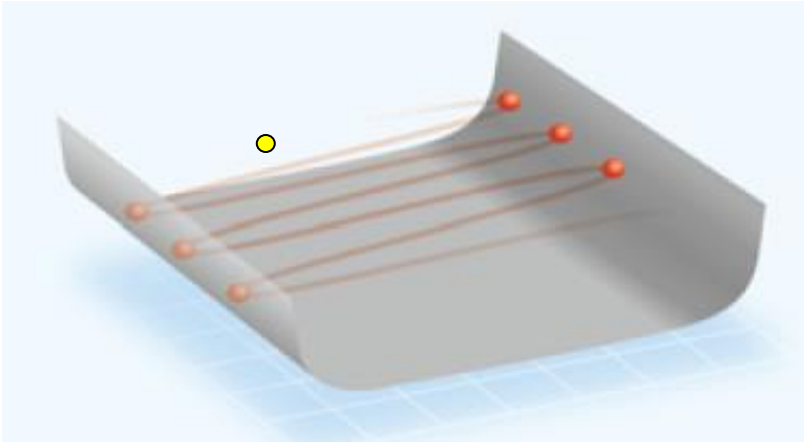
Like a rolling stone on a slope…

Conventional collision cell

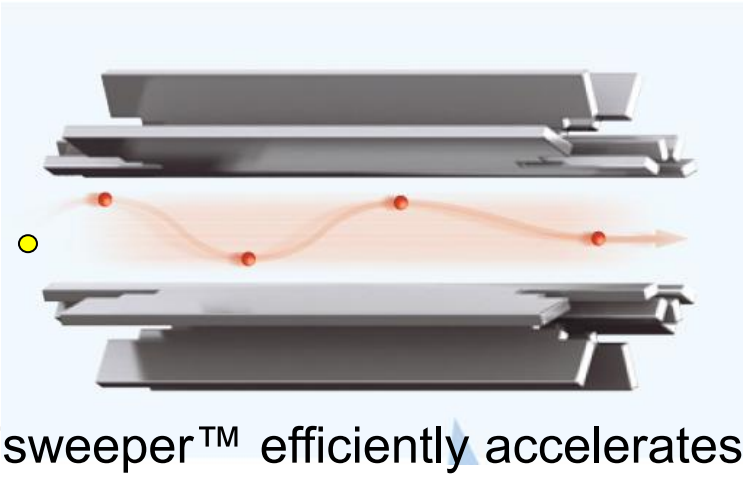


Ions lose momentum due to collision with gas.

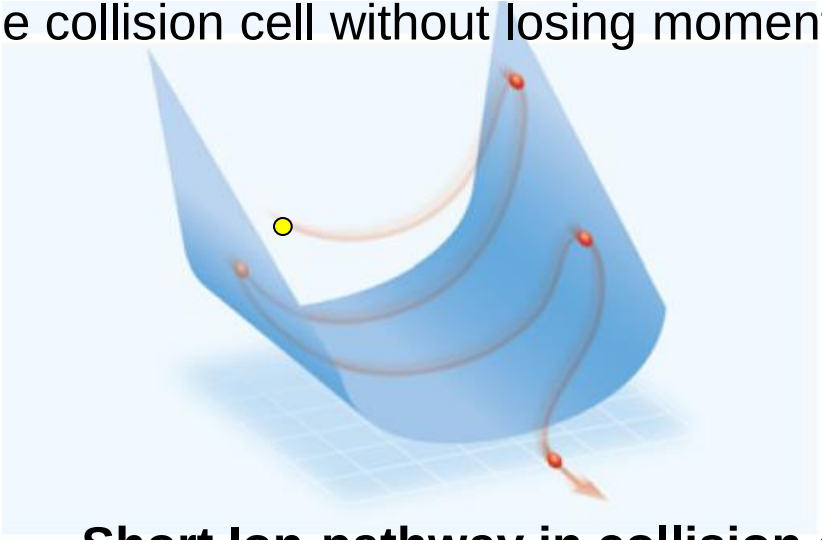


Long Ion-pathway in collision cell
>Entrance and Exit-potential are equal<

UFsweeper collision cell

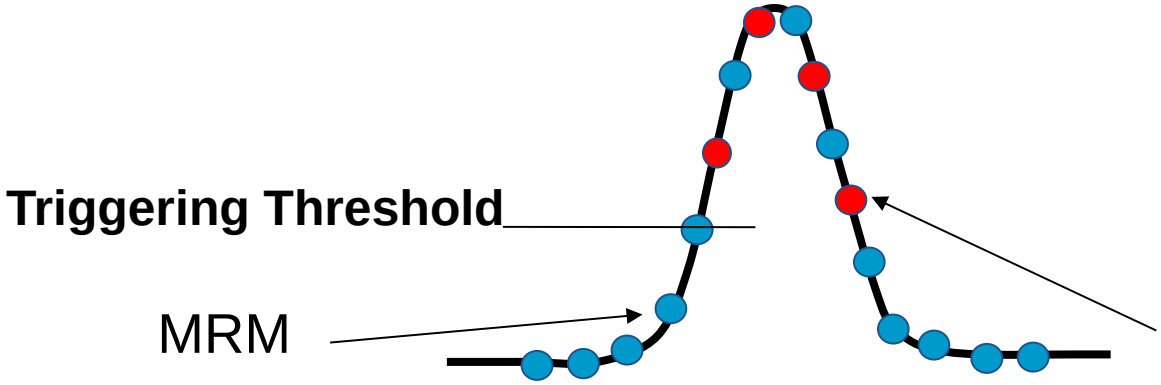


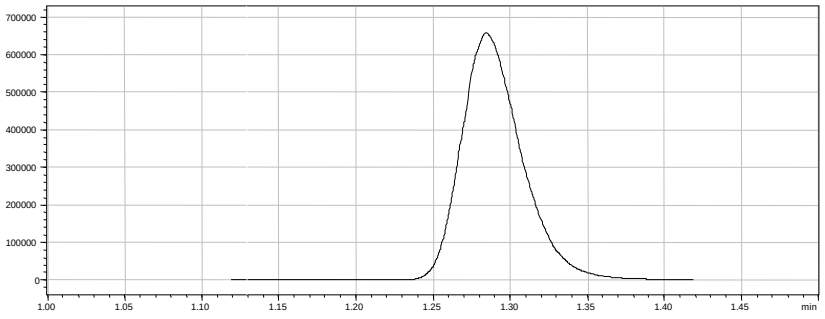
UFsweeper™ efficiently accelerates ions out of the collision cell without losing momentum.



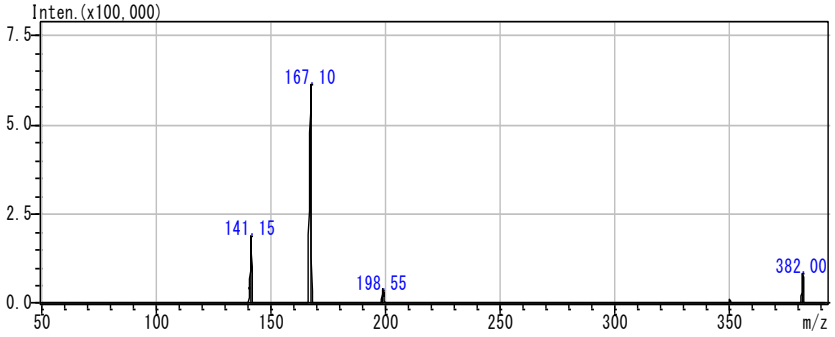
Short Ion-pathway in collision cell
>Entrance and Exit-potential are different<

UF-Technology: qualitative / quantitative data





Quantitative data



Qualititative data

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Chronology of UF-Technology

GLOBAL LAUNCH LCMS-8030

First mass spectrometry company to achieve a scan speed of 15,000u/sec and polarity switching time of 15msec

2010 AUGUST

LCMS-8040

Increased sensitivity by a factor of 5 compared to the LCMS-8030

2012 MAY

LCMS-8050

First mass spectrometry company to achieve 5msec polarity switching time and a scan time of 30,000u/sec. Increased sensitivity by 30 times compared to LCMS-8030

2013 AUGUST

LCMS-8060

A new vision in sensitivity. It simply changes everything. Increased sensitivity by 90 times compared to LCMS-8030

2015 ASMS 2015 MAY

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LCMS 8060

Heated ESI

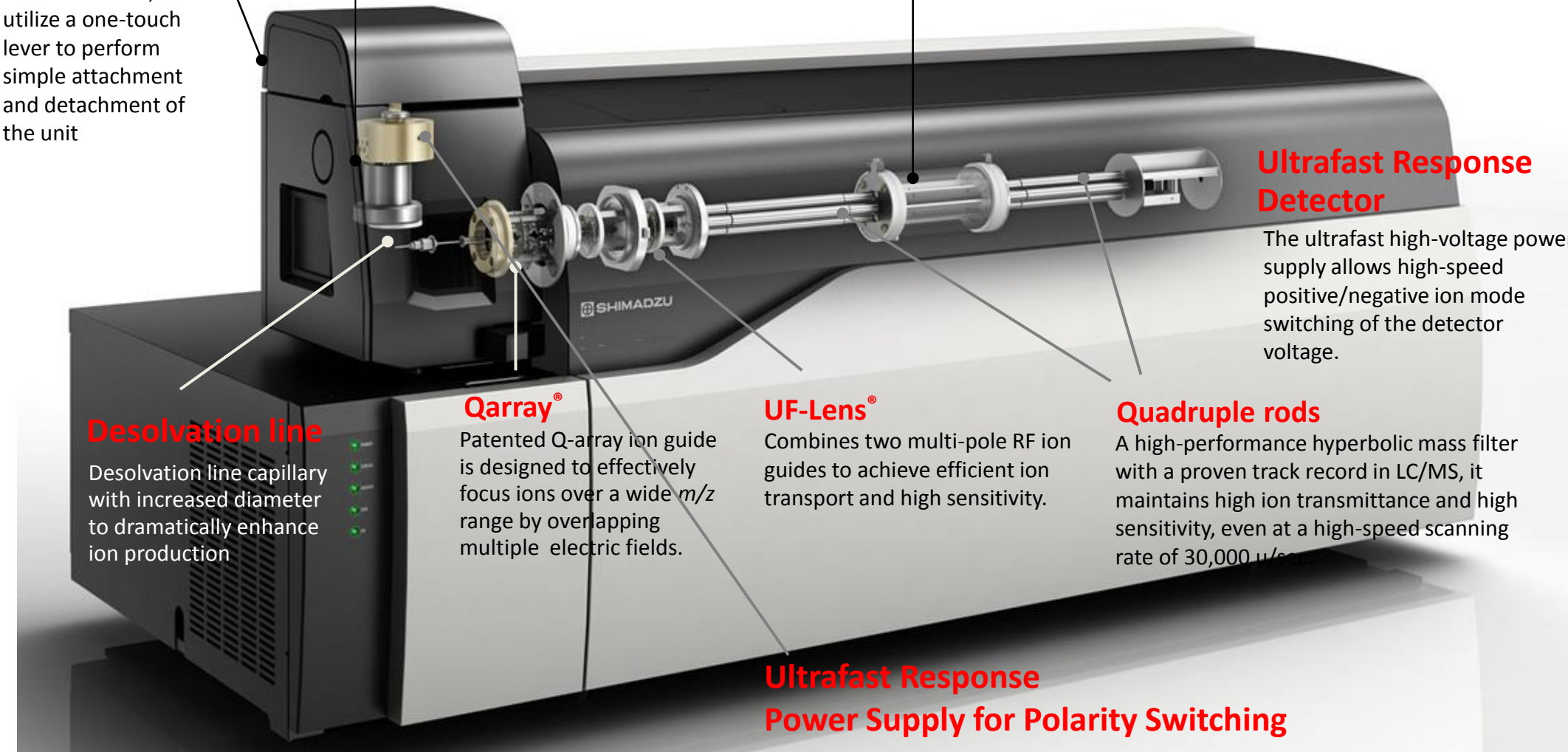
High-temperature gas supplements the nebulizer gas, improves desolvation efficiency. This facilitates the ionization of a wide range of compounds.

UFsweeper® Ⅲ Collision Cell

A high-sensitivity, high-speed collision cell, the proprietary **UFsweeper III** accelerates ions out of the collision cell without loss of momentum. Achieving fast sweeping on successive scans, it offers twice the CID efficiency of UFsweeper II, maintains signal intensity, and suppresses crosstalk, even for high-speed or simultaneous multi-component analysis.

Ionization Unit

Designed without cables or tubes; utilize a one-touch lever to perform simple attachment and detachment of the unit



Ultrafast Response Detector

The ultrafast high-voltage power supply allows high-speed positive/negative ion mode switching of the detector voltage.

Desolvation line

Desolvation line capillary with increased diameter to dramatically enhance ion production

Qarray®

Patented Q-array ion guide is designed to effectively focus ions over a wide *m/z* range by overlapping multiple electric fields.

UF-Lens®

Combines two multi-pole RF ion guides to achieve efficient ion transport and high sensitivity.

Quadruple rods

A high-performance hyperbolic mass filter with a proven track record in LC/MS, it maintains high ion transmittance and high sensitivity, even at a high-speed scanning rate of 30,000 u/sec.

Ultrafast Response Power Supply for Polarity Switching

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„Plug in“ Source

- Cable and tube free ion source
- Fast and easy source exchange

APCI-8060

ESI-8060

DUIS-8060

SHIMADZU

LCMS 8060

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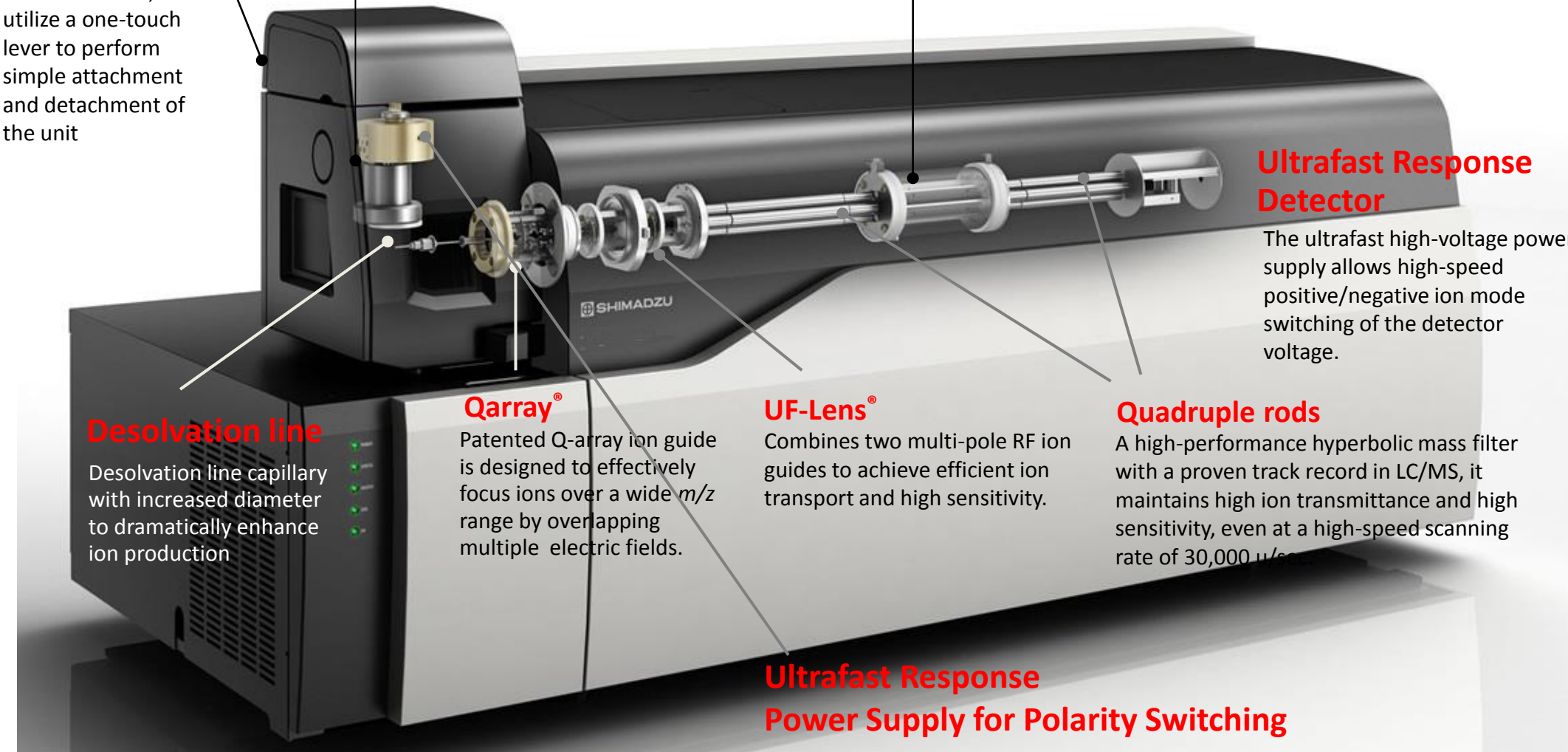

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Ultrafast Response Power Supply for Polarity Switching

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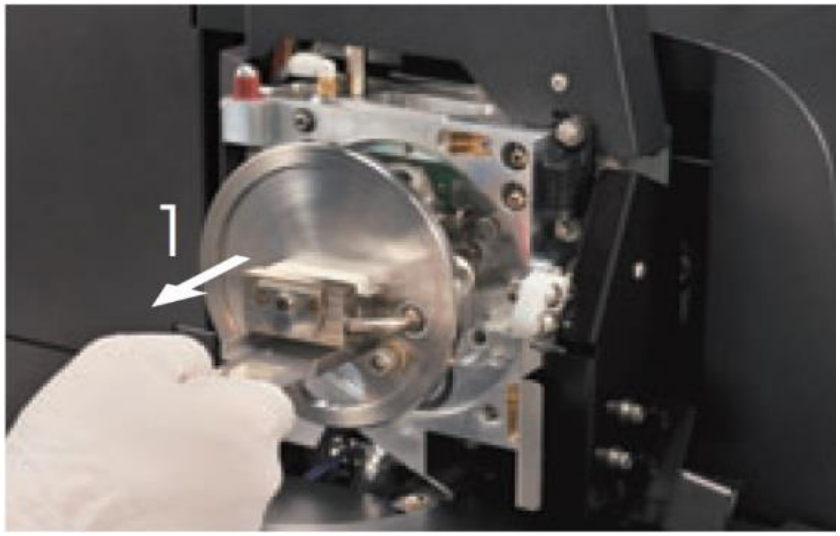
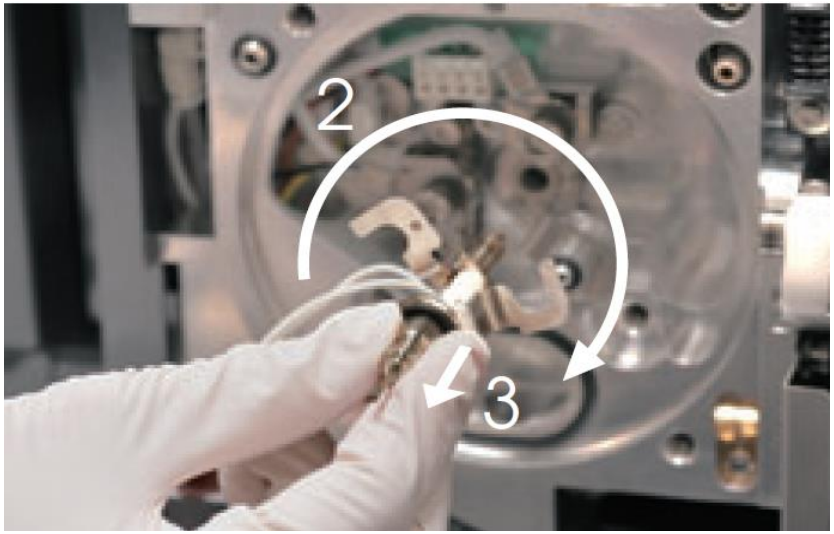
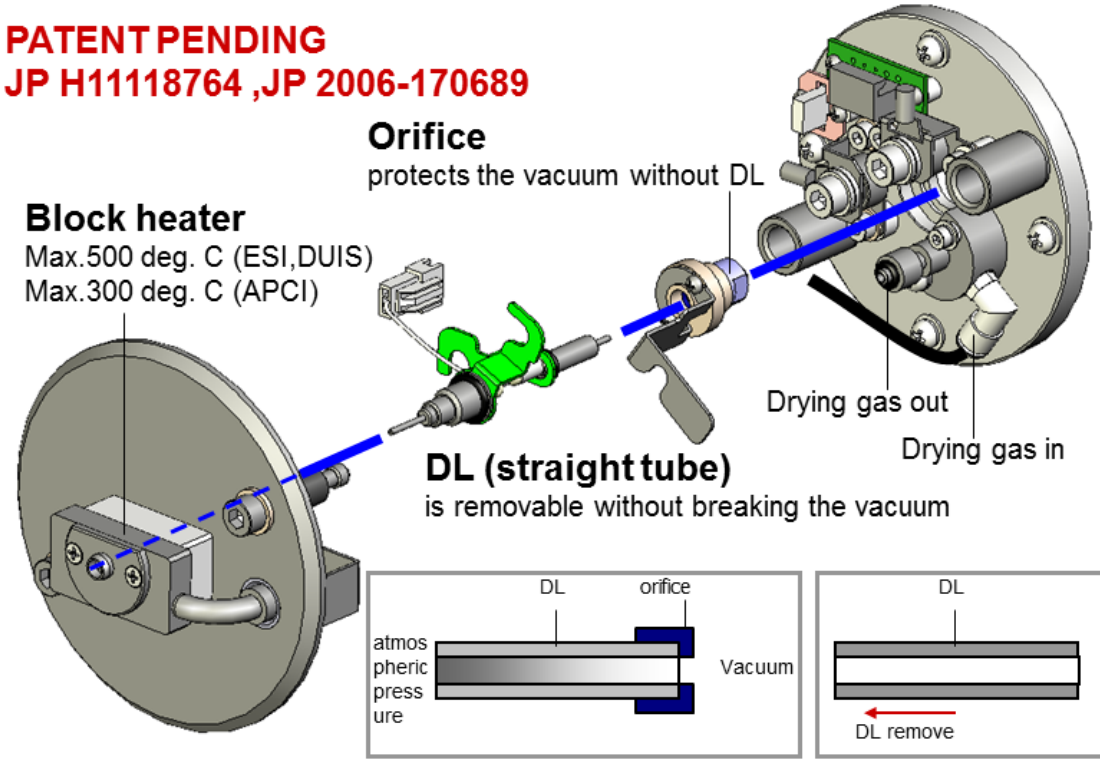
Desolvation Line exchange





- **Easy**
- **Quick**
- **Vent free!**

PATENT PENDING
JP H11118764 ,JP 2006-170689



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- **Water monitoring: Decisione di esecuzione (UE) 2015/495**

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Safety

Regulatory bodies have increased the number of regulated pesticides and the maximum residue level allowed

1. Commission Regulation (EC). 2005. No 396/2005 of the European Parliament and of the Council, maximum residue levels of pesticides in or on food and feed of plant and animal origin. Official Journal of the European Union, L 70: 1-16

2. US Environmental Protection Agency, Electronic code of federal regulation: Title 40: Part 180 - tolerances and exemptions for pesticide chemical residues in food. http://www.ecfr.gov/cgi-bin/text-idx?c=ecfr&tpl=/ecfrbrowse/Title40/40cfr180_main_02.tpl

3. Japanese Ministry of Health, Labour and Welfare, Department of Food Safety. 2006. Director Notice about Analytical Methods for Residual Compositional Substances of Agricultural Chemicals, Feed Additives, and Veterinary Drugs in Food (Syoku-An No. 0124001 January 24, 2005; amendments May 26, 2006).

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Application News

No.C136

Liquid Chromatography Mass Spectrometry

Expanding Capabilities in Multi-Residue Pesticide Analysis Using The LCMS-8060

David R. Baker[1], Laëtitia Fages[2], Eric Capodanno[2], Neil Loftus[1]
[1]Shimadzu Corporation, UK; [2]Phytocontrol, France

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Materials

- Food extracts of mint, tomato and apple
- SAMPLE PREPARATION: QuEChERS protocol.
  Final extracts prepared in CH_3CN without any dilution.
- CALIBRATION CURVE: A six point calibration curve from 2 to 100 pg/µL generated using spiked IS (Atrazine-d5 and Diuron-d6)

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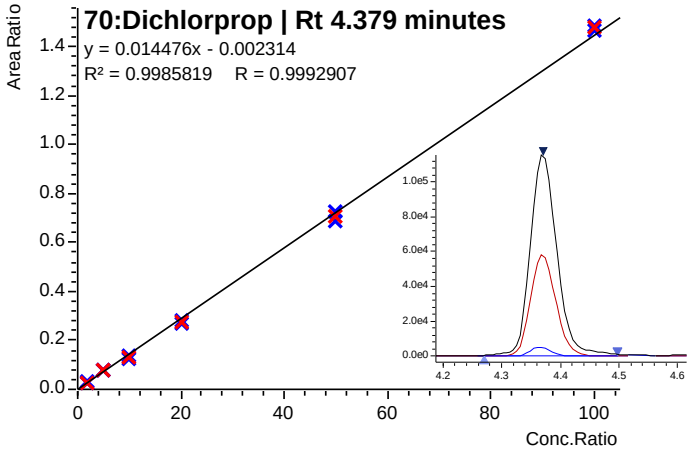
Methods:

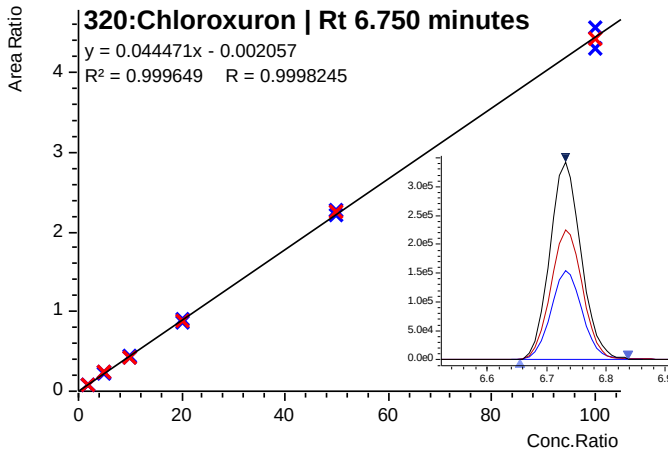
Liquid chromatography	
UHPLC	Nexera LC system
Analytical column	Restek Raptor Biphenyl (2.1 mm I.D. × 100 mm L., 2.7 µm)
Column temperature	35 °C
Flow rate	0.4 mL/min
Solvent A	2 mmol/L ammonium formate + 0.002 % formic acid - Water
Solvent B	2 mmol/L ammonium formate + 0.002 % formic acid - Methanol
Binary Gradient B.Conc.	3 % (0 min) - 10 % (1.00 min) - 55 % (3.00 min) - 100 % (10.50 - 12.00 min) - 3 % (12.01 - 15.00 min)
Injection volume	2 µL sample (plus 40 µL water)

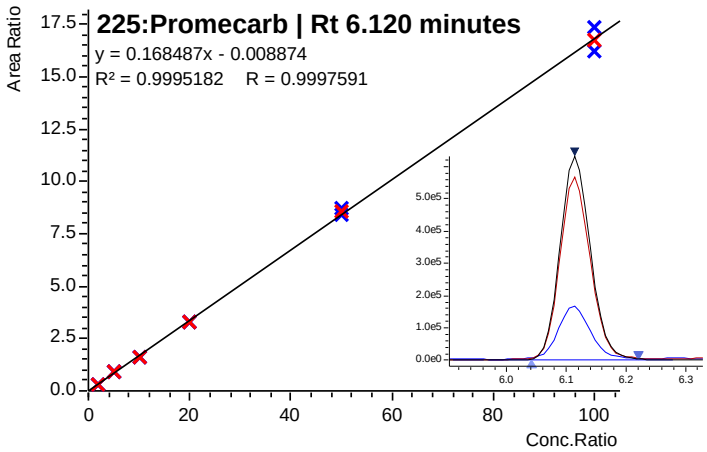
Mass spectrometry	
LC/MS/MS	LCMS-8060
Ionisation mode	Heated electrospray
Polarity switching time	5 msec
Pause time	1 msec
Total MRM transitions	1,919 (1,819 positive; 100 negative)
MRM Dwell	4 msec (target ion); 1 msec (reference ion)
Interface temperature	350 °C
Heating block	300 °C
Desolvation line	150 °C
Heating gas	10 L/min
Drying gas	10 L/min
Nebulizer gas	3 L/min

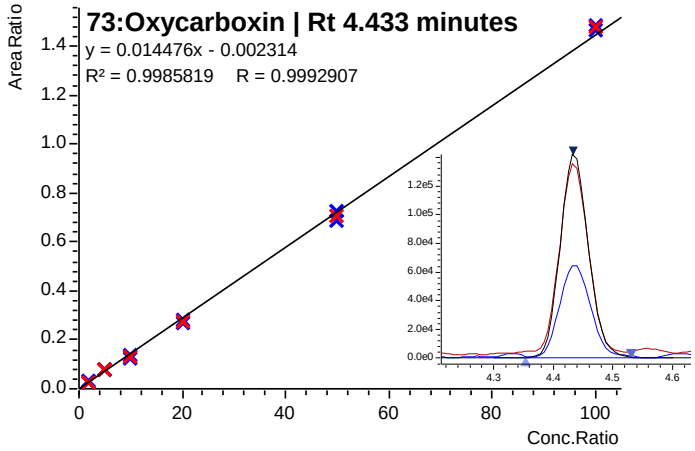
Results: LINEARITY

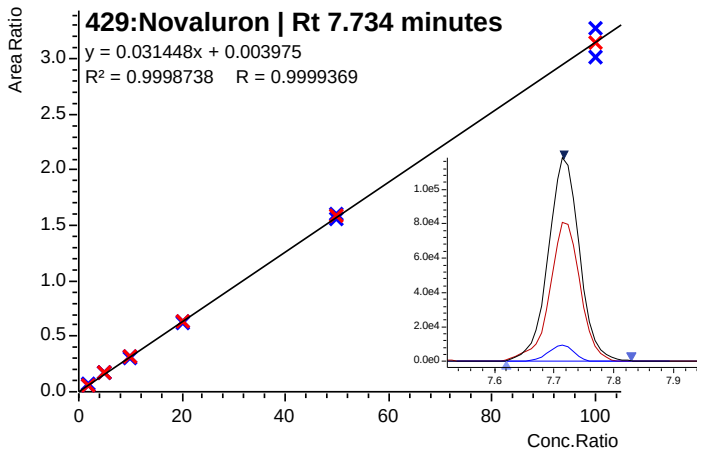
- Linearity was assessed over a six point calibration curve from 0.002 – 0.1 mg/kg (2 – 100 pg/µL).
- All 646 pesticides achieved excellent R^2 values greater than 0.99 in both tomato and mint spiked extracts with typical values greater than 0.996

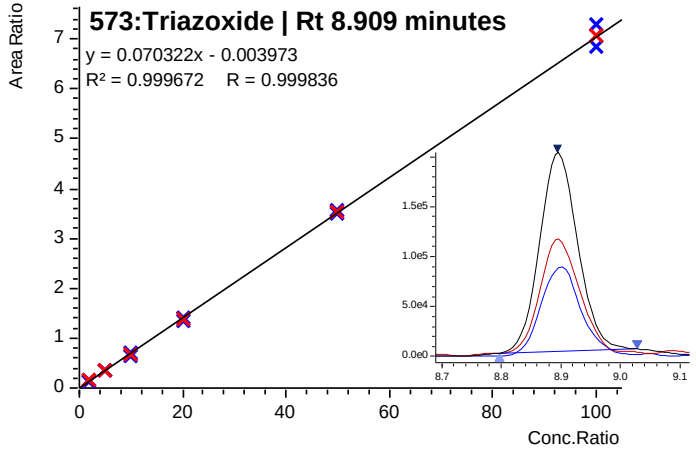








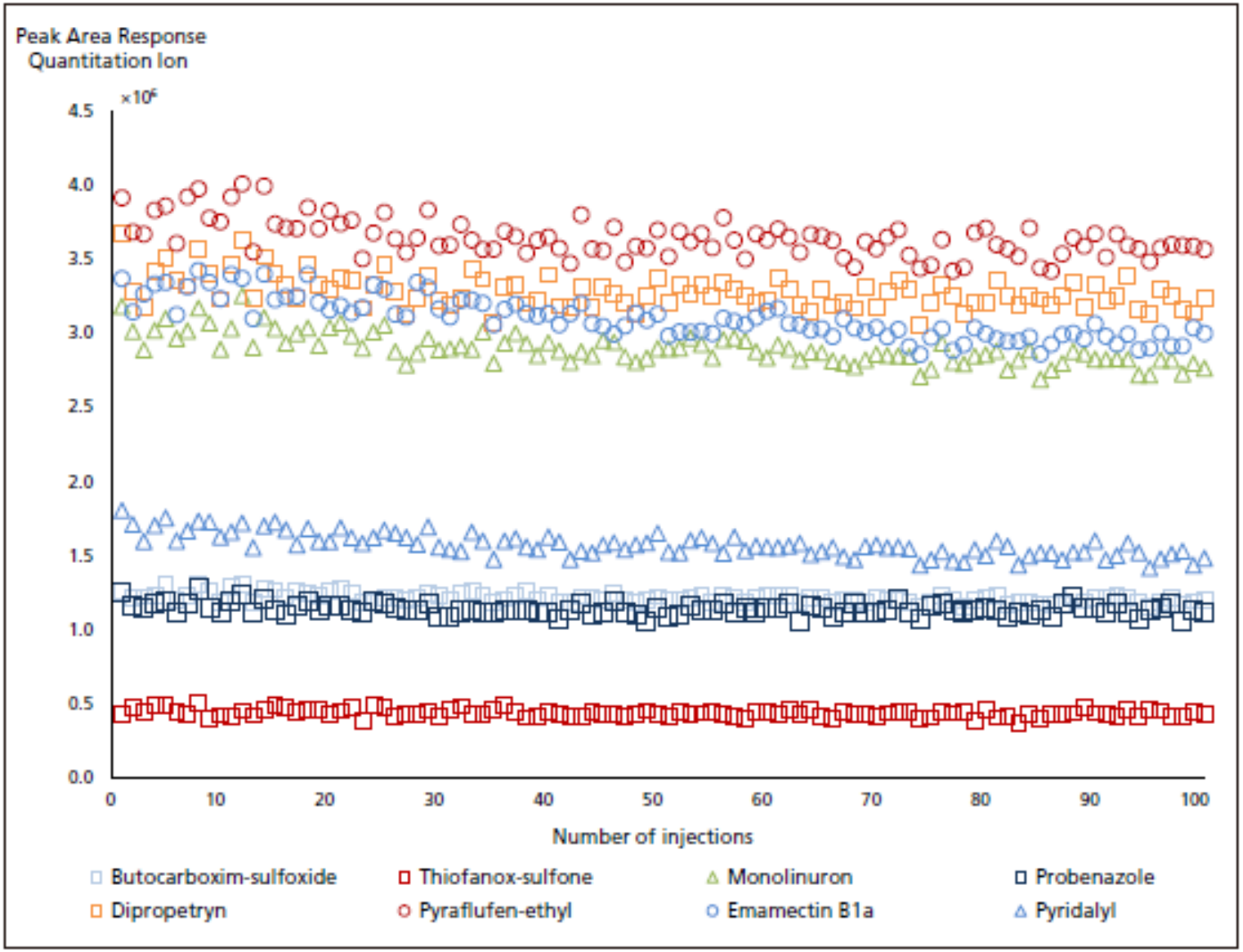




Linear fit and 1/C weighting for all compounds

Repeatability -1-

- To assess the robustness of the system and the developed method during routine analysis, repeat injections of a mint matrix sample spiked with 646 pesticides at 0.050 mg/kg, were analysed over a 24 hour period



Repeatability -2-

- To assess the robustness of the system and the developed method during routine analysis, repeat injections of a mint matrix sample spiked with 646 pesticides at 0.050 mg/kg, were analysed over a 24 hour period

Compound Name	CAS Number	Formula	M	Polarity	MRM Quantitation Ion	RT (mins)	Average Peak Area	%RSD (n=100)
Butocarboxim-sulfoxide	34681-24-8	C7H14N2O3S	206.0725	+	207.10 > 75.10	3.042	1,220,391	2.6
Thiofanox-sulfone	39184-59-3	C9H18N2O4S	250.0987	+	268.10 > 57.00	4.001	442,724	5.7
Monolinuron	1746-81-2	C9H11ClN2O2	214.0509	+	215.10 > 99.10	4.985	2,904,116	3.7
Probenazole	27605-76-1	C10H9NO3S	223.0303	+	224.00 > 41.05	5.995	1,145,189	3.5
Dipropetryn	4147-51-7	C11H21N5S	255.1518	+	256.20 > 144.05	6.999	3,289,597	3.4
Pyraflufen-ethyl	129630-19-9	C15H13Cl2F3N2O4	412.0204	+	413.00 > 339.00	8.004	3,653,333	3.5
Emamectin B1a	138511-97-4	C56H81NO15	1007.5606	+	886.40 > 158.20	9.008	3,109,562	4.5
Pyridalyl	179101-81-6	C18H14Cl4F3NO3	488.9680	-	491.90 > 109.05	10.171	1,579,422	5.0

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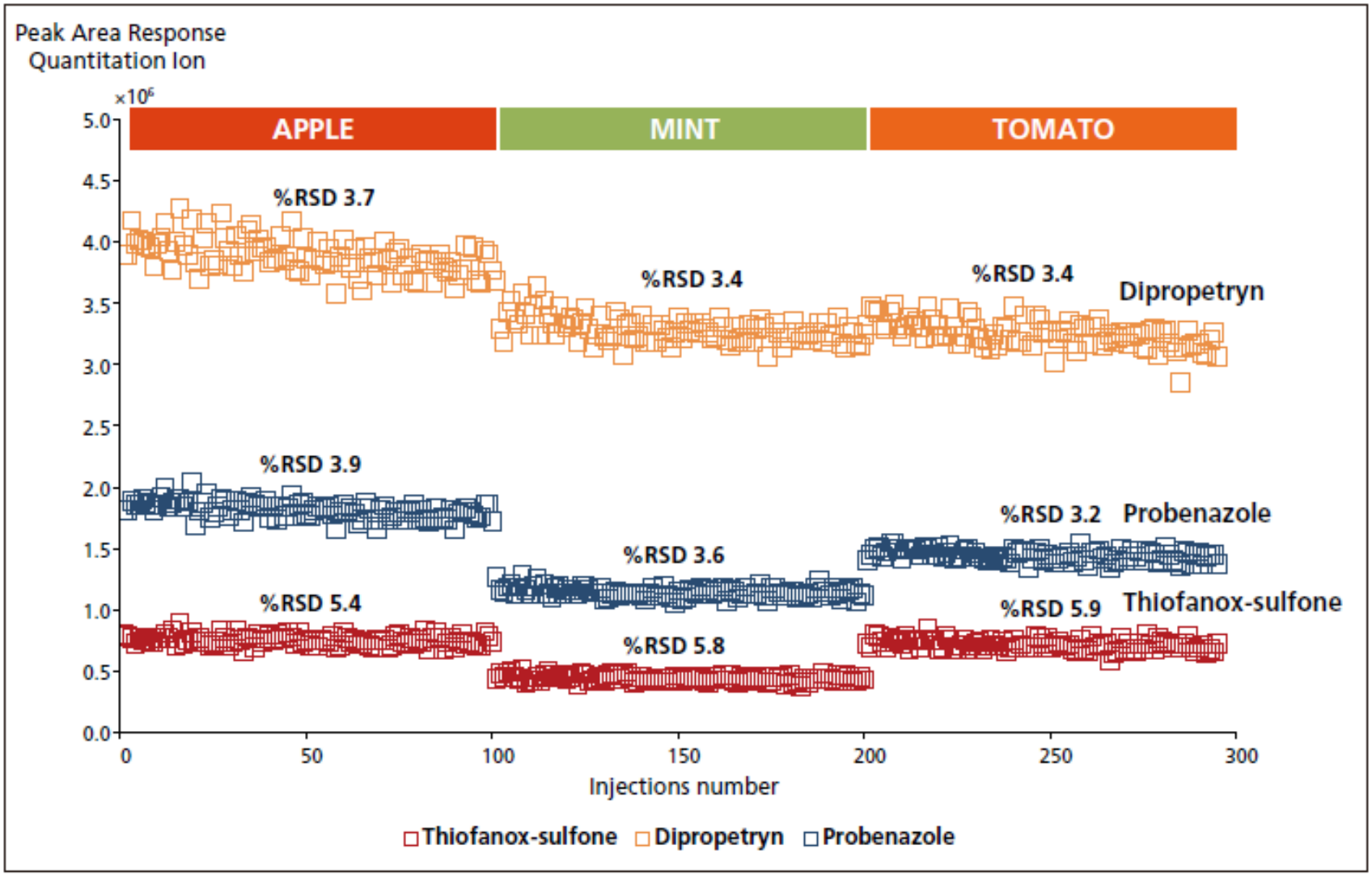
Response to differing matrices -1-



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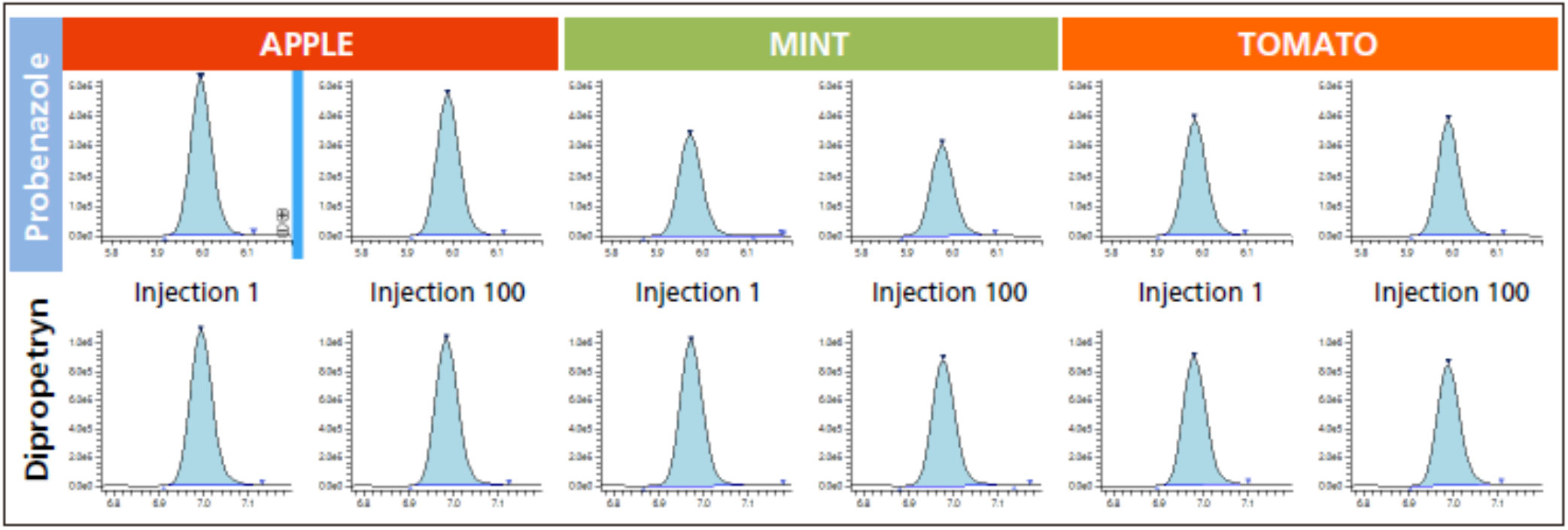
Response to differing matrices -2-



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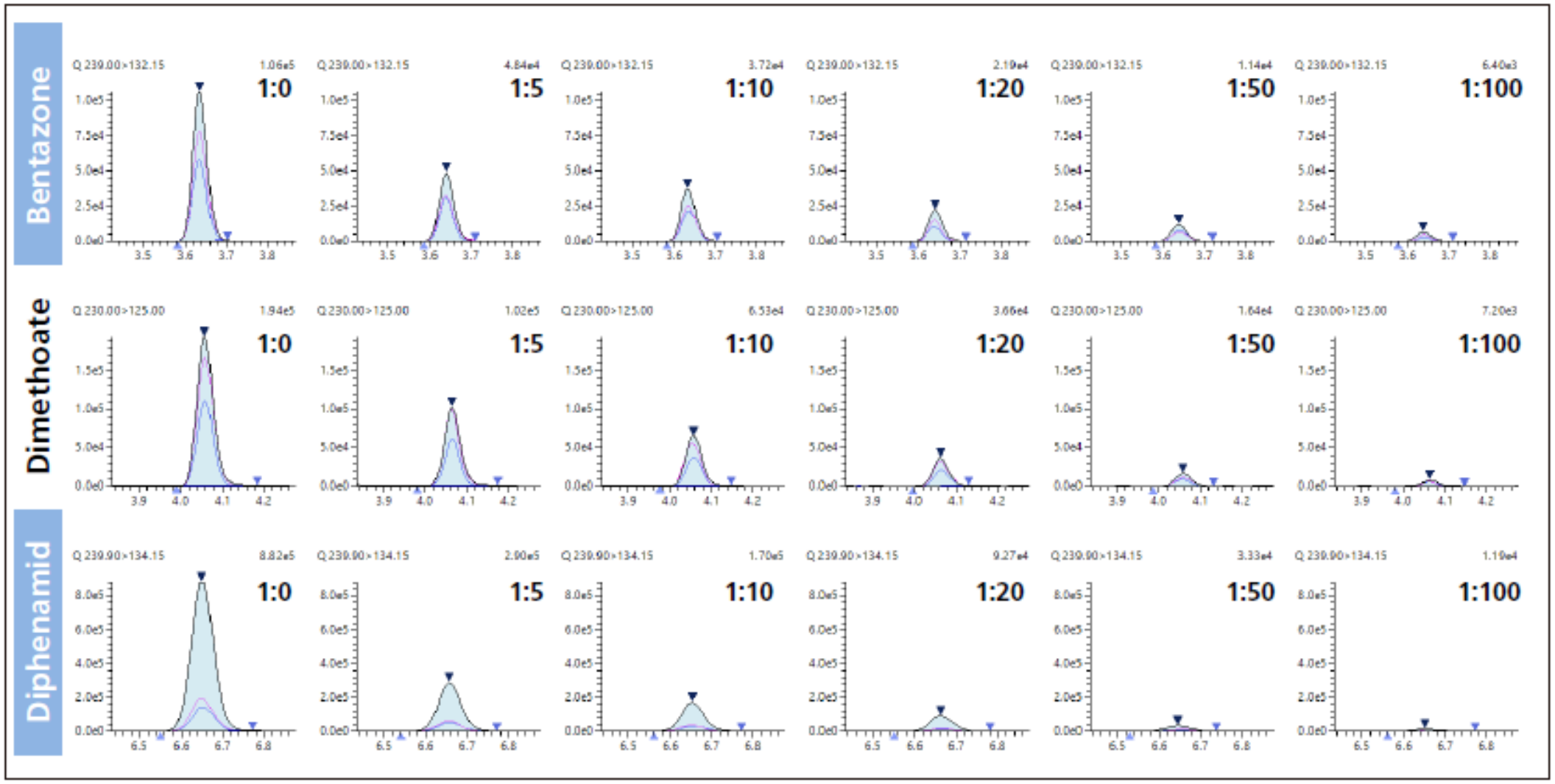
Matrix effects -1-



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Matrix effects -2-

				Dilution series					
Compound	CAS	Formula	M	0	1:5	1:10	1:20	1:50	1:100
				Recovery					
Bentazone	25057-89-0	C10H12N2O3S	240.0569	32.1	44.6	65.5	72.7	91.7	98.1
Demeton-S-methyl-sulfone	17040-19-6	C6H15O5PS2	262.0099	51.1	78.5	89.6	91.1	114.2	116.8
Dimethoate	60-51-5	C5H12NO3PS2	228.9996	36.2	65.3	88.5	92.2	92.4	94.2
Isocarbamid	30979-48-7	C8H15N3O2	185.1164	28.8	57.1	81.8	98.7	102.5	96.4
Vamidothion	2275-23-2	C8H18NO4PS2	287.0415	53.6	76.3	98.2	98.5	101.5	114.1
Thiazafluron	25366-23-8	C6H7F3N4OS	240.0293	32.8	62.9	80.5	84.2	87.1	97.4
Demeton-S-methyl	919-86-8	C6H15O3PS2	230.0200	57.8	82.1	93.1	87.6	108.5	102.4
Sebuthylazine	7286-69-3	C9H16ClN5	229.1094	28.7	53.3	69.8	79.8	88.5	95.8
Flutriafol	76674-21-0	C16H13F2N3O	301.1027	27.3	46.1	71.4	76.1	81.8	87.3
Furametpyr	123572-88-3	C17H20ClN3O2	333.1244	48.3	69.8	86.9	86.2	97.6	101.9
Fenobucarb	3766-81-2	C12H17NO2	207.1259	60.9	79.2	100.7	96.1	102.8	103.9
Benodanil	15310-01-7	C13H10INO	322.9807	50.9	69.8	86.3	96.5	102.4	94.8
Terbuthylazine	5915-41-3	C9H16ClN5	229.1094	50.4	66.6	83.2	87.2	89.8	91.0
Dimethachlor	50563-36-5	C13H18ClNO2	255.1026	75.1	86.1	106.0	107.1	106.2	108.0
Dimethenamid	87674-68-8	C12H18ClNO2S	275.0747	72.6	84.9	102.9	100.0	103.6	97.3
Furalaxyl	57646-30-7	C17H19NO4	301.1314	82.2	89.1	106.6	108.6	106.2	102.4
Bixafen	581809-46-3	C18H12Cl2F3N3O	413.0310	66.8	79.3	99.0	95.6	103.7	97.1
Triflumuron	64628-44-0	C15H10ClF3N2O3	358.0332	54.2	71.8	95.5	84.9	95.3	101.7
Epoxiconazole	133855-98-8	C17H13ClFN3O	329.0731	61.6	77.2	98.8	95.3	90.0	101.2
Teflubenzuron	83121-18-0	C14H6Cl2F4N2O2	379.9742	41.8	50.9	80.1	86.8	100.0	97.7

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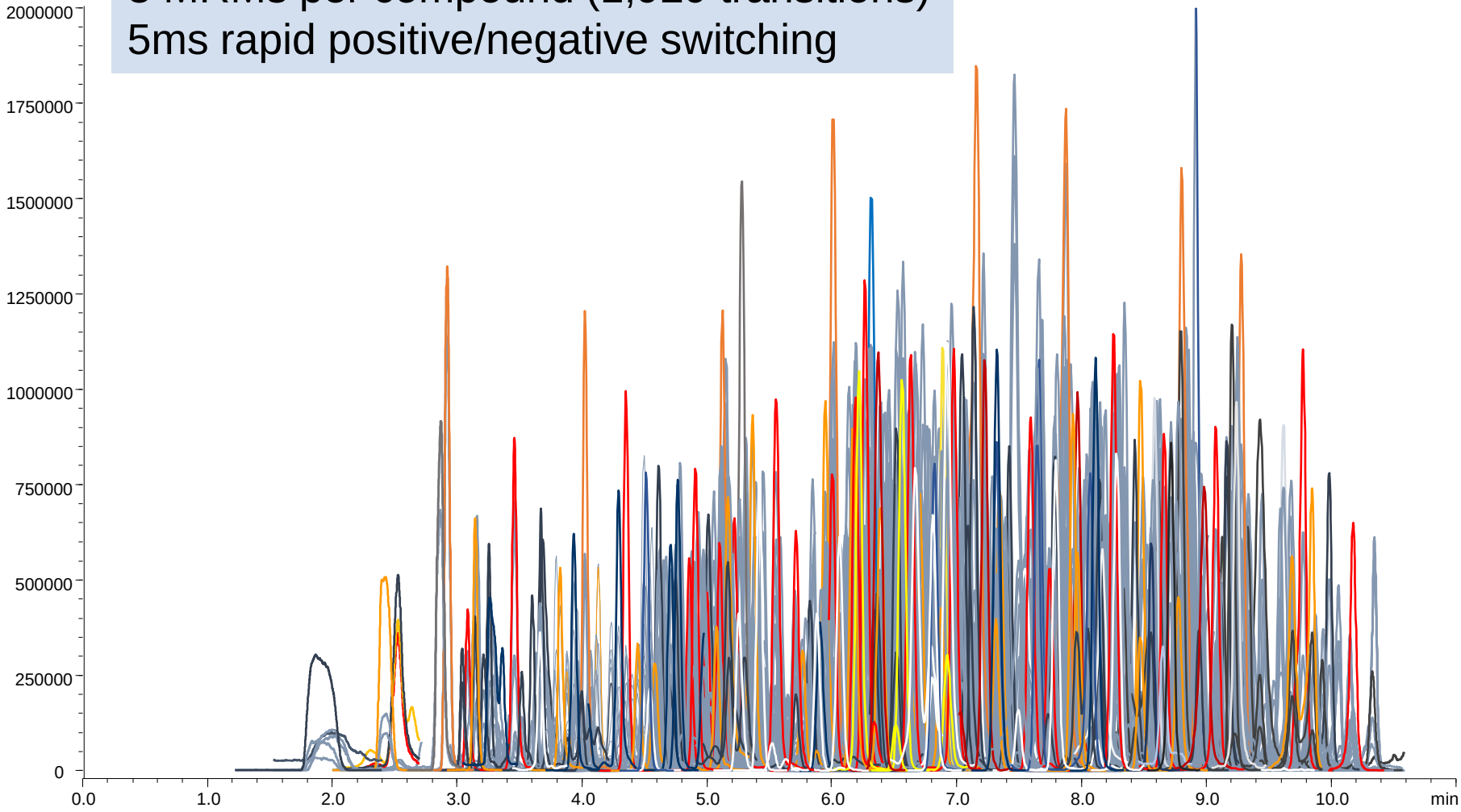
Pesticides Solutions

646pesticides in 10.5 minutes
3 MRMs per compound (1,929 transitions)
5ms rapid positive/negative switching



646 pesticides spiked into a mint extract at 0.010 mg/kg

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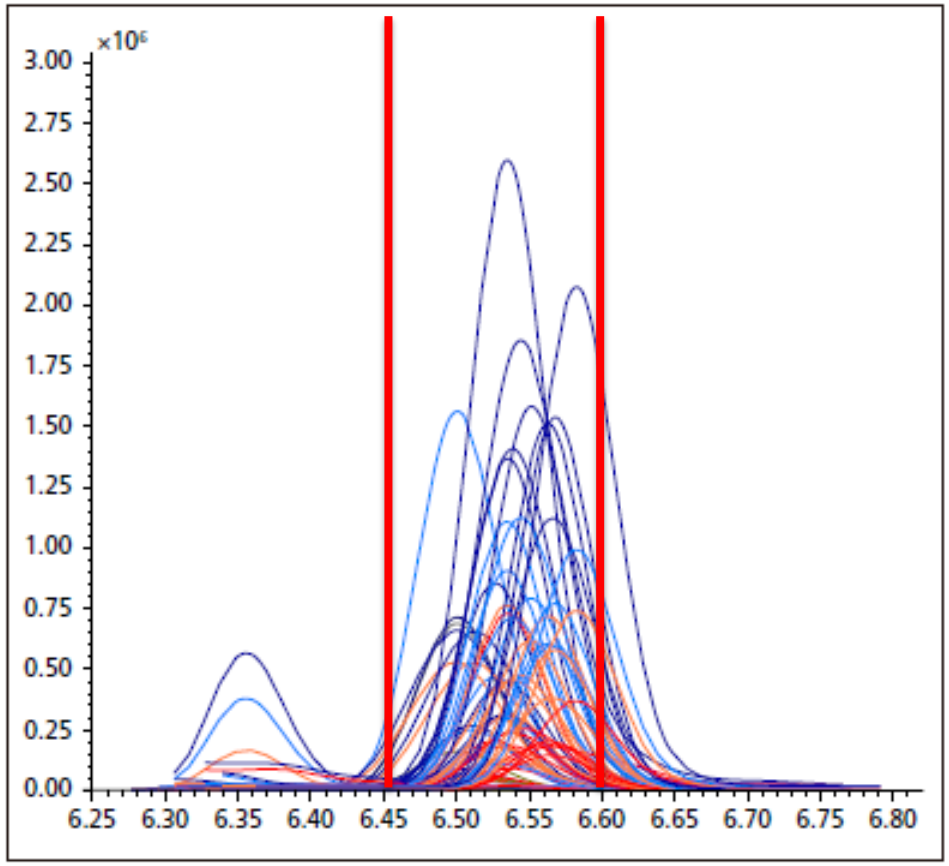
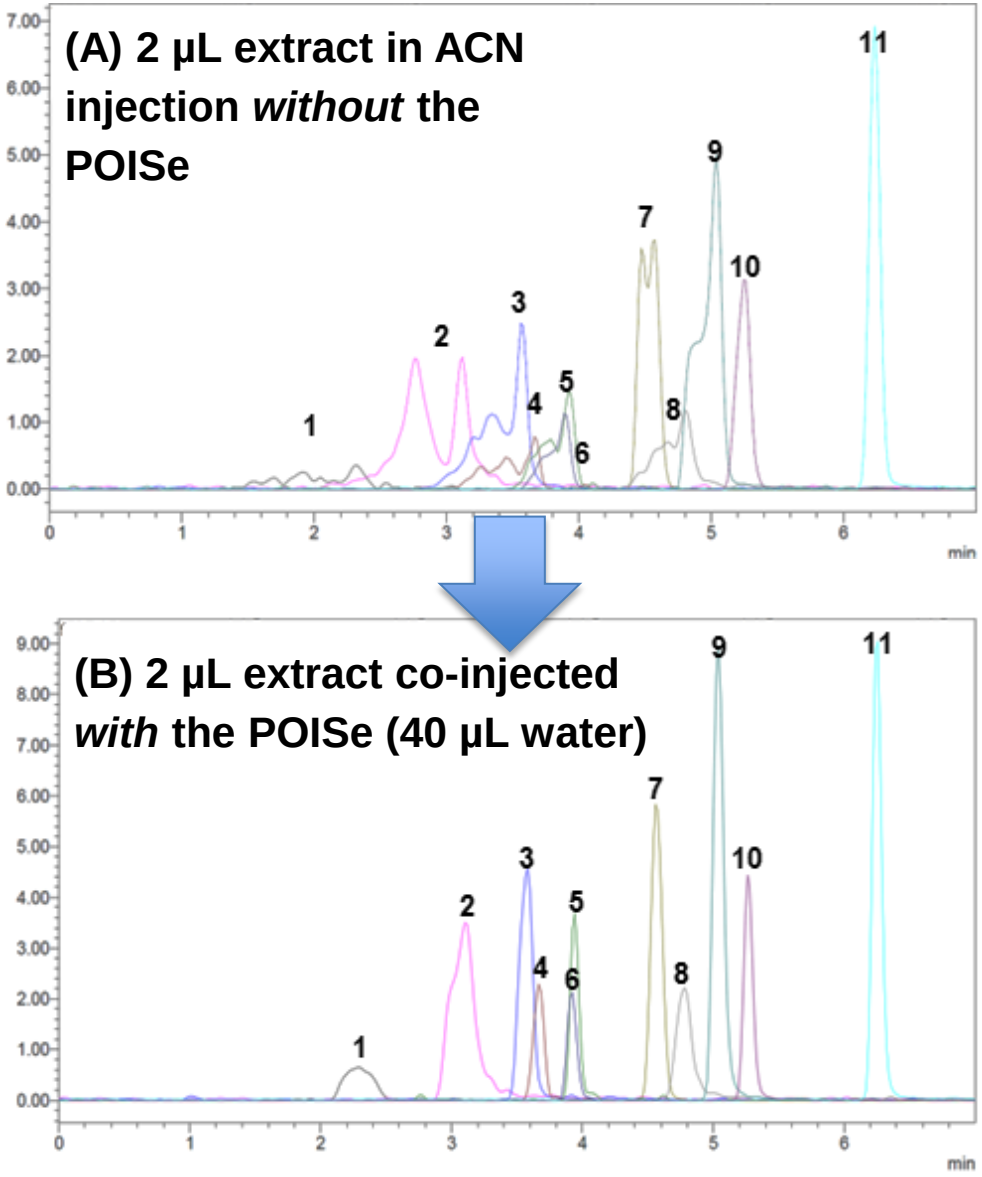
LCMS-8060 SPEED/Polarity switching

Between 6.45 and 6.60 min 220 MRMtransitions overlapped.
199 MRMs positive mode and 21 MRMs negative mode.
25 compounds eluted
Avg peak area RSD% was <3%



Compound Name	CAS number	Formula	RT	Average Peak Area	%RSD (n=6)
Trinexapac-ethyl	95266-40-3	C13H16O5	6.45	1,780,015	3.1
Iprovalicarb	140923-17-7	C18H28N2O3	6.46	1,442,486	2.8
Dodemorph	1593-77-7	C18H35NO	6.47	658,920	4.2
Fluopyram	658066-35-4	C16H11ClF6N2O	6.47	2,439,146	1.9
Flutolanil	66332-96-5	C17H16F3NO2	6.48	3,372,285	2.7
Trifloxysulfuron	145099-21-4	C14H14F3N5O6S	6.48	1,822,340	2.5
Azaconazole	60207-31-0	C12H11Cl2N3O2	6.50	1,580,445	2.0
Terbutryn	886-50-0	C10H19N5S	6.50	755,446	3.4
Prometryn	7287-19-6	C10H19N5S	6.50	1,300,193	2.6
Azimsulfuron	120162-55-2	C13H16N10O5S	6.50	2,498,050	1.8
Metominostrobin	133408-50-1	C16H16N2O3	6.51	2,929,500	1.7
Thifluzamide	130000-40-7	C13H6Br2F6N2O2S	6.51	193,982	5.9
Nicarbazin	330-95-0	C13H10N4O5	6.52	973,101	2.6
Bromobutide	74712-19-9	C15H22BrNO	6.53	1,829,781	2.1
Saflufenacil	372137-35-4	C17H17ClF4N4O5S	6.53	465,224	2.3
Cyproconazole	94361-06-5	C15H18ClN3O	6.54	1,174,967	1.7
Clomazone	81777-89-1	C12H14ClNO2	6.54	3,409,656	1.7
Fensulfothion	115-90-2	C11H17O4PS2	6.54	4,267,514	1.4
Oxasulfuron	144651-06-9	C17H18N4O6S	6.54	2,911,533	1.1
Rimsulfuron	122931-48-0	C14H17N5O7S2	6.55	4,722,065	1.8
Fenthion-oxon	6552-12-1	C10H15O4PS	6.55	3,075,195	1.4
Nitrothal-isopropyl	10552-74-6	C14H16NO6Na	6.56	2,199,581	3.0
Chlorantraniliprole	500008-45-7	C18H14BrCl2N5O2	6.57	2,407,025	2.7
Fipronil-sulfone	120068-36-2	C12H4Cl2F6N4O2S	6.57	2,843,708	2.0
Valifenalate	283159-90-0	C19H27ClN2O5	6.59	3,845,335	1.9

Performance Optimising Injection Sequence



No.	Compound
1	Methamidophos
2	Propamocarb
3	Omethoate
4	Butocarboxim sulfoxide
5	Aldicarb sulfoxide
6	Dinotefuran
7	Oxamyl
8	DMPF
9	Demeton-S-methyl sulfoxide
10	Demeton-S-methyl sulphone
11	Ethiofencarb sulphone

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Pesticides Solutions

Library entries	
Compound information	Compound Name Synonyms Japanese name Chinese name CAS Chemical Formula Mono-isotopic mass Theoretical *m/z* ([M+H]+, [M+Na]+, [M+K]+, [M+NH_4]+, [M-H]-) Activity InChI InChIKey
MS/MS parameters	Ionization mode Q1 (*m/z*) Q3 (*m/z*) Q1 Pre Bias CE Q3 Pre Bias
Web links	Alanwood.net PAN Pesticide Database Chemical Book ChemSpider

Fast sample preparation
(QuECheRS)
- *Reliable for different matrix*
- *High extraction efficiency*
- *Customizable procedure*

Complete MRM library
- *750 Compounds*
- *>6000 MRM transitions*
- *Detailed chemical description*

Easy customization
User can choice compounds to detect

Ready to use *LCMS-MS method*
- *LC conditions*
- *MS conditions*
- *Integration parameters*
- *Automatic Report*

Shimadzu high end Triple Quadrupole

Quantification of 647 pesticides in 10.5 minutes
- *High sensitivity*
- *Elevated repeatability*
- *Robust performance over several days*

- Method package for pesticides analysis
- **Polar pesticides: how to approach them**
- Water monitoring: Decisione di esecuzione (UE) 2015/495

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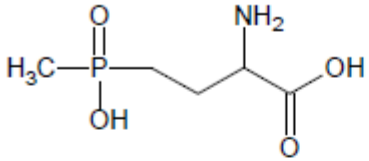
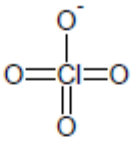
Highly polar pesticides

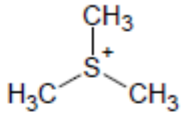
Glyphosate



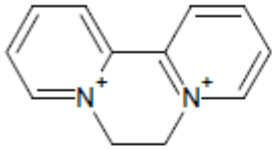
Perchlorate



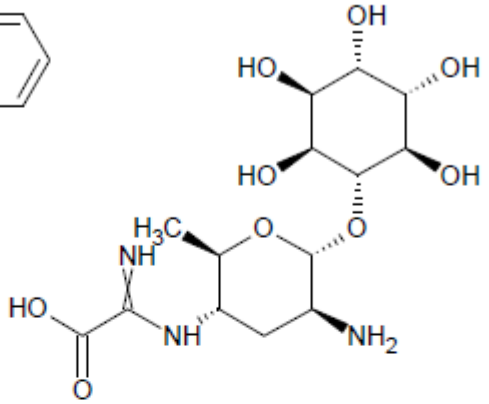
Trimesium



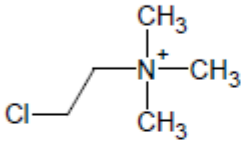
Diqaut



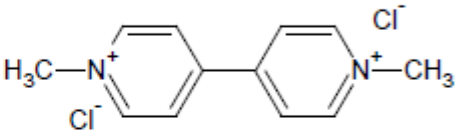
Kasugamycine



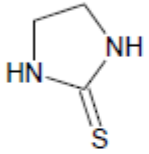
Chlormeqaut



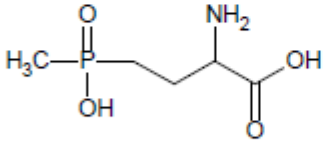
Paraquat



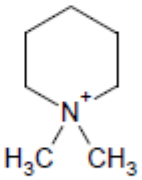
ETU



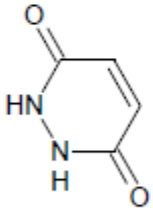
Glufosinate



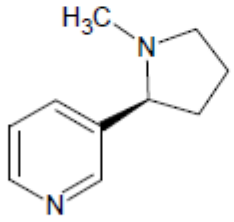
Mepiquat



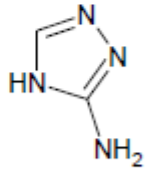
Maleic hydrazide



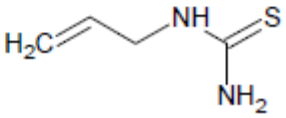
Nicotine



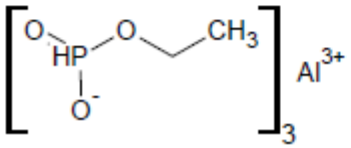
Amitrole



PTU



Fosethyl aluminium



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Materials

- Food extracts of apple
- SAMPLE PREPARATION: chopping, freezing, homogeneizing, adding 1% FA in MeOH solution and centrifuge
- LINEARITY CURVE: Six point curve from 5 to 200 pg/µL generated by spiking samples.
- CALIBRATION CURVE: using deuterated IS

Method development:

- COLUMNS:

- SIELC Obselisc R
- Hypercarb PGC
- SeQuant ZiC-HILIC
- SeQuant ZiC-cHILIC
- Scherzo SM-C18
- Scherzo SW-C18
- Fortis Phenyl
- Luna Phenyl Hexyl
- Restek IBD

- MOBILE PHASES & ADDITIVES:

- Acetic acid
- Formic Acid
- Ammonium formate
- Ammonium acetate
- Ammonium hydroxide

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Final methods:

Liquid chromatography				
	Method 1		Method 2	
UHPLC	Nexera UHPLC system		Nexera UHPLC system	
Analytical column	ZIC-HILIC (100 x 2.1mm, 3.5µm)		Hypercarb PGC (100mm x 2.1mm, 5µm)	
Mobile phase	A = Water 20mM ammonium formate and 0.3% formic acid		A = Water 1% acetic acid	
	B = Acetonitrile		B = Methanol 1% acetic acid	
Gradient	Time (mins)	%B	Time (mins)	%B
	0	97	0	0
	5.8	68	10	30
	9	15	15	35
	10	15	17.5	68
	10	97	18	100
	16	Stop	22	100
			22.1	0
			33	Stop
Column temp.	35°C		35°C	
Injection volume	6µL (40µL acetonitrile co-injected)		5µL	
Flow rate	0.4mL/min		0.3mL/min	
Mass spectrometry				
LC/MS/MS	LCMS-8050			
Ionisation mode	Heated electrospray			
Polarity switching time	5 ms			
Pause time	1 ms			
Dwell times	5-50ms			
Interface temperature	350°C			
Heating block	300°C			
Desolvation line	200°C			
Gas	Heating gas 10 L/min; drying gas 10 L/min; Nebulising gas 3 L/min			

High Polar Pesticides: method 1

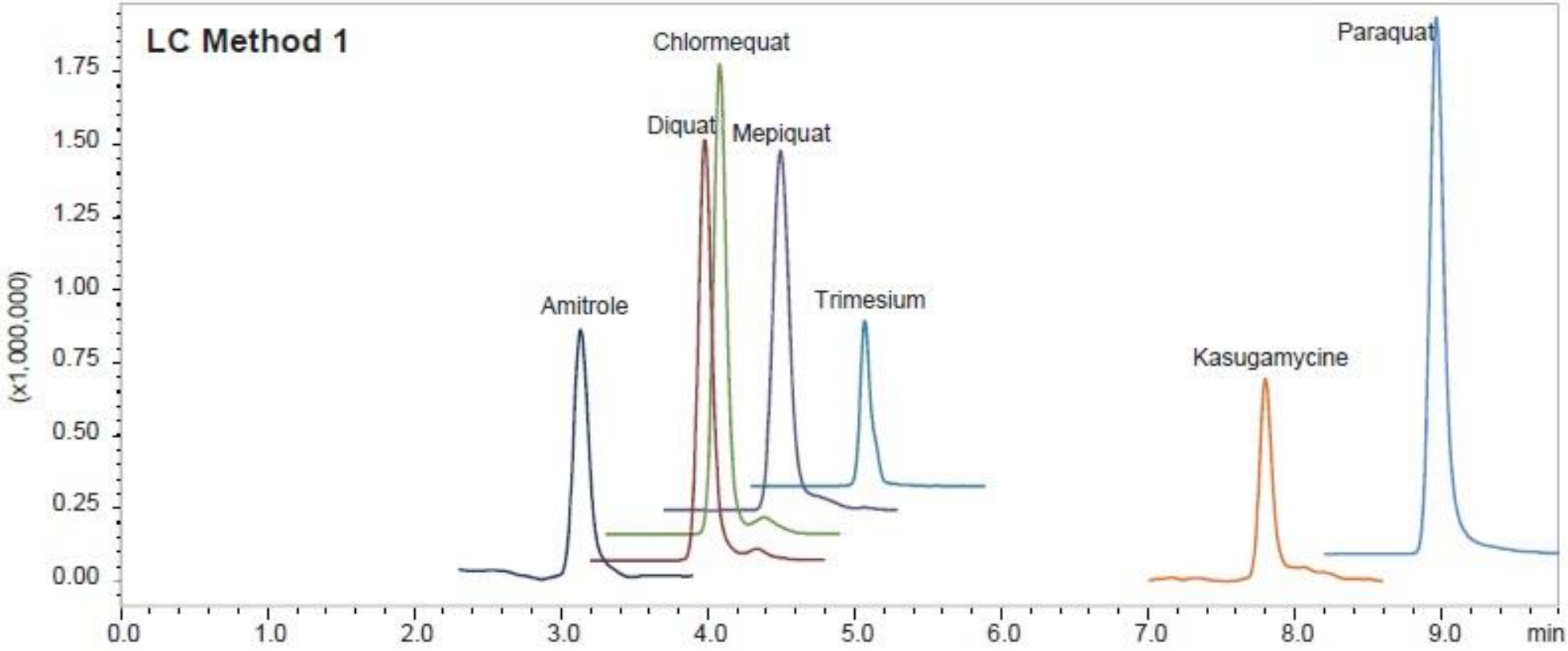

Figure 2 . Target analytes at 0.05mg/kg in apple matrix using a ZIC-HILIC based separation (LC Method 1)

All compounds were quantified in the range 0.005 – 0.2 mg/kg with correlation coefficients greater than 0.9975

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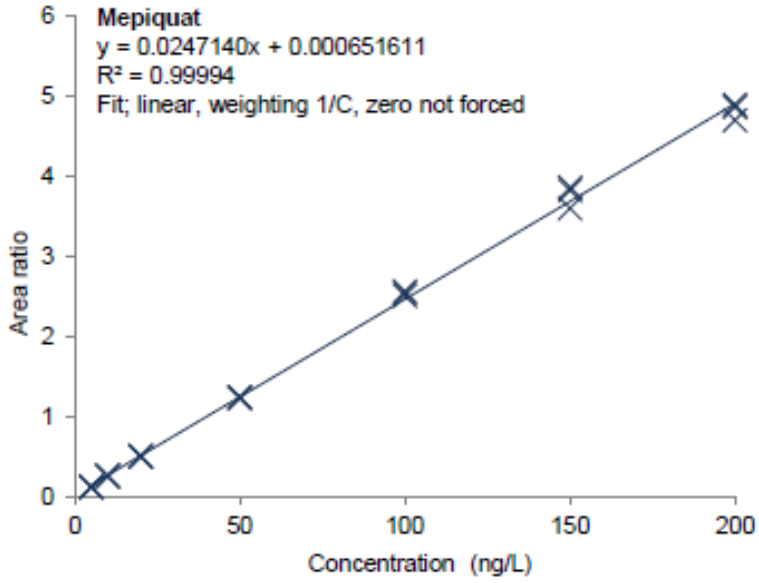
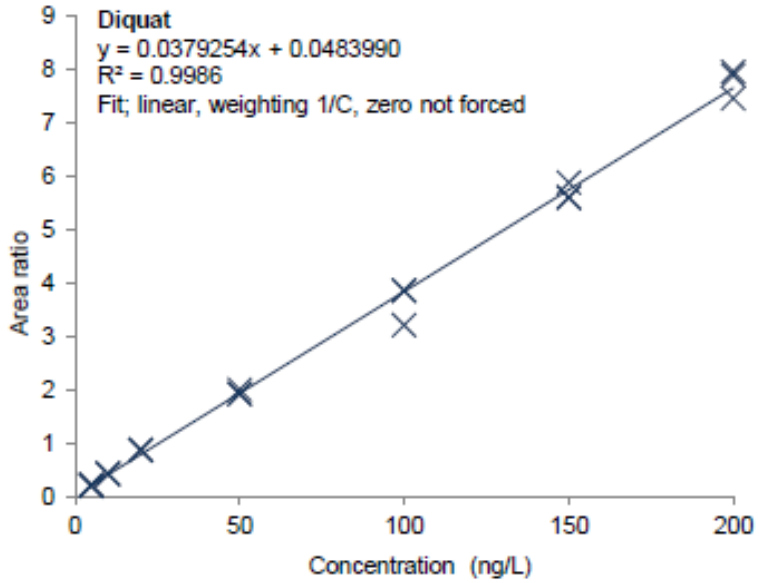
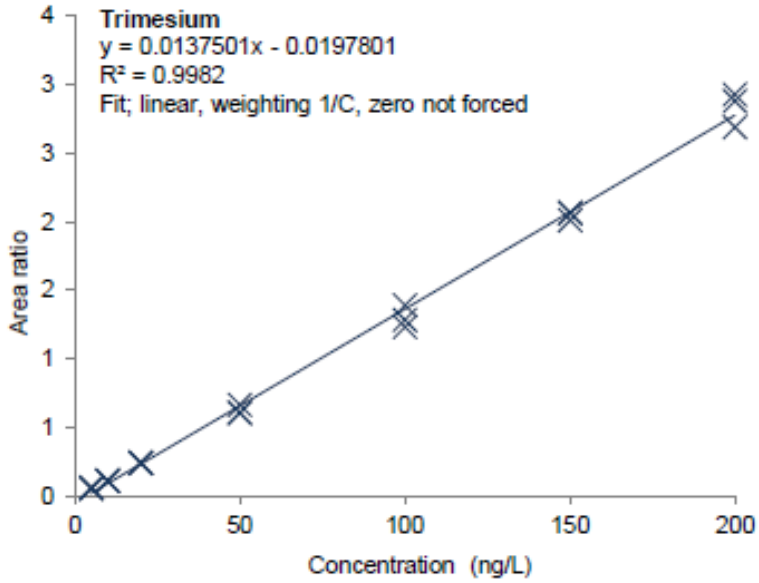
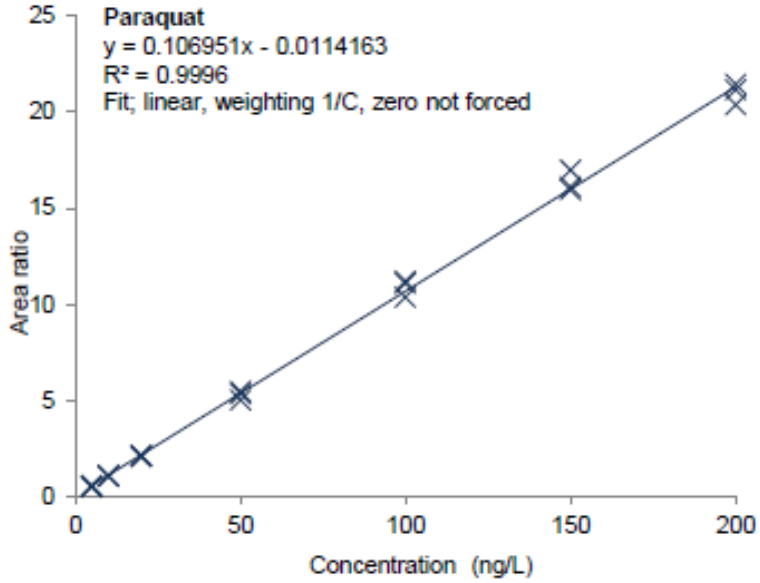
Linearity results method 1

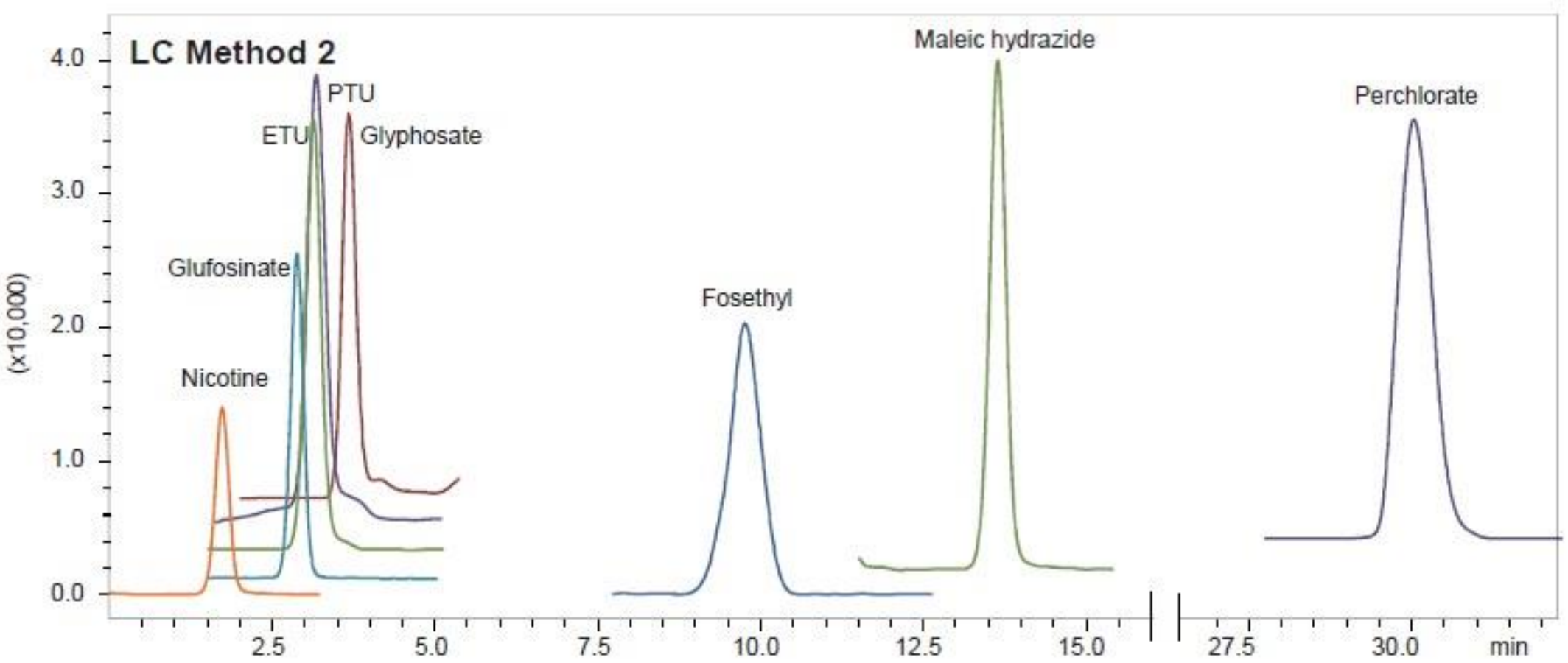






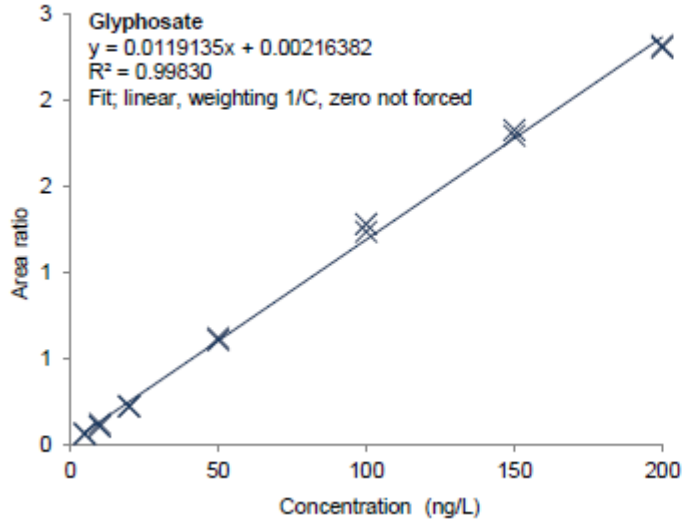


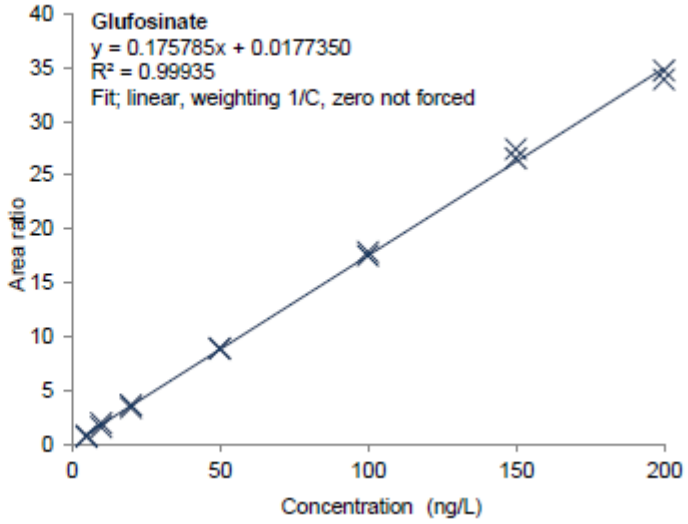
High Polar Pesticides: method 2

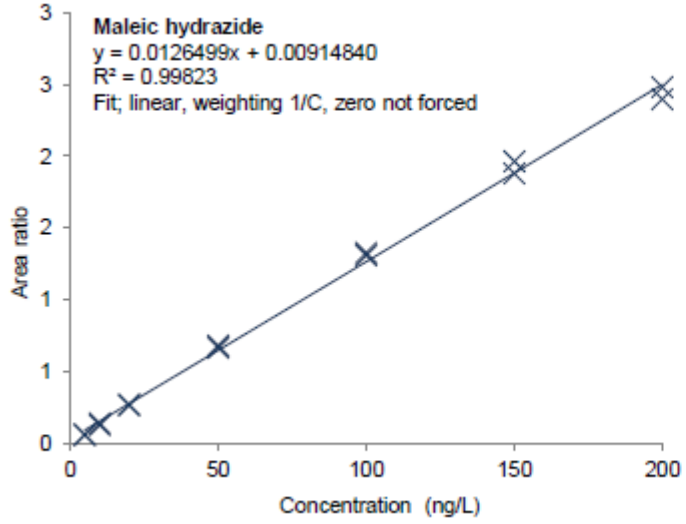


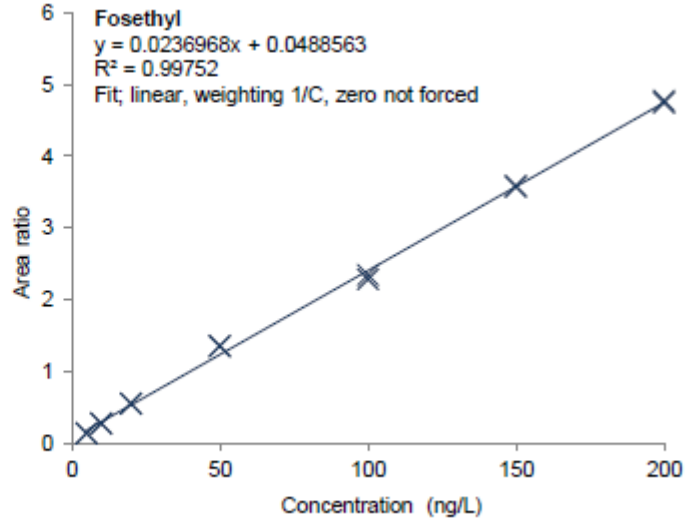
All compounds were quantified in the range 0.005 – 0.2 mg/kg with correlation coefficients greater than 0.9975

Linearity results method 2









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Linearity

Compound	R^2	Fit type	Weight	Method
Diquat	0.9986	Linear	1/C	Method 1
Chlormequat	0.9988	Linear	1/C	Method 1
Amitrole	0.9981	Quadratic	1/C	Method 1
Kasugamycine	0.9992	Linear	1/C	Method 1
Daminozide	0.9995	Quadratic	1/C	Method 1
Mepiquat	0.9993	Linear	1/C	Method 1
Paraquat	0.9995	Linear	1/C	Method 1
Trimesium	0.9981	Linear	1/C	Method 1
ETU	0.9998	Linear	1/C	Method 2
Fosethyl	0.9975	Linear	1/C	Method 2
Gluphosinate	0.9993	Linear	1/C	Method 2
Glyphosate	0.9983	Linear	1/C	Method 2
Maleic hydrazide	0.9982	Linear	1/C	Method 2
Nicotine	0.9984	Linear	1/C	Method 2
Perchlorate	0.9998	Linear	1/C	Method 2
PTU	0.9991	Linear	1/C	Method 2

- 3 MRM transitions/compound (only 2 for kasugamicyne
- All polar pesticides quantified at 0.01 mg/kg → Lower than EU MRL required (0.02-0.1 mg/kg) !!!
- Sensitivity is easily reached without derivatization → it is also possible to dilute the sample extract and reduce matrix effect

- Method package for pesticides analysis
- Polar pesticides: how to approach them
- **Water monitoring: Decisione di esecuzione (UE) 2015/495**

DECISIONE DI ESECUZIONE (UE) 2015/495 DELLA COMMISSIONE

del 20 marzo 2015

che istituisce un elenco di controllo delle sostanze da sottoporre a monitoraggio a livello dell'Unione nel settore della politica delle acque in attuazione della direttiva 2008/105/CE del Parlamento europeo e del Consiglio

[notificata con il numero C(2015) 1756]

(Testo rilevante ai fini del SEE)

Elenco di controllo delle sostanze da sottoporre a monitoraggio a livello dell'Unione di cui all'articolo 8 *ter* della direttiva 2008/105/CE

Denominazione della sostanza o del gruppo di sostanze	Numero CAS (1)	Numero UE (2)	Metodi di analisi indicativi (3) (4) (5)	Limite massimo ammissibile del metodo di rilevazione (ng/l)
17-alfa-etinilestradiolo (EE2)	57-63-6	200-342-2	SPE — LC-MS-MS su grandi volumi	0,035
17-beta-estradiolo (E 2), estrone (e 1)	50-28-2, 53-16-7	200-023-8	SPE — LC-MS-MS	0,4
diclofenac	15307-86-5	239-348-5	SPE — LC-MS-MS	10
2,6-di-terz-butil-4-metilfenolo	128-37-0	204-881-4	SPE — GC-MS	3 160
4-metossicinnamato di 2-etilesile	5466-77-3	226-775-7	SPE — LC-MS-MS oppure GC-MS	6 000
Antibiotici macrolidi (6)			SPE — LC-MS-MS	90
Metiocarb	2032-65-7	217-991-2	SPE — LC-MS-MS oppure GC-MS	10
Neonicotinoidi (7)			SPE — LC-MS-MS	9
Ossadiazone	19666-30-9	243-215-7	LLE/SPE — GC-MS	88
Tri-allato	2303-17-5	218-962-7	LLE/SPE — GC-MS oppure LC-MS-MS	670

DECISIONE DI ESECUZIONE (UE) 2015/495 DELLA COMMISSIONE

del 20 marzo 2015

che istituisce un elenco di controllo delle sostanze da sottoporre a monitoraggio a livello dell'Unione nel settore della politica delle acque in attuazione della direttiva 2008/105/CE del Parlamento europeo e del Consiglio

[notificata con il numero C(2015) 1756]

(Testo rilevar ni del SEE)

Elenco di controllo delle sostanze da sott nitoraggio a livello dell'Unione di cui all'articolo 8 *ter* 008/105/CE

Denominazione della sostan gruppo di sostanz	ero		etodi di analisi indi-cativi (3) (4) (5)	imite massimo ammis-sibile del metodo di rilevazione (ng/l)
			LC-MS-MS su lumi	0,035
17-			S-MS	0,4
diclof			LC-MS-M	10
	128-37-0	204-881-4	SP	
	5466-77-3	226-775-7	SPE — LC-MS-MS oppure GC-MS	
			SPE — LC-MS-MS	90
	2032-65-7	217-991-2	SPE — LC-MS-MS oppure GC-MS	10
Neonicotinoidi (7)			SPE — LC-MS-MS	9
Ossadiazone	19666-30-9	243-215-7	LLE/SPE — GC-MS	88
Tri-allato	2303-17-5	218-962-7	LLE/SPE — GC-MS oppure LC-MS-MS	670

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Excellence in Science

Thanks for your kind attention

Veronica Mainini
LCMS Application Support, Shimadzu Italy
vmainini@shimadzu.it

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C146-E306

For LabSolutions Version 5.82 and Later

LC/MS/MS Method Package for Residual Pesticides Ver. 2

- World's largest compound panel (646 pesticides in a single method)
- Ultra-high-speed method, with detection in 10.5 minutes
- Ultra-high-speed detection delivers robust and reproducible data quality for extended pesticide programs
- Pretreatment program to improve the shape of peaks for polar pesticides
- Excellent data stability in combination with the LCMS-8000 series

LCMS-8060

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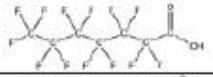
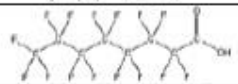
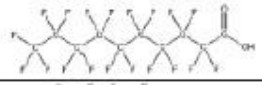
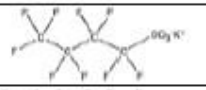
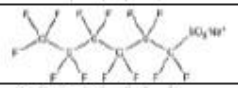
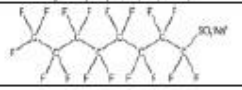
Water Safety

Name	Abbreviation	Structure	Retention Time	Transitions
Perfluoro-n-hexanoic acid	PFHxA		1.28	313>119 313>269
Perfluoro-n-heptanoic acid	PFHpA		1.63	363>169 363>319
Perfluoro-n-octanoic acid	PFOA		1.91	413>169 413>369
Perfluoro-n-nonanoic acid	PFNA		2.15	463>219 463>419
Perfluoro-n-decanoic acid	PFDA		2.36	513>269 513>469
K Perfluoro-n-butanesulfonate	L-PFBS		1.02	299>80 299>99
Na Perfluoro-n-hexanesulfonate	L-PFHxS		1.70	399>80 399>99
Na Perfluoro-n-octanesulfonate	L-PFOS		2.18	499>80 499>99

Perfluorinated Compounds

LCMS-8050,analytes were ionized using negative mode electrospray ionization. The method required only 3.15 minutes.

Linearity from 2.5-25 fg (S/N>10) to 3200 fg on column