Multi residue pesticide screening in fruit and vegetables using the G6490A QQQ system

Easy, reliable quantitation and identification of pesticides in Food Samples using LC-MS/MS and library search

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Pesticides screening – the state of the art

Current regulations and residue situation

- **EU regulation**
  - Maximum residue levels regulated in commision regulation (EC) 396/2005
    - appendix II – IV regulates >170 000 maximum residue limits (matrix-pesticide combinations)
  - European and national monitoring programs are in place also regulated by (EC) 396/2005
  - 173 notifications related to pesticide residues have been entered in the Rapid Alert System for Food and Feed (RASFF) in 2009
- **US regulation**
  - 40 CFR Part 180:
    Regulates tolerances and exemptions from tolerances for pesticide chemicals in food. Specifies allowed methodologies for analysis
  - Special regulations are in place for:
    - Organic food
    - Baby food

Pesticides screening – the state of the art

Method validation – the SANCO guidelines

Method needs to be validated for at least one representative matrix from each commodity group

Commodity group	Commodity categories	Typical representative commodities
High water content	12 categories, e.g. fruiting vegetables/cucurbits	Tomatoes, peppers, cucumber
High oil content	3 categories, e.g. Oily fruits and products	Olives, avocados
High starch / low water content	2 categories, e.g. cereal grain and products	Wheat, maize, rice, breakfast cereals
High acid content	3 categories, e.g. citrus fruit	Lemons, mandarins, oranges
High sugar / low water content	Dried fruit	Raisins, fruit jams
Difficult or unique commodities		Hops, coffee, tea, spices

Pesticides screening – the state of the art

Pesticide ranking published by EURL for pesticides

"Check your scope" ranking for pesticides

- Listing includes more than 1100 compounds
  - Pesticides currently used or used in the past
  - Pesticide metabolites of importance
- Ranking of pesticides based on:
  - Toxicological data (toxicological endpoints and endocrine disruptive activity)
  - Residue situation in crops (reporting from labs in Europe and RASFF notifications)
  - Agricultural usage (including potential for misuse and persistent pesticides)
- Analytical information

	Compounds	Exclusive method
LCMS amenable	683	212
GCMS amenable	552	156
GCMS and LCMS amenable	381	
No good method mentioned*	252	

* rated as difficult or not possible for GCMS and LCMS or no data available for both methods

Outline

Why is utmost sensitivity required for pesticide analysis?

- Analyze a large number of relevant compounds with single injection (even those with lower abundancies)
- To show improved LOQs for pesticides in complex matrices
- To show suitability of 6490 for analysis of baby food
- To show pecision of 6490 on this application
- To show that the 6490 allows to inject less, thereby
  - Reduce matrix effects to get better accuracies for quantitation based on solvent calibration
  - Improve robustness
- To demonstrate confirmation of questionable compounds in complex matrices

Agilent G6490A QQQ system

New developments for utmost sensitivity

- Ionization and Ion Transfer Technology
  - Agilent Jet Stream Ion Generation
  - Hexabore capillary
  - Dual ion funnel (iFunnel) technology
    - Two stages for ion focusing and gas removal
    - Improvements for wide *m/z* range transmission
    - Low capacitance

- Collision Cell
  - Hexapole field axial focusing curved collision cell
    - Tapered cell structure for increased ion acceptance at entrance
    - Reduced noise

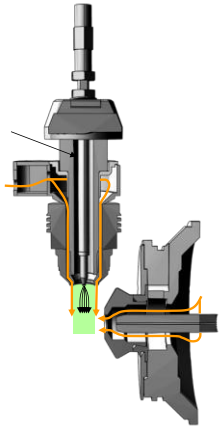
- Improved Quad Drive Electronics
  - Improved Quad DC frequency response
  - Higher RF power capability
  - Quad drive frequency increased to 1.4 MHz

Agilent iFunnel technology

Captures 6 to 10 times more ions

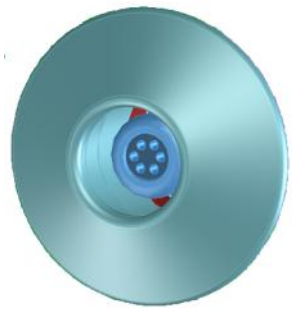
Agilent Jet Stream

- Thermal confinement of ESI plume to create ion rich zone
- Efficient desolvation to create gas phase ions
- Effective ionization across broad range of analyte classes including many APCI compounds



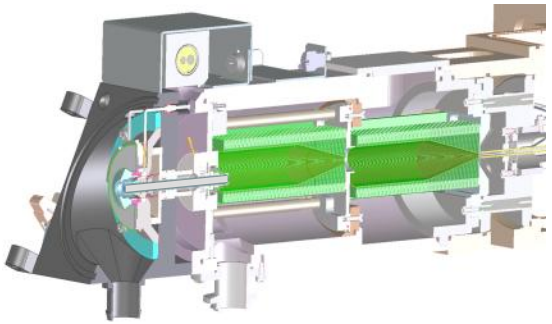
Hexabore Capillary

- Six bores and half the length means much less restriction
- Samples 6 to 10 times more ion rich gas from the source with 6 capillaries
- Captures the majority of the gas from the source region



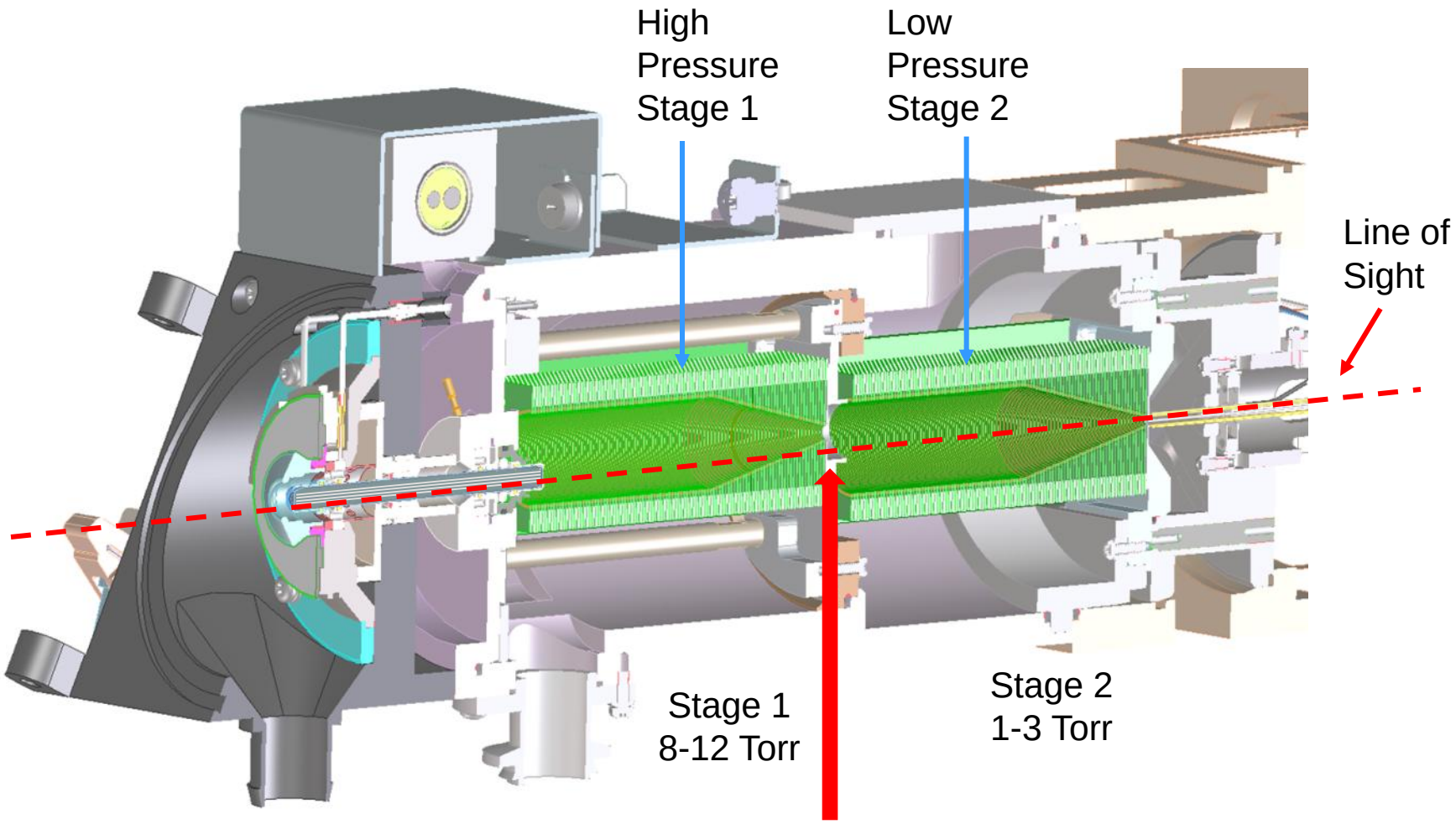
Dual Ion Funnel

- Removes the gas but captures the ions
- Makes skimmer and one compound dependant parameter obsolete
- Removes neutral noise
- Low capacitance design allows for fast polarity switching



Agilent iFunnel technology

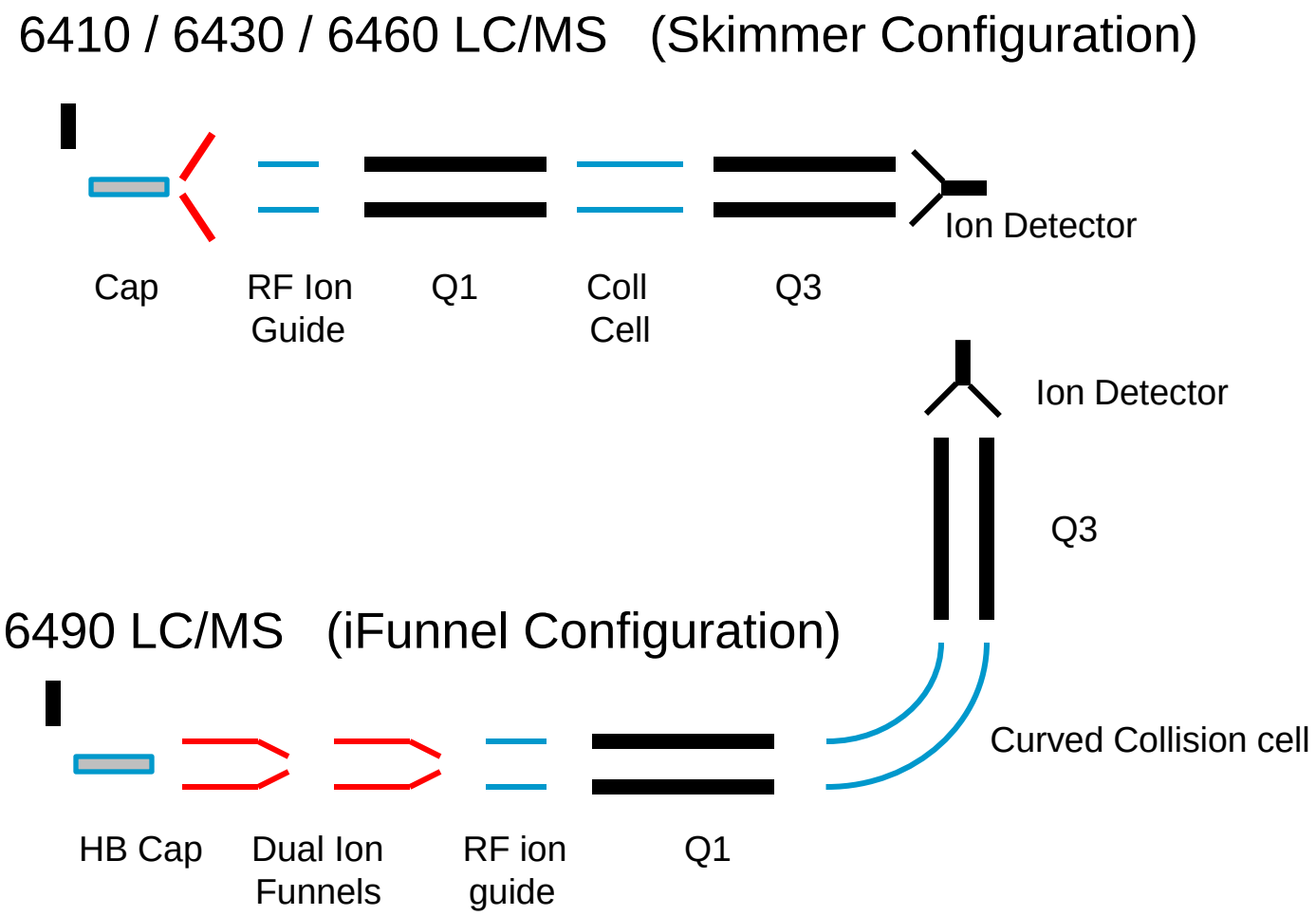
Two stage ion funnel manages the gas load



Offset ion funnels to prevent neutrals from going straight through to MS

Agilent triple quadrupole instruments

Instrument configurations



Agilent Dynamic MRM application kits

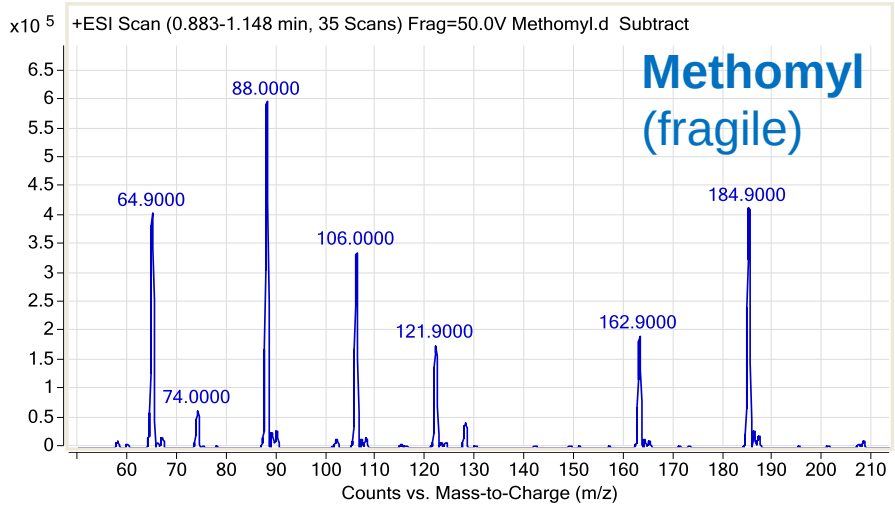
Our approach to make you more productive

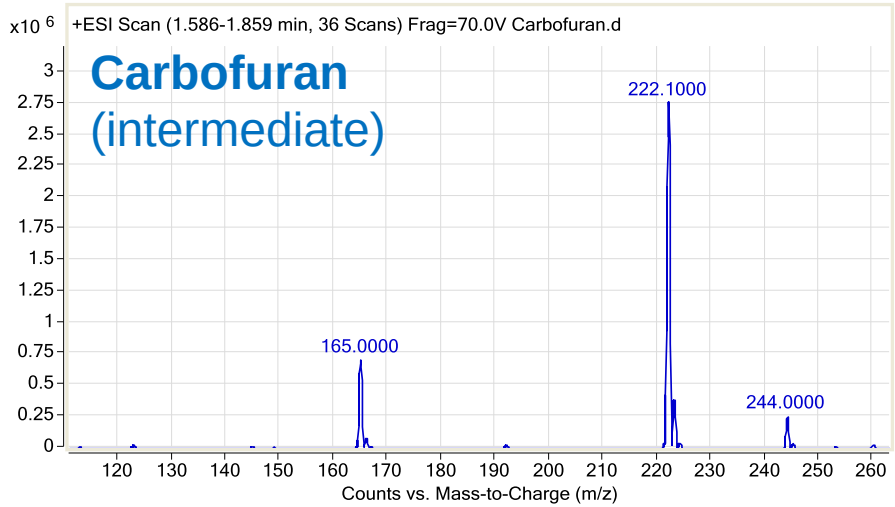
G1733AA - Pesticide DMRM
Data Base Kit

- Database with conditions, transitions, and retention times for 600 compounds
- Pre-configured methods for 300 pesticides for different LC configurations
- ZORBAX Eclipse Plus UHPLC column
- Small suite positive and negative ion test mix for method validation and adjustment
- Extensive documentation and free trial SampliQ QuEChERS kits

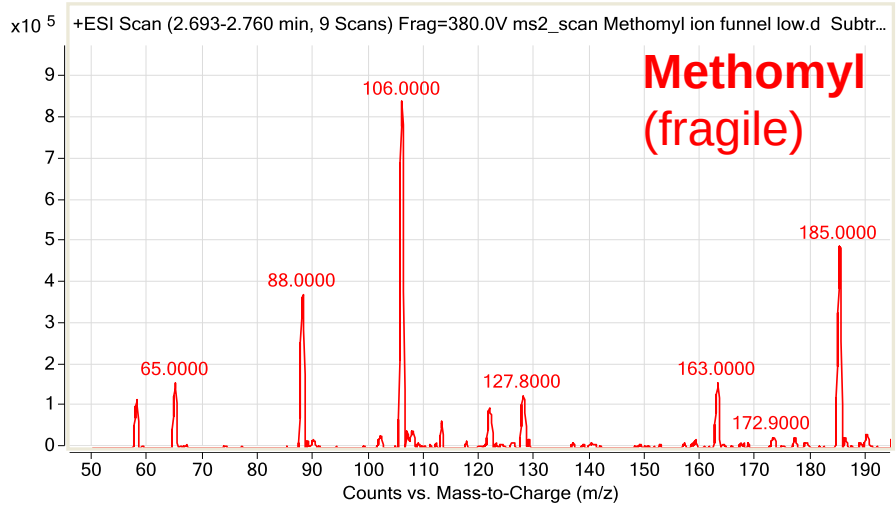
Universal transmission of ions with iFunnel

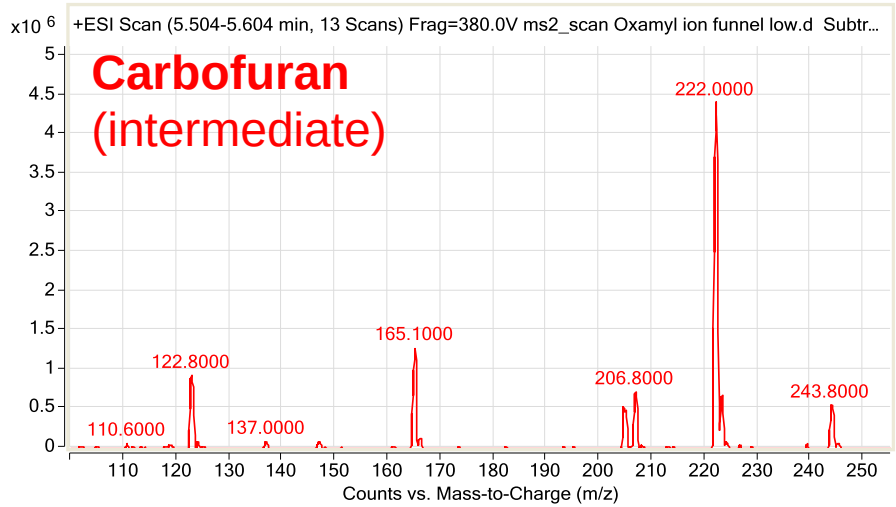
Full scan spectra 6460 (optimized FragV)





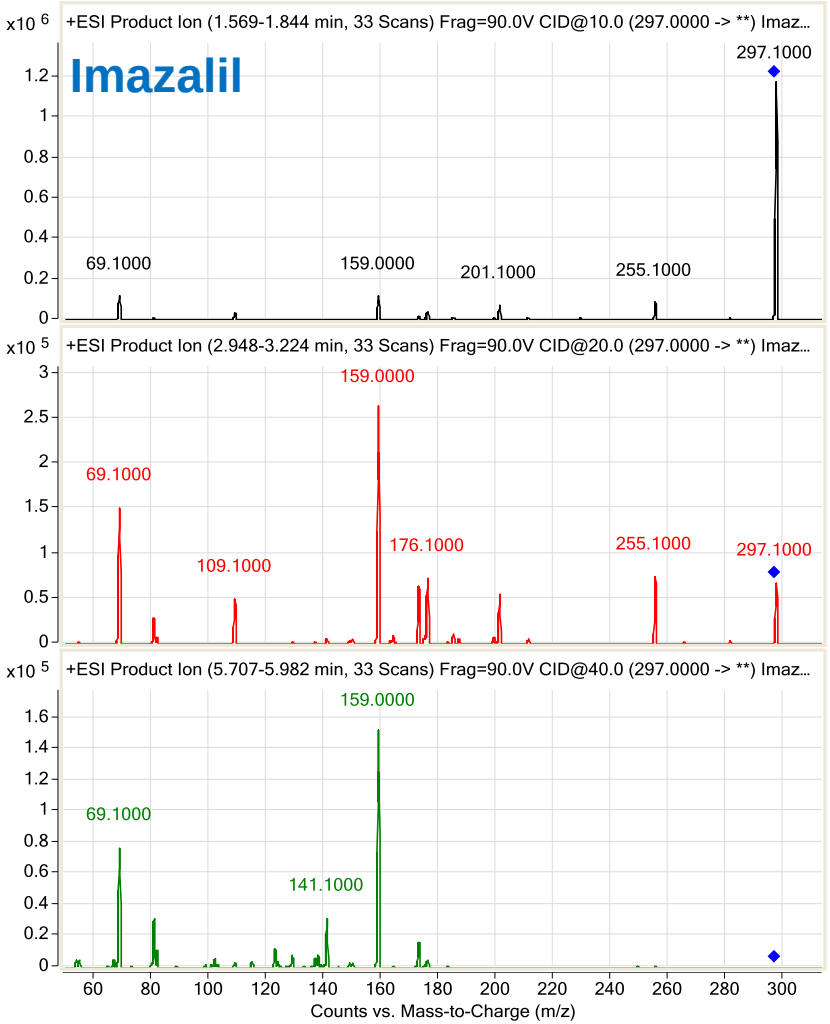
Full scan spectra 6490



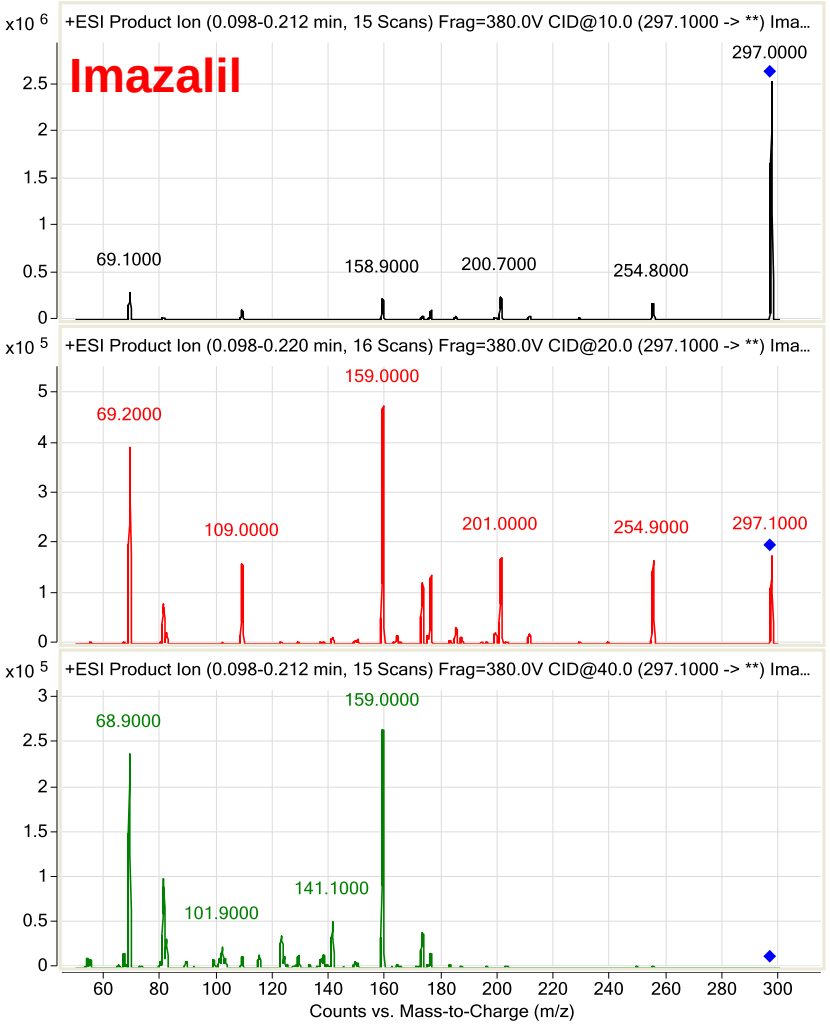


Linear vs. curved collision cell: Comparable behavior

Product ion spectra 6460 (optimized FragV)

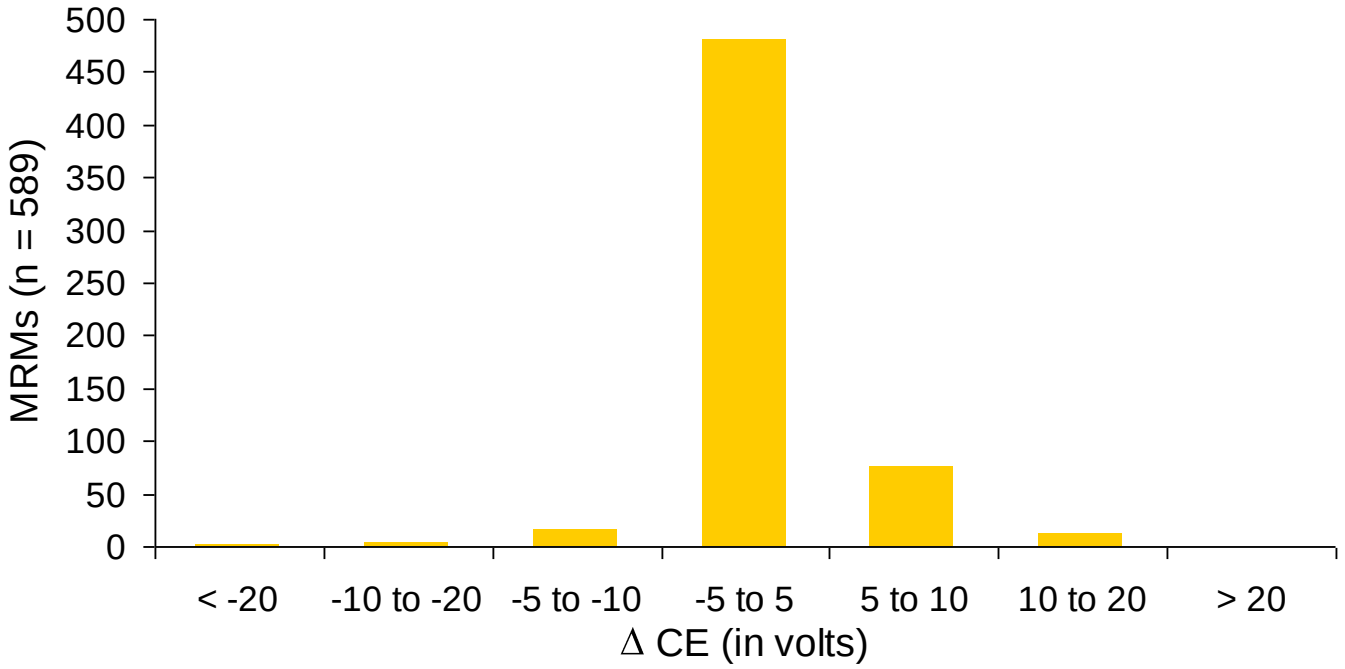


Product ion spectra 6490



Linear vs. curved collision cell: Comparable behavior

Collision energy optimization via MassHunter Optimizer for 6460 vs. 6490



- < 0.4% of all MRMs show CE difference of more than 20 V
- 2.5 % of all MRMs show CE differences between 10 and 20 V
- 15.4 % of all MRMs show CE differences between 5 and 10 V
- 81.7% of all MRMs show CE differences of less than 5 V

Multi residue pesticide method

Compounds included in method

Acephat	Butocarboxim-sulfoxid	Desmedipham	Fenamiphos-sulfon	Flusilazol	Metamitron	Oxadiazon	Proquinazid	Terbutylazin
Acetamiprid	Buturon	DMSA	Fenamiphos-sulfoxid	Flutolanil	Metazachlor	Oxadixyl	Prosulfocarb	Tetraconazol
Acrinathrin	Cadusaphos	Dichlofluanid	Fenarimol	Flutriafol	Metconazol	Oxamyl	Pymetrozin	Thiabendazol
Aldicarb	Carbaryl	Dichlorvos	Fenazaquin	Foramsulfuron	Methabenzthiazuron	Oxasulfuron	Pyraclostrobin	Thiacloprid
Aldicarb-sulfon	Carbendazim	Diclofop-methyl	Fenbuconazol	Formetanat-Hydrochlorid	Methacrifos	Oxydemeton-sulfon	Pyrazophos	Thiamethoxam
Aldicarb-sulfoxid	Carbofuran 3 hydroxy	Dicrotophos	Fenbutatinoxid	Formothion	Methamidophos	Paclobutrazol	Pyridaben	Thifensulfuron-methyl
Alloxydim	Carbofuran	Diethofencarb	Fenhexamid	Fosthiazat	Methidathion	Paraoxon-methyl	Pyridaphenthion	Thiodicarb
Amidosulfuron	Carbosulfan	Difenoconazol	Fenobucarb	Fuberidazol	Methiocarb	Penconazol	Pyridat	Thiofanox sulfon
Aminopyralid	Carfentrazone-ethyl	Difenoxuron	Fenoxaprop free acid	Furathiocarb	Mthiocarb-sulfon	Pencycuron	Pyrifenox	Thiofanox sulfoxid
Amitraz	Chlorantraniliprol	Diflubenzuron	Fenoxycarb	Halosulfuron-methyl	Methiocarb-sulfoxid	Pendimethalin	Pyrimethanil	Thiofanox
Asulam	Chlorfenvinphos	Diflufenican	Fenpiclonil	Haloxyfop free acid	Methomyl	Pethoxamid	Pyriproxifen	Thiophanat
Atrazin	Chlorfluazuron	Dimefuron	Fenpropimorph	Hexaconazol	Methoxyfenozid	Phenmedipham	Pyroxsulam	Thiophanat-methyl
Avermectin B1a Metabolite	Chloridazon (Pyrazon)	Dimethenamid	Fenpyroximat	Hexaflumuron	Metobromuron	Phenthoat	Quinalphos	Tolclophos-methyl
Avermectin B1a	Chlorimuron-ethyl	Dimethoat	Fenthion	Hexythiazox	Metolachlor	Phorat	Quinmerac	Tolylfluanid
Avermectin B1b	Chloroxuron	Dimethomorph	Fenthion-oxon	Imazalil	Metosulam	Phosalon	Quinoxyfen	Topramezone
Azimsulfuron	Chlorsulfuron	Dimoxystrobin	Fenthion-oxon-sulfon	Imidacloprid	Metoxuron	Phosmet	Quizalfop free acid	Tralkoxydim
Azinphos-ethyl	Chlozolinat	Diniconazol	Fenthion-oxon-sulfoxid	Indoxacarb	Metrafenon	Phosmet-oxon	Quizalofop-ethyl	Triadimefon
Azinphos-methyl	Chromafenozid	Dioxathion	Fenthion-sulfon	Ipconazol	Metribuzin	Phosphamidon	Rimsulfuron	Triadimenol
Azoxystrobin	Clethodim	Diuron	Fenthion-sulfoxid	Iprodion	Metsulfuron-methyl	Phoxim	Rotenone	Triasulfuron
Beflubutamid	Clofentezin	EPN	Flazasulfuron	Iprovalicarb	Mevinphos	Picoxystrobin	Sethoxydim	Triazofos
Benalaxyl	Clomazon	Epoxyconazol	Flonicamid	Isoproturon	Molinat	Pinoxaden	Siduron	Tribenuron-methyl
Benfuracarb	Clopyralid	Ethaboxam	Florasulam	Isoxaflutol	Monocrotophos	Piperonyl butoxid	Silthiopham	Trichlorfon
Bensulfuron-methyl	Clothianidin	Ethiofencarb	Fluazifop free acid	Kresoxim methyl	Monolinuron	Pirimicarb	Simeconazol	Tricyclazol
Benthiavalicarb	Cyazofamid	Ethiofencarb-sulfon	Fluazifop-P-butyl	Lenacil	Monuron	Pirimiphos-methyl	Spinosad	Trifloxystrobin
Bifenazat	Cycloxydim	Ethiofencarb-sulfoxid	Flufenacet	Linuron	Myclobutanil	Pirmicarb-desmethyl	Spirotetramat	Triflumizol
Bifenox	Cyhexatin	Ethion	Flufenoxuron	Lufenuron	Napropamid	Prochloraz	Spiroxamin	Triflumuron
Bispyribac	Cymoxanil	Ethiprol	Flumetsulam	Malaoxon	Neburon	Profenophos	Sulfosulfuron	Triflusulfuron-methyl
Bitertanol	Cyproconazol	Ethirimol	Fluometuron	Mandipropamid	Nicosulfuron	Promecarb	Tebuconazol	Triforin
Bromacil	Cyprodinil	Ethofumesat	Fluopicolid	Mecarbam	Nitenpyram	Propamocarb	Tebufenozid	Trinexapac-ethyl
Bromuconazol	Cyromazin	Ethoprophos	Fluoroglycofen-ethyl	Mepanipyrim	Novaluron	Propaquizafop	Tebufenpyrad	Triticonazol
Bupirimat	Daminozid	Etofenprox	Fluoxastrobin (E)	Mesosulfuron-methyl	Nuarimol	Propargite	Teflubenzuron	Tritosulfuron
Buprofezin	DEET	Famoxadon	Fluquinconazol	Mesotrione	Ofurace	Propiconazol	Tembotrion	Zoxamid
Butocarboxim	Demeton-S-methyl	Fenamidon	Fluroxypyr	Metaflumizone	Omethoat	Propoxur	Tepraloxydim	
Butoxycarboxim	Demeton-S-methyl-sulfon	Fenamiphos	Flurtamon	Metalaxyl	Orthosulfamuron	Propyzamid	Terbutryn	

313 compounds including 9 isomers

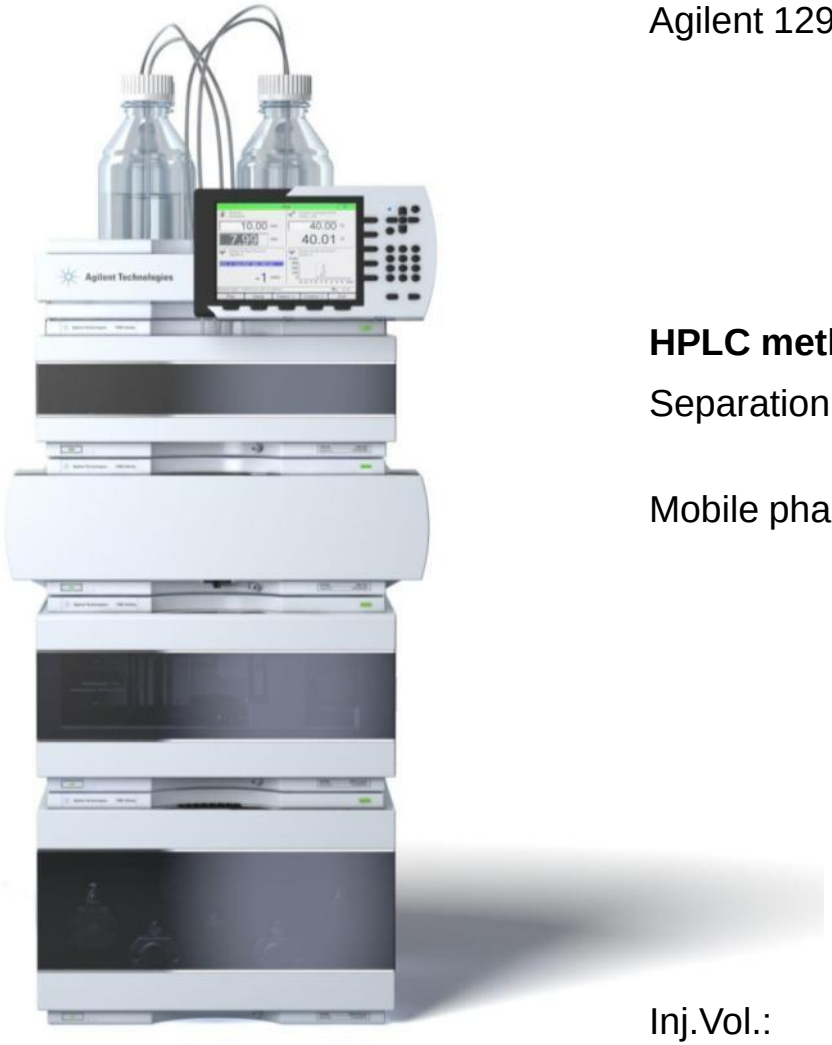
Pesticide screening and quantitation
Sample preparation

Samples have been prepared according §64 LFGB „QuEChERS“ without modification:

- 10 g of homogenized sample have been extracted with 10 ml acetonitrile. For wheat flour and black tea sample amount has been reduced to 5 or 2 g, respectively and samples have been fortified with 10 ml water before extraction.
- Lemon sample has been neutralized by addition of 600 µl 5N NaOH
- Addition of MgSO4, NaCl, sodium citrate, centrifuge (5 min @ 3000 rpm)
- Clean-up by dispersive SPE. Transfer of 6 ml of the supernatant to a d-SPE tube with 900 mg MgSO4, 150 mg PSA, for pepper, black tea and rucola in addition 15 or 45 mg graphitized carbon black are added.
- After centrifugation 5 ml of the supernatant are stabilized with 50 µl formic acid (5% in acetonitrile)

Multi residue pesticide method

HPLC method



Agilent 1290 Infinity LC system consisting of:

- binary pump
- wellplate sampler
- column compartment
- diode array detector (not used)

HPLC method

Separation column:	ZORBAX Eclipse Plus C-18 RRHD column, 100 x 2.1 mm, 1.8 µm @ 25°C	
Mobile phase:	A: 5 mM ammonium formate	
	B: methanol + 5 mM ammonium formate	
	Flow:	0.6 ml/min
	Gradient:	0.00 min 5 % B
		0.20 min 5 % B
		2.20 min 50 % B
		10.50 min 100 % B
		13.00 min 100 % B
		13.10 min 5 % B
		15.00 min 5 % B
Inj.Vol.:	2 µl	

Multi residue pesticide method

MS method

Spray chamber conditions:

Gas temp.:	120°C
Dry gas:	15 l/min
Nebulizer:	35 psi
Sheath gas temp:	375°C
Sheath gas flow:	12 l/min

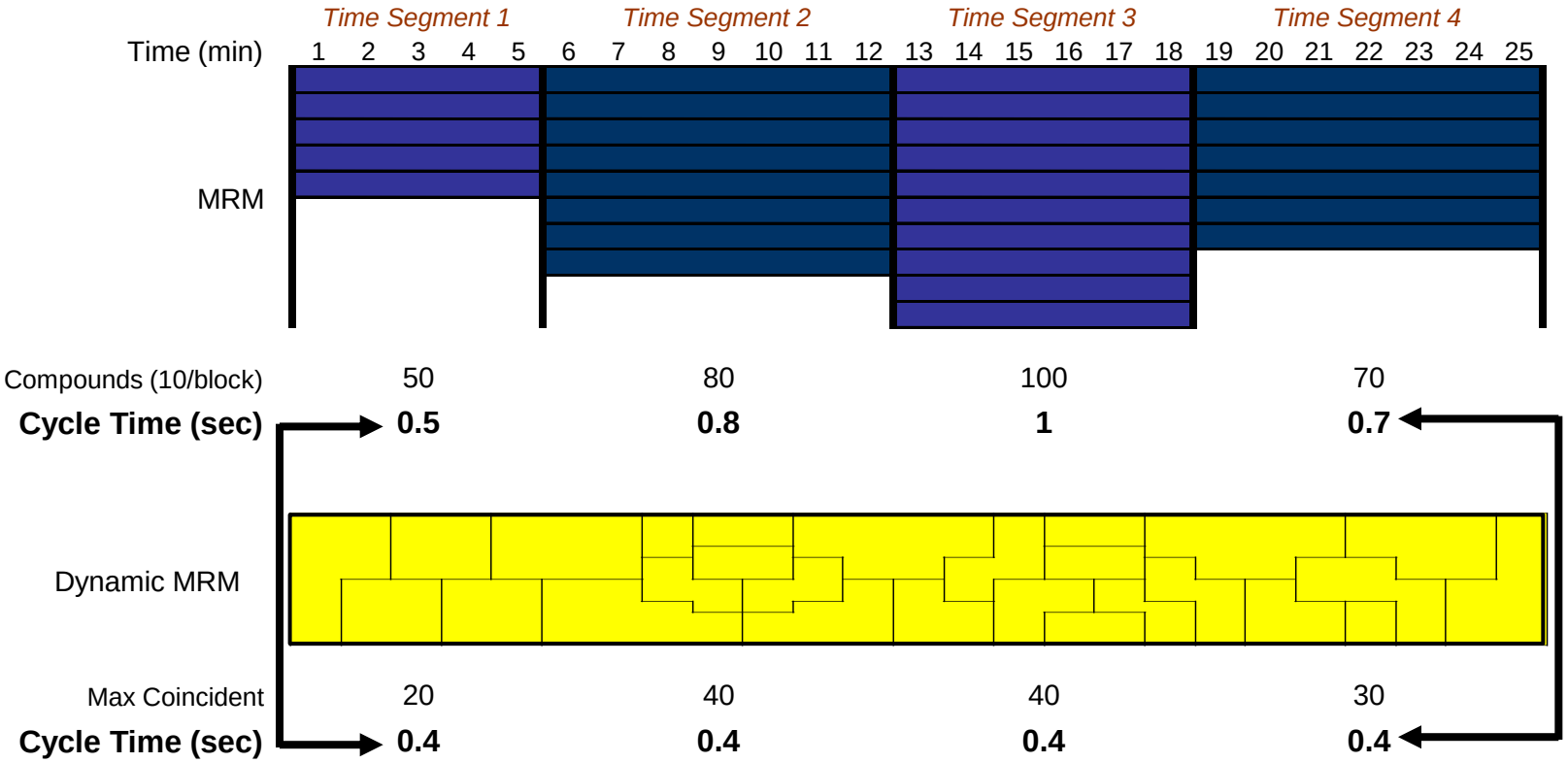
	Positive	**Negative**
CapVoltage:	3500 V	3000 V
Nozzle voltage	300 V	500 V

Automatic setup of MRM tables based on selected cycle time, retention times and retention time windows for the individual compounds

- Cycle time 600 ms
- Interscan delay 3.5 ms
- Total No. of MRMs 635
- Maximum No. Of concurrent MRMs 74
- Minimum Dwell time 4.61 ms
- Maximum Dwell time 296.5 ms

Multi residue pesticide method

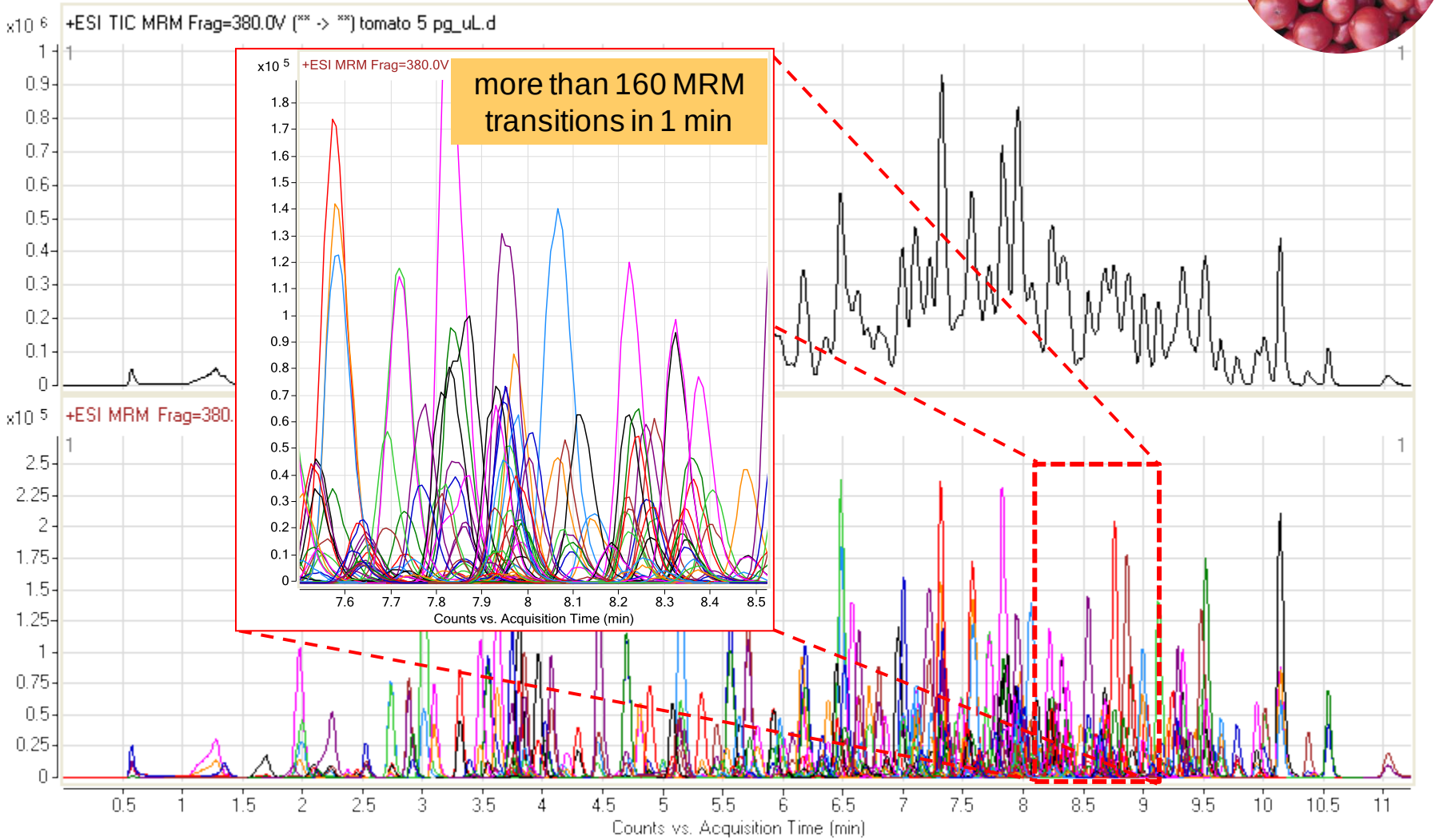
Comparison of MRM and Dynamic MRM



- 2 x shorter cycle times supports narrow chromatographic peaks, more analytes or longer dwell per analyte.

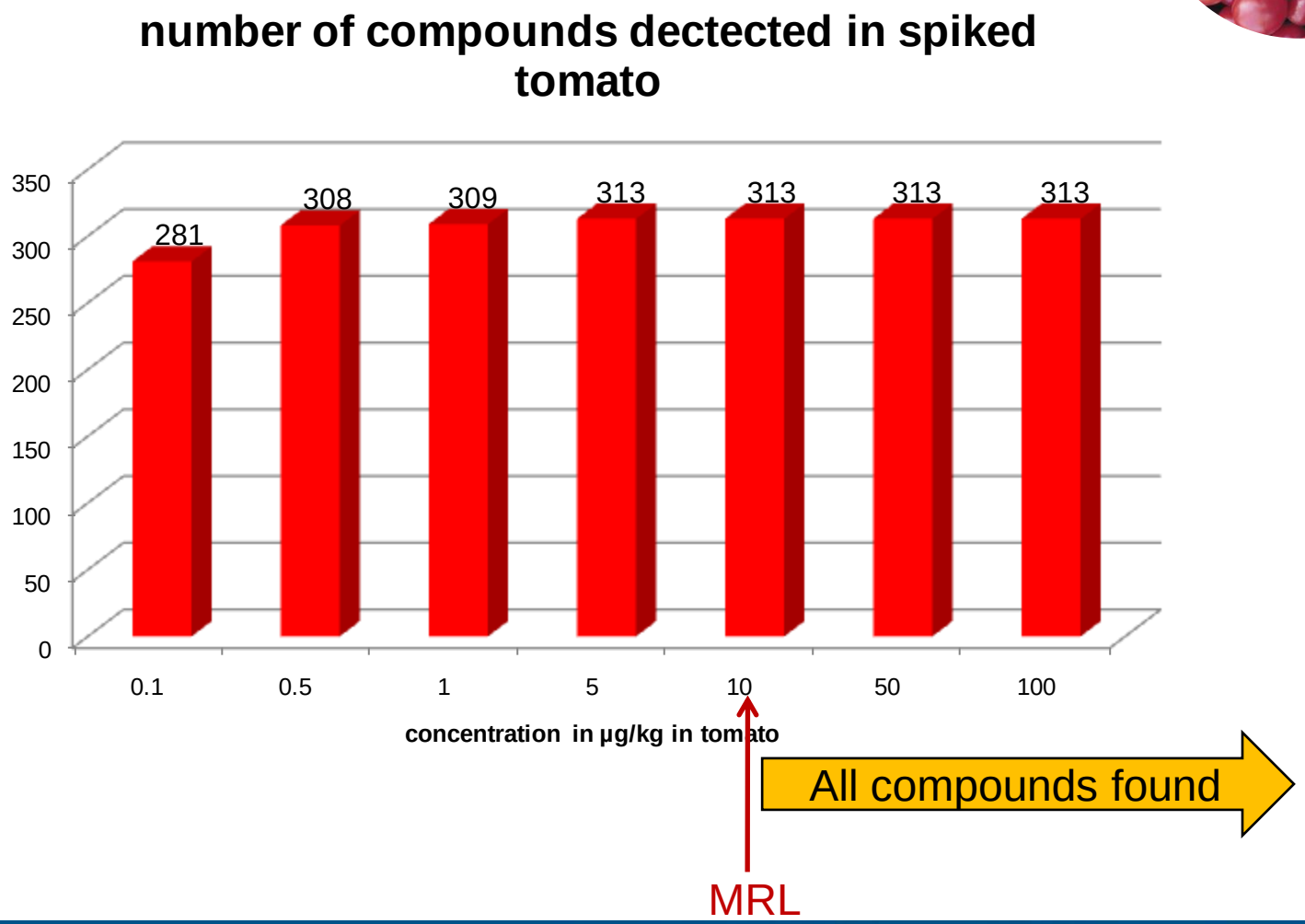
Multi residue pesticide method

MRM traces for tomato extract spiked at 10 µg/kg



Results for tomato extract

Coverage of method for tomato matrix

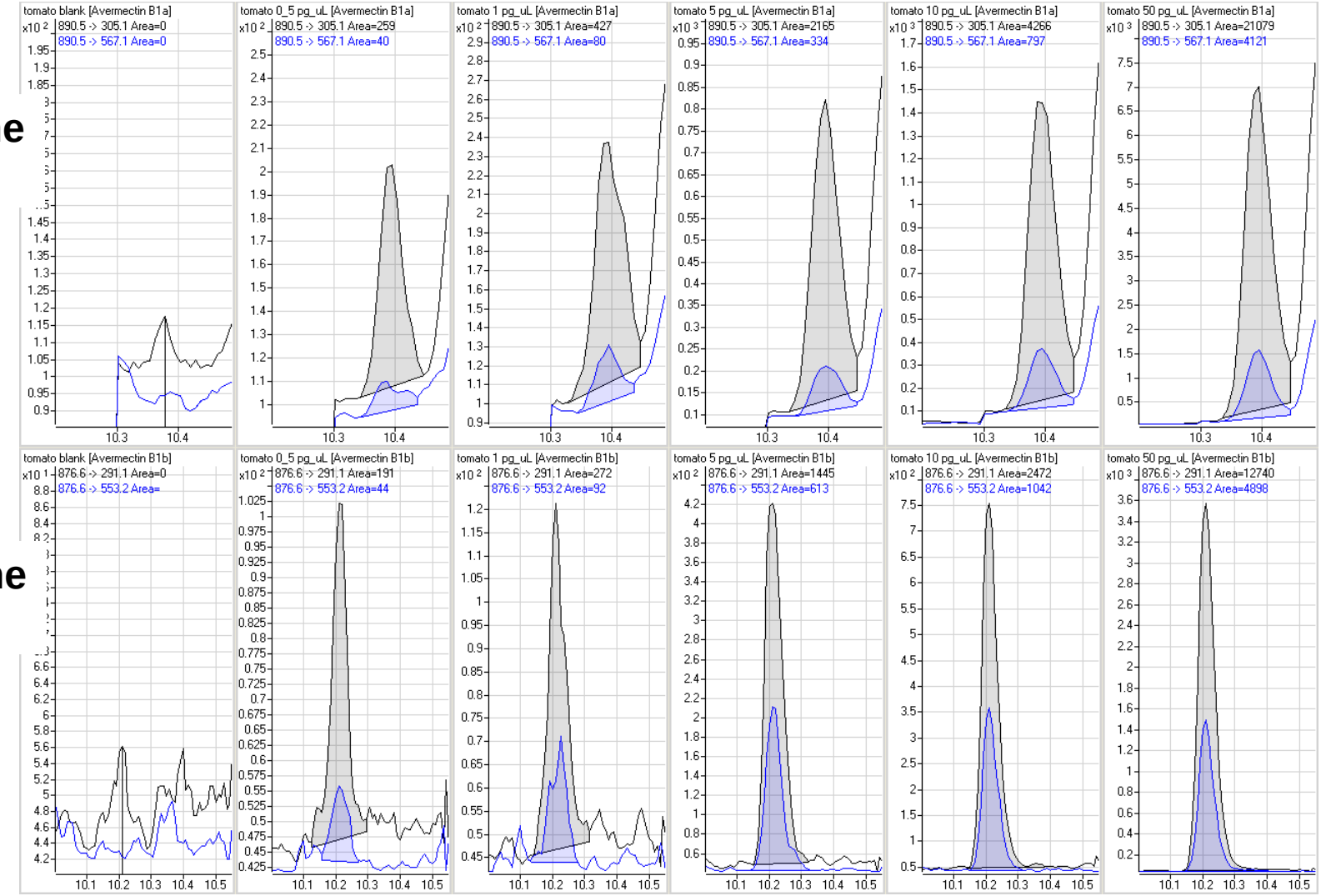


Results for tomato extract

Avermectine B1a and B1b

Avermectine B1a

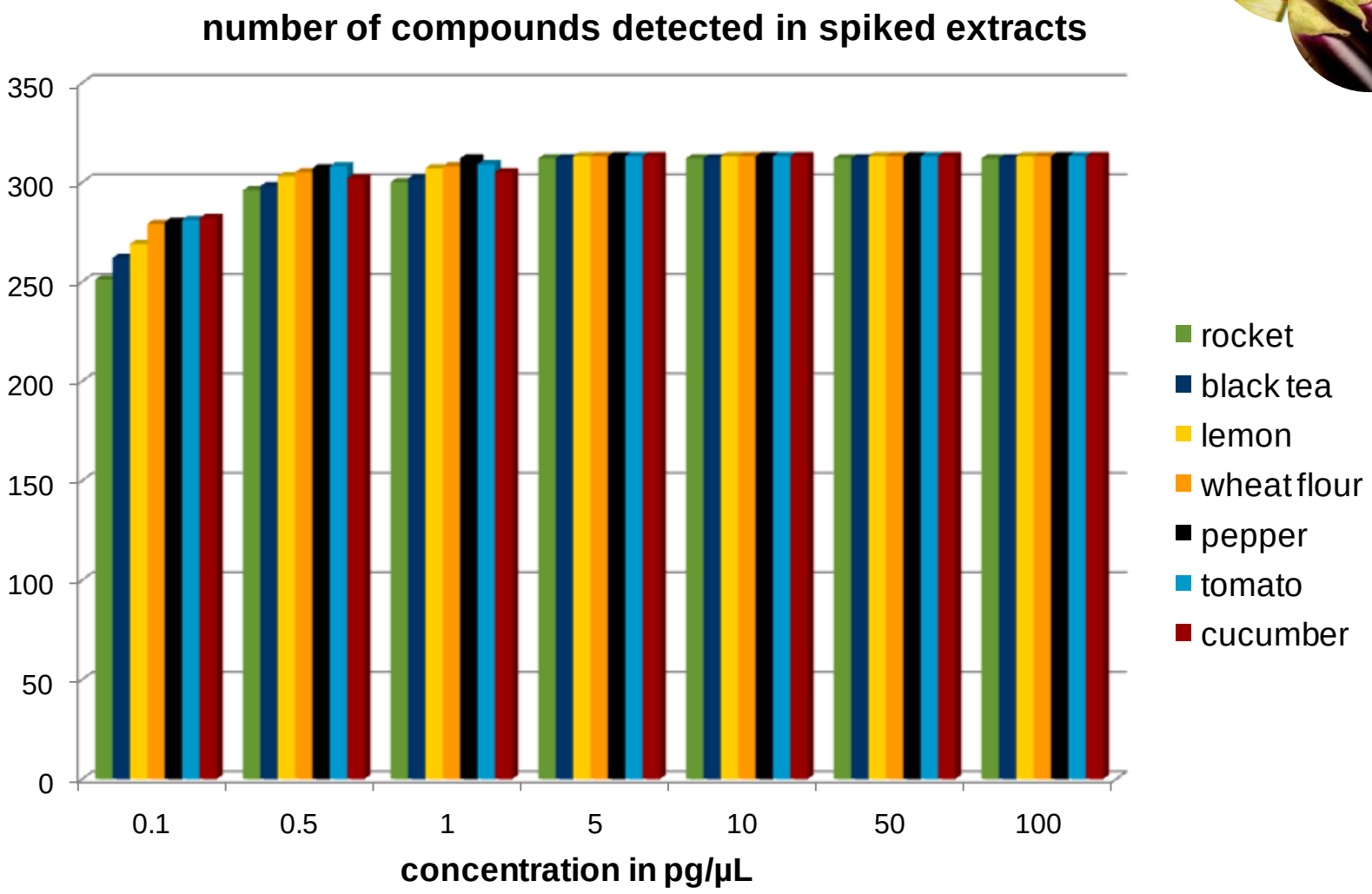
Avermectine B1b



blank | 0.5 µg/kg | 1 µg/kg | 5 µg/kg | 10 µg/kg | 50 µg/kg

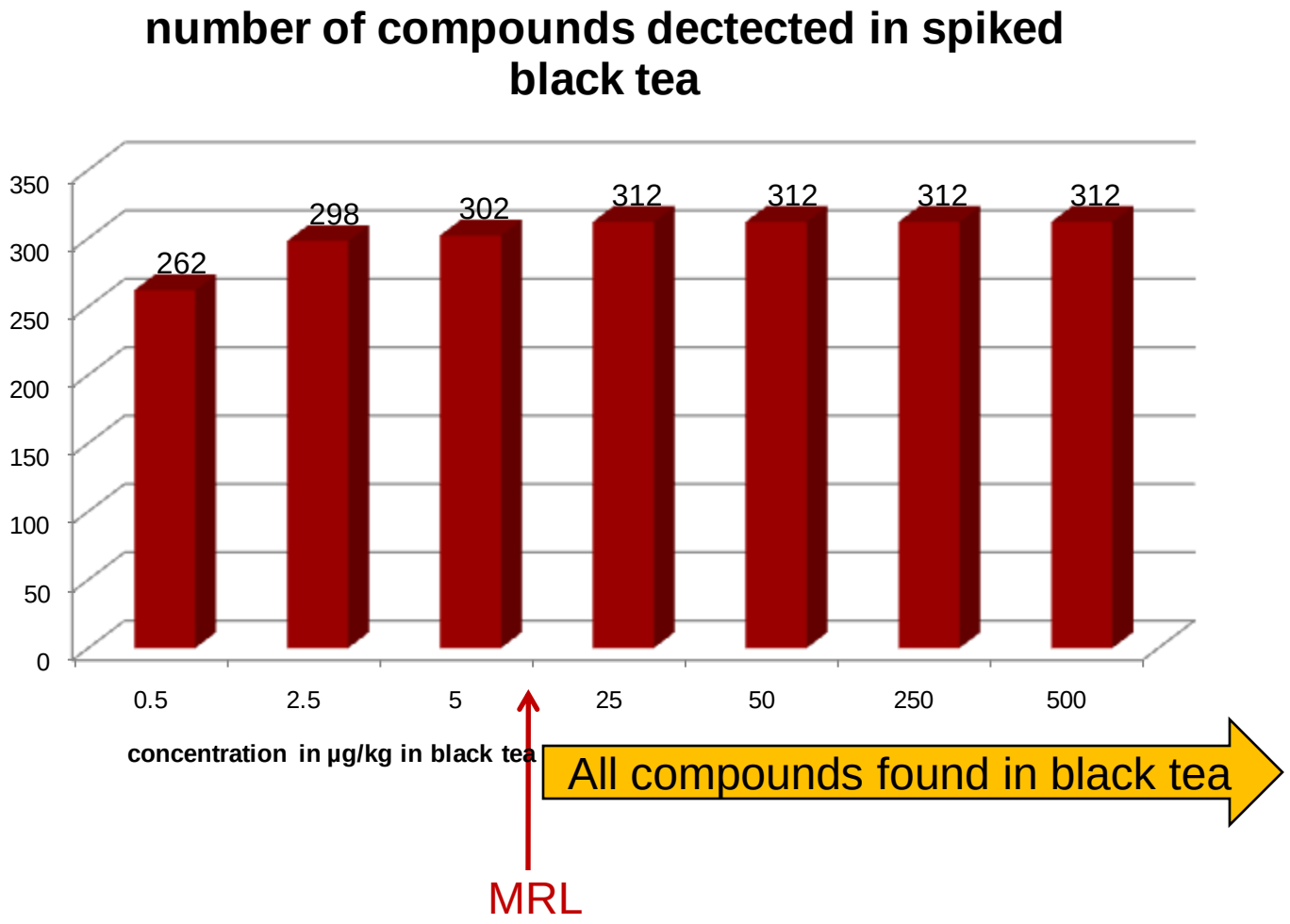
Results for all matrices

Coverage of method for different matrices



Results for black tea

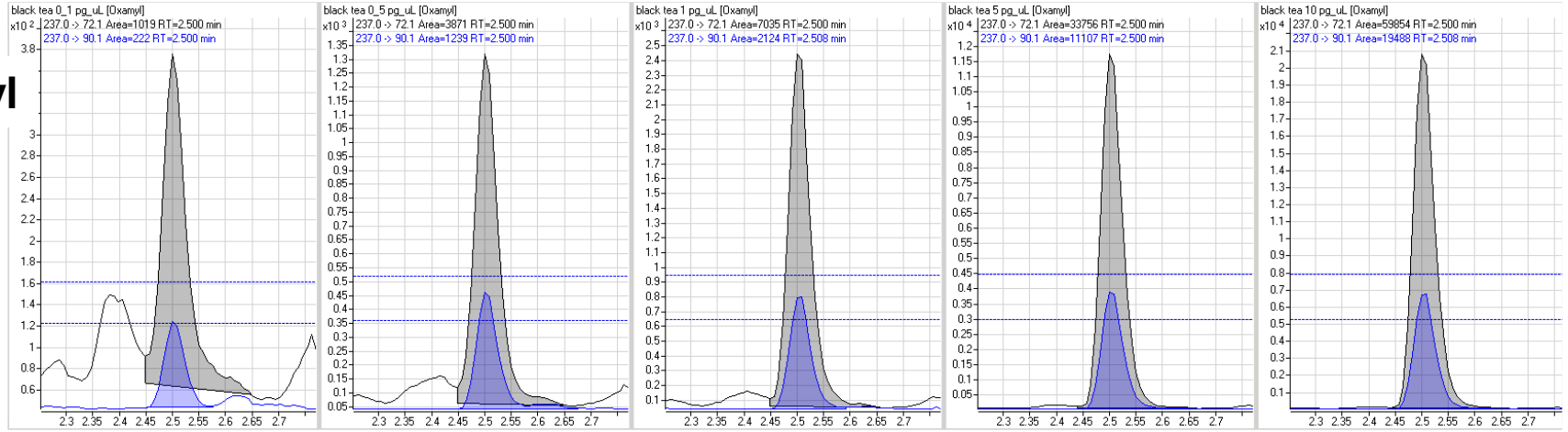
Coverage of method for black tea



Results for black tea

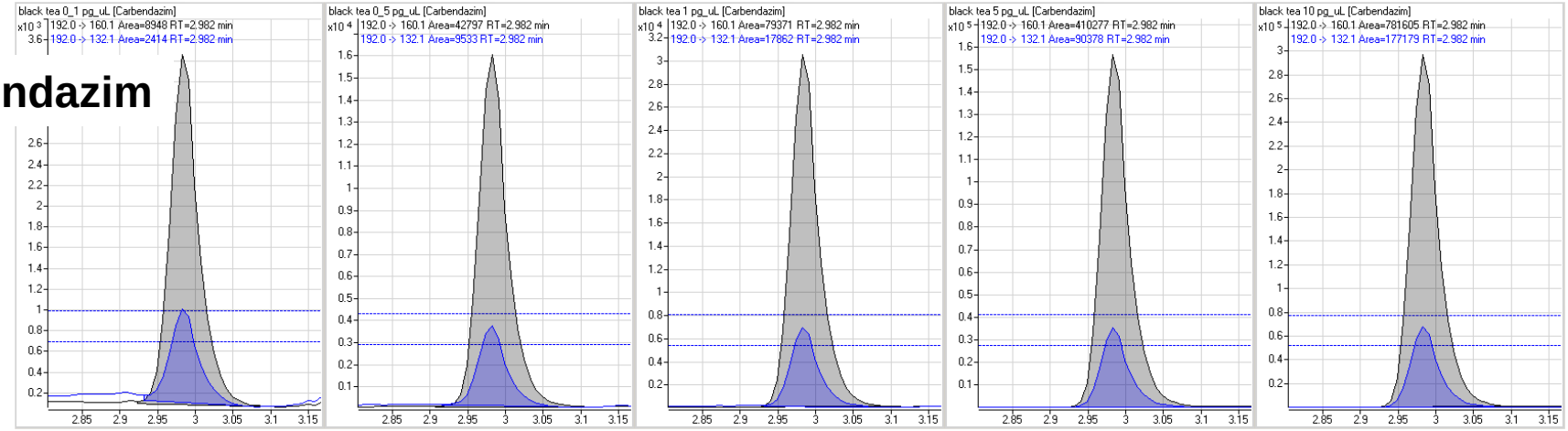
Oxamyl and Carbendazim (High in “Check Your Scope” ranking)

Oxamyl



0.5 µg/kg | 2.5 µg/kg | 5 µg/kg | 25 µg/kg | 50 µg/kg

Carbendazim

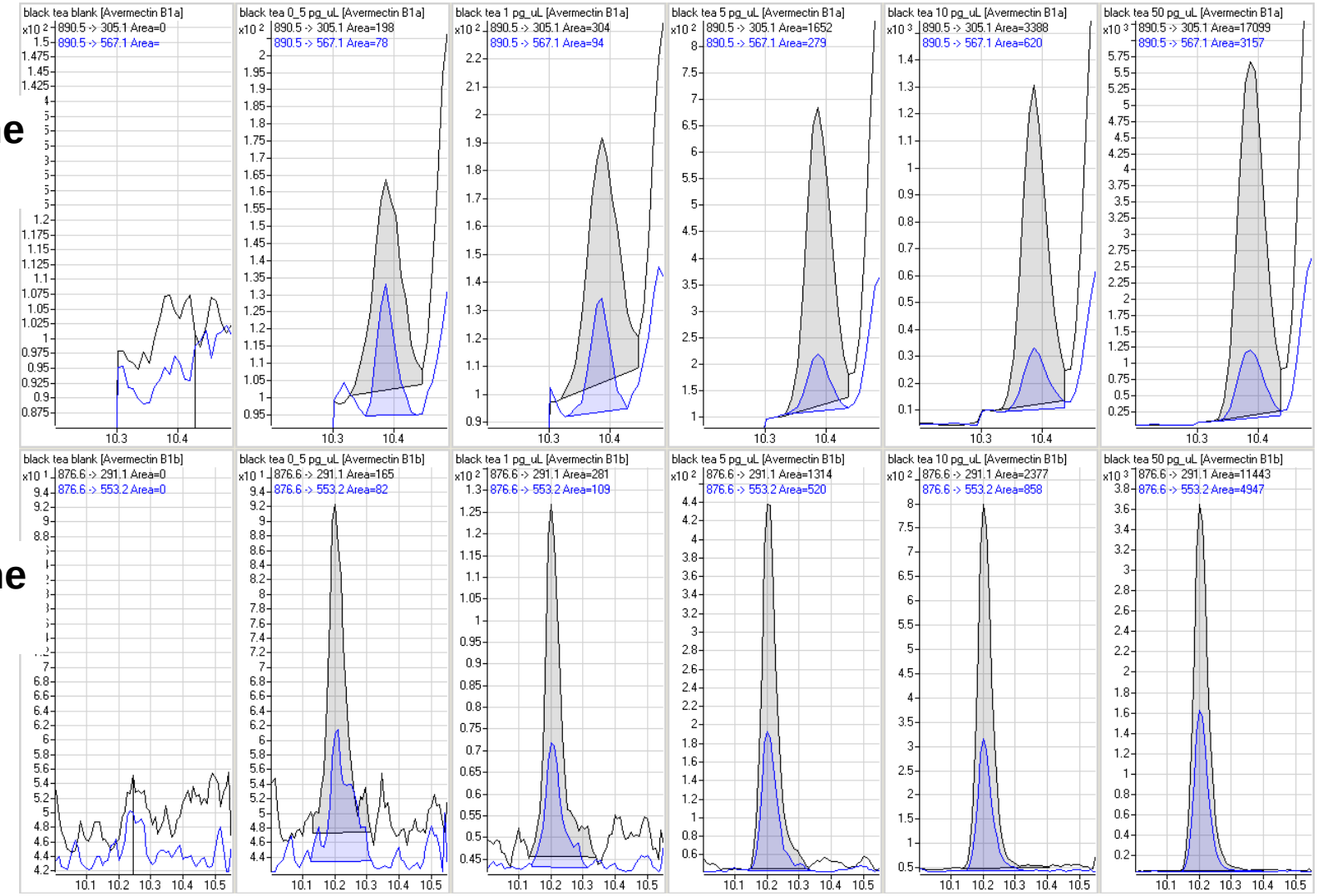


Results for black tea

Avermectine B1a and B1b

Avermectine B1a

Avermectine B1b

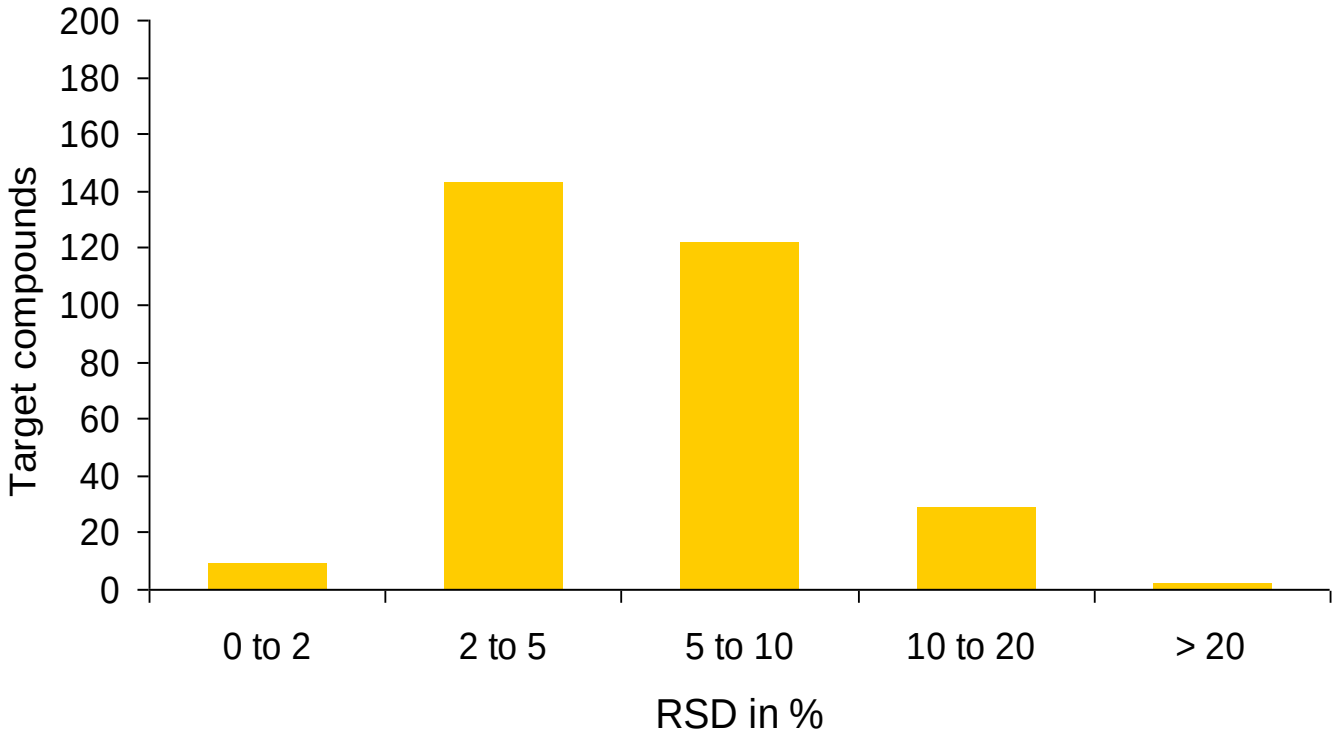


blank | 2.5 µg/kg | 5 µg/kg | 25 µg/kg | 50 µg/kg | 250 µg/kg

Results for black tea

Method performance characteristics for black tea extracts

- Replicate injection of black tea extract spiked at 5 µg/kg (n =8)

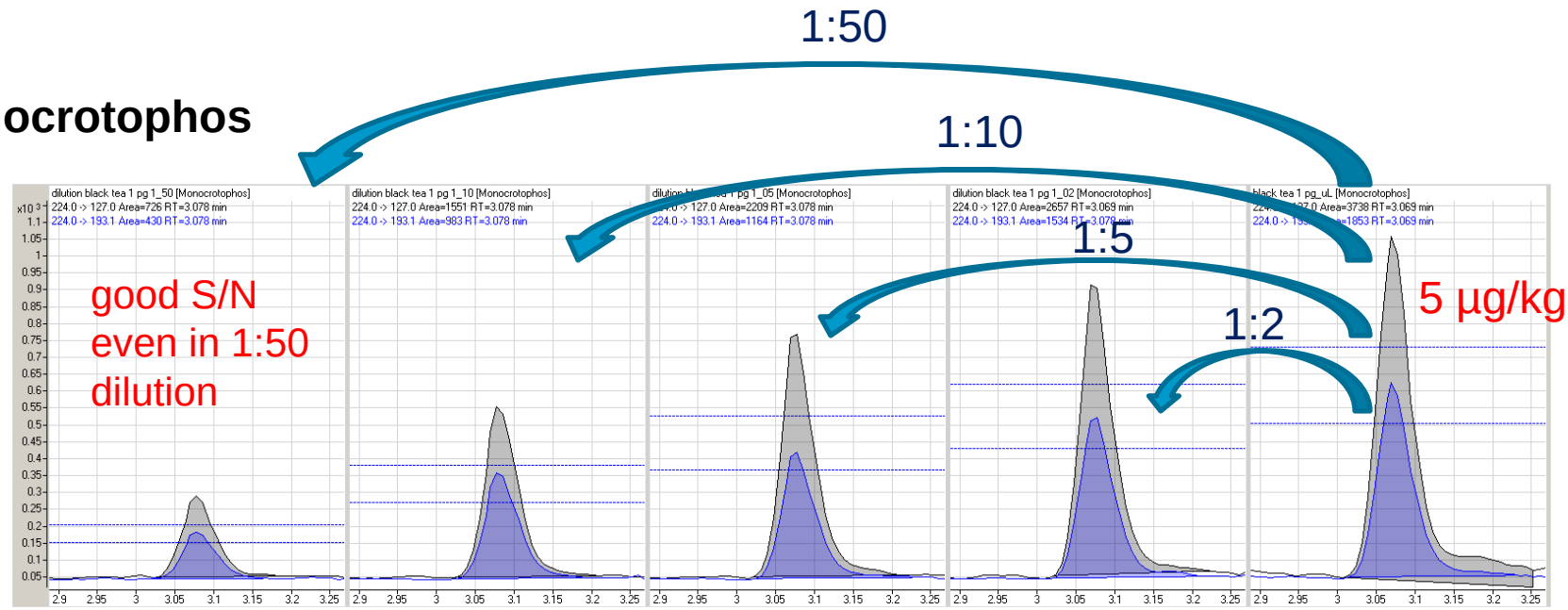


- At 50% of the MRL 303 of 305 pesticides have RSD values within the SANCO criteria of 20% with most of the compounds (n = 274) showing RSDs below 10%

Dilution of black tea extract

Results for monocrotophos

Monocrotophos

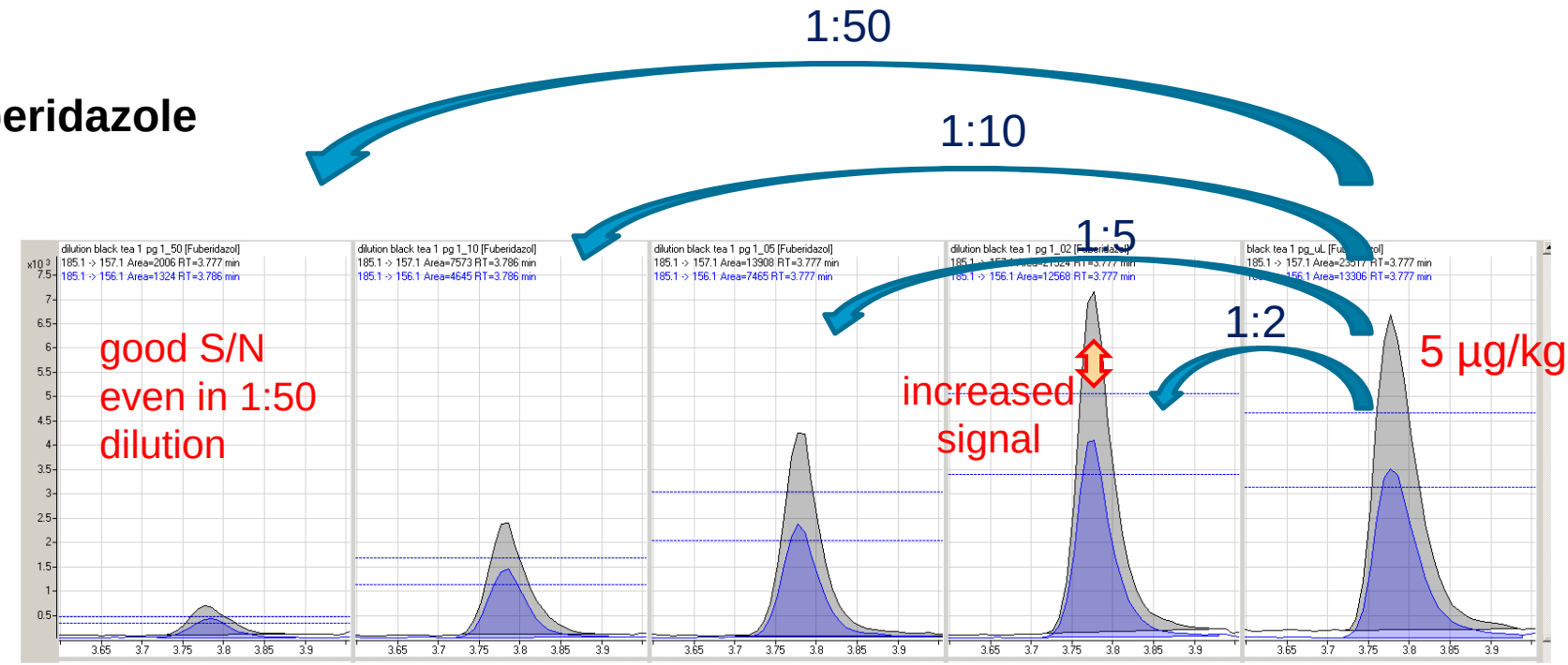


40 fg o.c. | 200 fg o.c. | 400 fg o.c. | 1 pg o.c. | 2 pg o.c.

Dilution of black tea extract

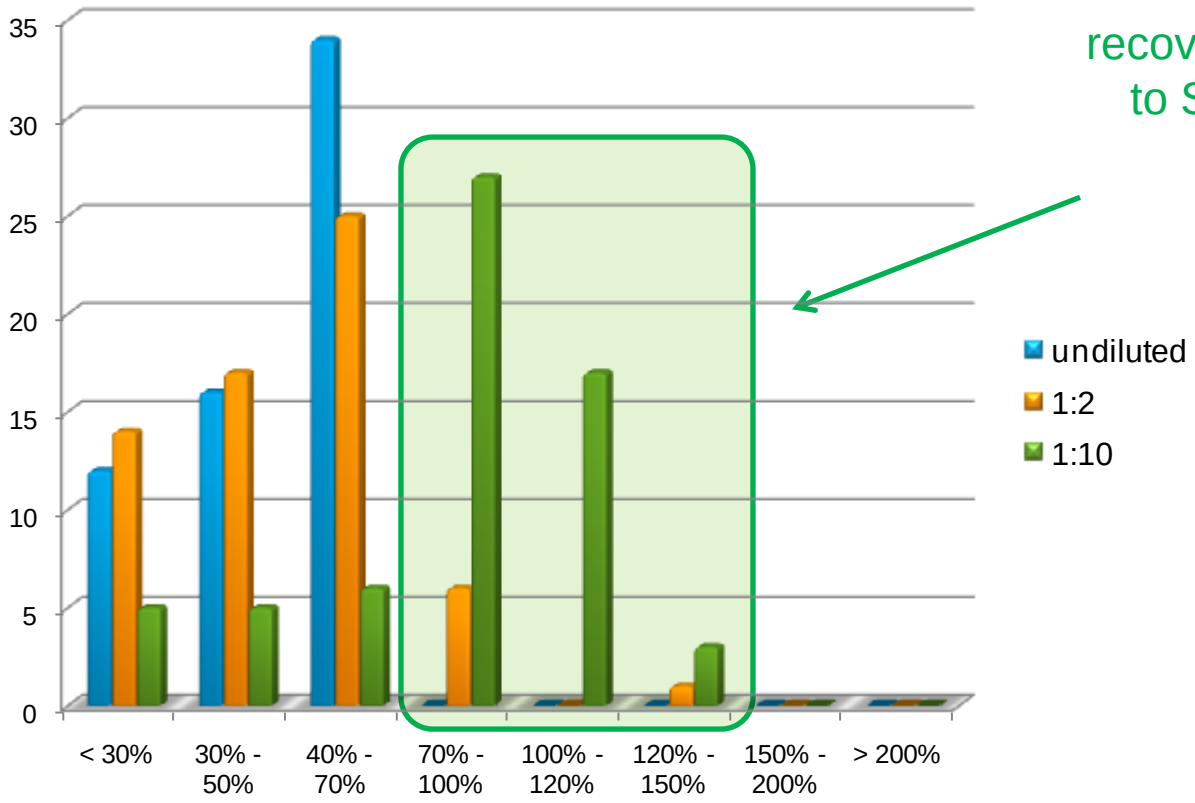
Results for fuberidazole

Fuberidazole



Dilution of black tea extract spiked at 1 pg/ul

Equivalent to 5 ug/kg – only compounds with recovery less than 70% are shown



recovery range according to SANCO document (70% - 120%)

→ significantly better recoveries after dilution for compounds with strong ion suppression in the undiluted tea extract

Multi residue pesticide method

Results of dilution experiments of tea extracts

- Dilution is a possible way to overcome matrix effects like ion suppression
- This allows solvent calibration and still have a method which can be validated according to SANCO recovery requirements (> 70%)
- With any dilution an improved robustness of the method can be expected due to the lower matrix amount which is introduced into the ionization source

Multi residue pesticide method

Other conclusions

- These results show that the 1290/6490 can analyse a range of food types for well over 300 priority pesticides and can detect all compounds down to their MRL achieving **excellent precision even for challenging matrix types.**
- The unique package that enables this cabability is:

1. 1290 UHPLC.
2. Dynamic MRM.
3. Jet Stream/Ion Funnel Ion sampling.
4. Curved Collision cell with ion focussing and Linear acceleration for speed and sensitivty in detection.

Is it Possible to Simultaneously Obtain Qualitative and Quantitative Results?

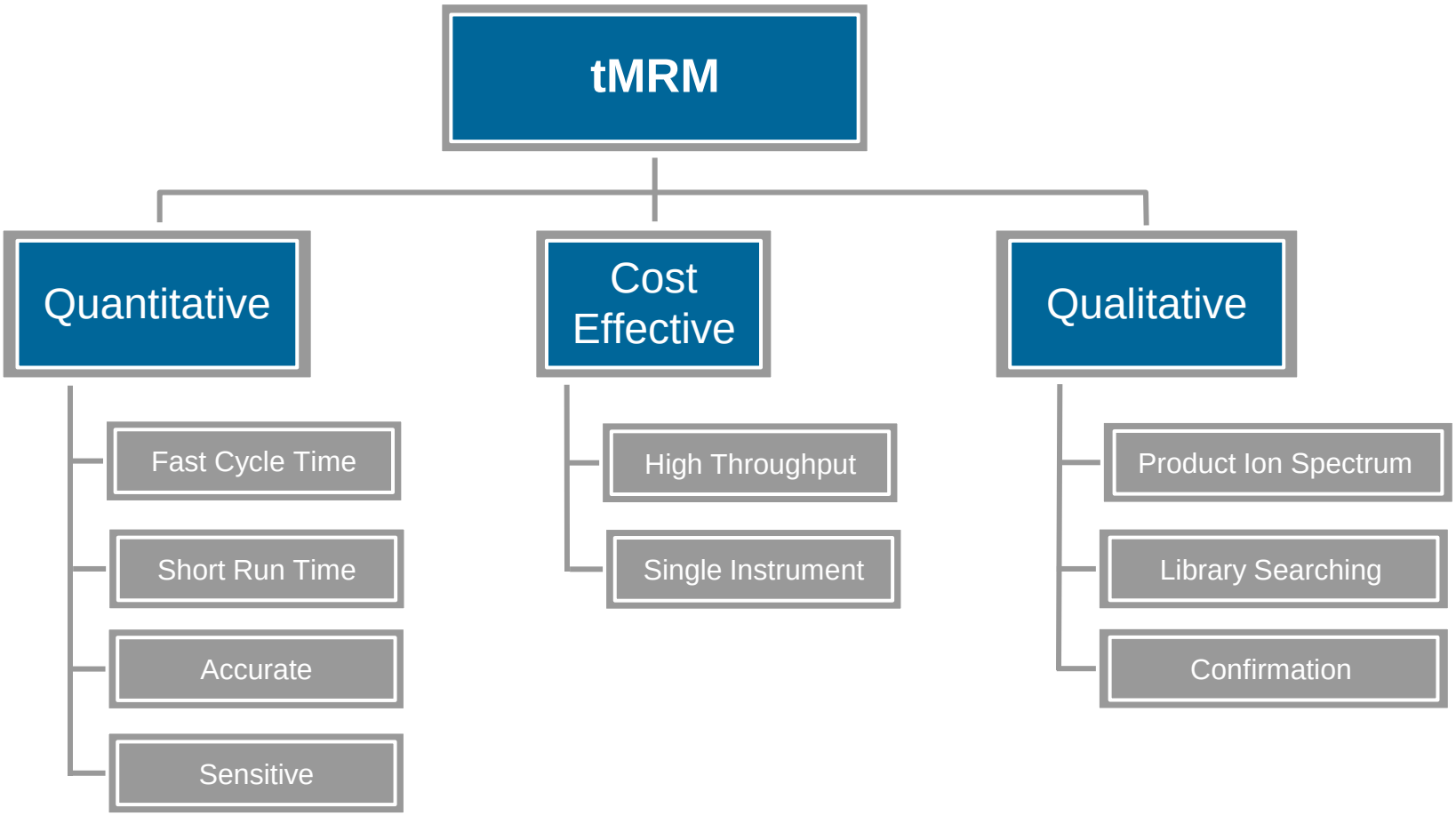
Unknown Screening – what's in the sample?

Qual/Quan: Screening and Quantitation?

Quantitation – how much compound(s) is in the sample?

Non-Selective ⟵ ⟶ Selective

The Ideal Analytical Solution



6400 Triple Quadrupole Product Line

Excellent Value and Performance

6420 Triple Quadrupole LC/MS

- Robust, Easy-to-Use
- Lowest cost of ownership
- Automate compound optimization

6430 Triple Quadrupole LC/MS

- Fast, robust,
- Targeted Protein Quantitation
- Fast polarity switching

6460 Triple Quadrupole LC/MS

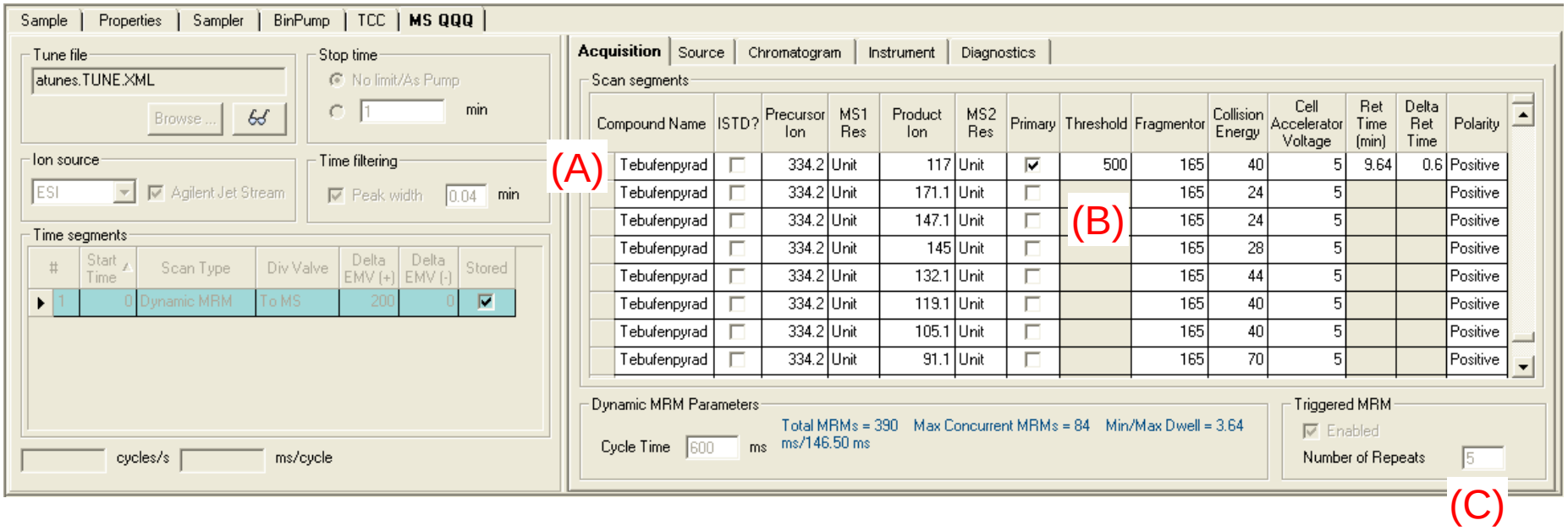
- Agilent Jet Stream – sub fg sensitivity
- Fast polarity switching
- Largest mass range for a premium Triple Quad

6490 Triple Quadrupole LC/MS

- iFunnel – zeptomole sensitivity
- Curved hexapole collision cell – reduced noise
- Perfect for the most demanding applications
- Fast polarity switching

Triggered MRM Parameters

Primary transitions (A) with defined threshold (B) trigger additional transitions for given number of repeats (C).

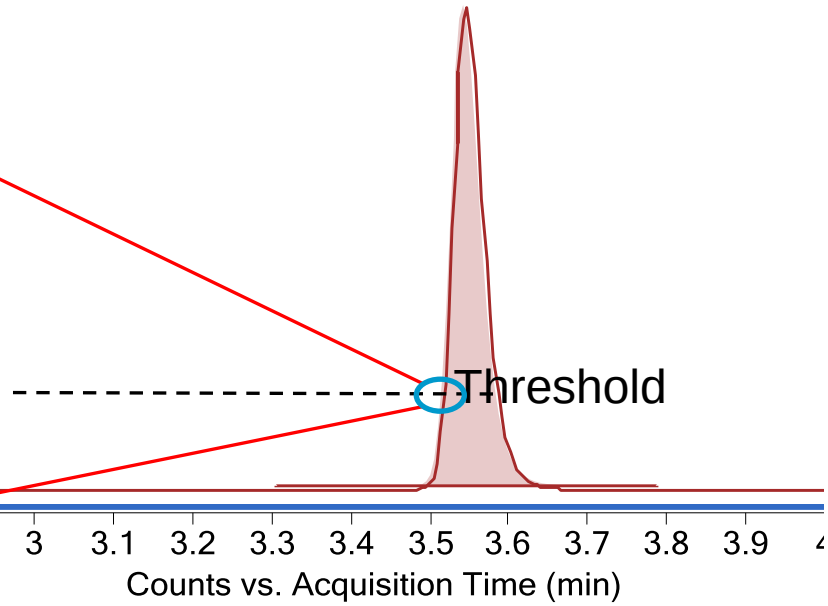


Triggered MRM (tMRM)

Triggered cycle (above threshold)

Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Primary	Threshold	Fragmentor	Collision Energy	Cell Accelerator Voltage
Deoxynivalenol	☐	297.1	Unit	249.1	Unit	☑	100	95	4	3
Deoxynivalenol	☐	297.1	Unit	203.1	Unit	☑	100	95	8	4
Deoxynivalenol	☐	297.1	Unit	175	Unit	☐		95	16	7
Deoxynivalenol	☐	297.1	Unit	161	Unit	☐		95	20	4
Deoxynivalenol	☐	297.1	Unit	129	Unit	☐		95	44	4
Deoxynivalenol	☐	297.1	Unit	115.1	Unit	☐		95	68	3
Deoxynivalenol	☐	297.1	Unit	91	Unit	☐		95	44	6
Deoxynivalenol	☐	297.1	Unit	77	Unit	☐		95	70	3

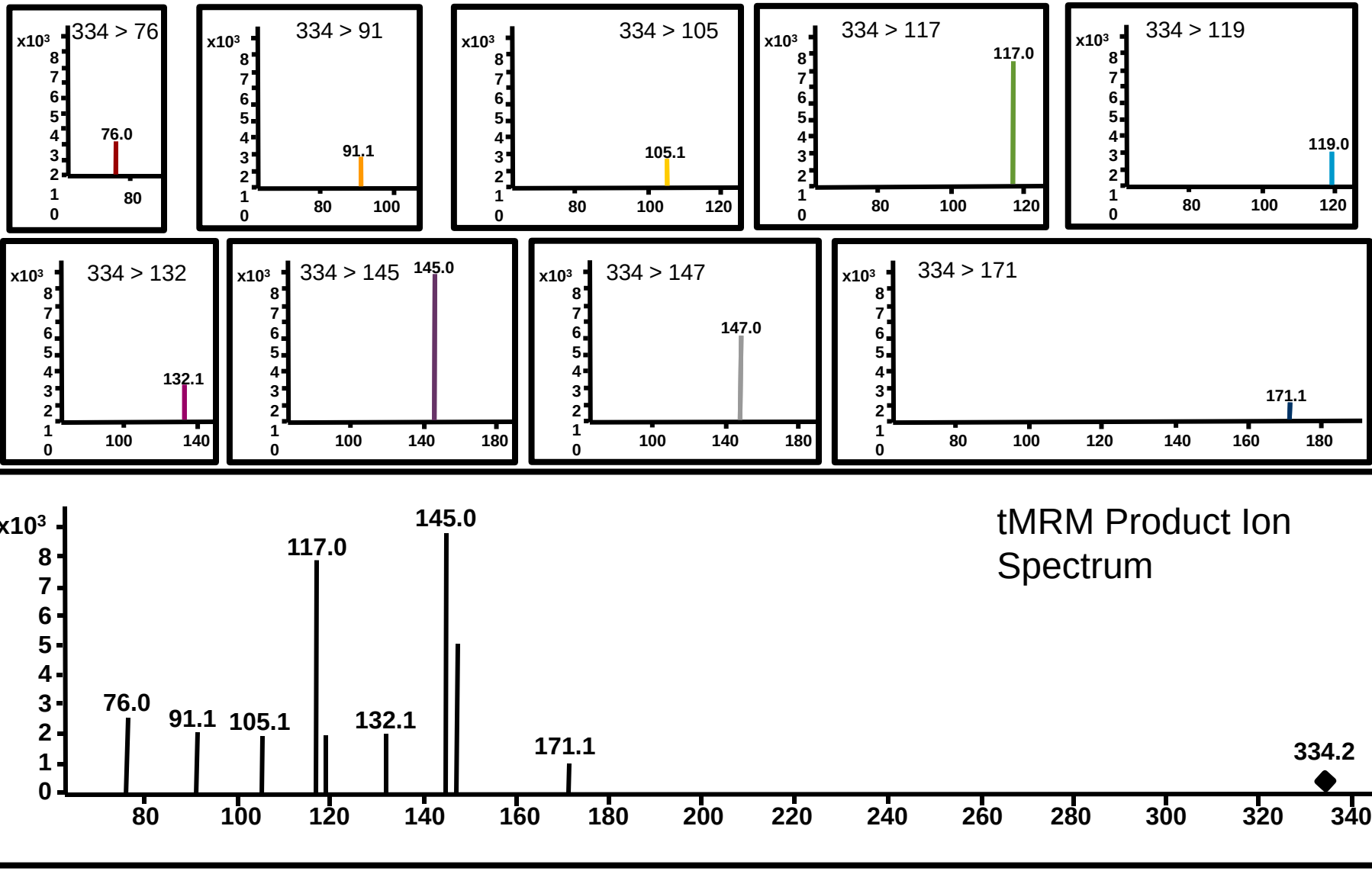
Additional MRMs used for compound confirmation



Primary cycle (below threshold)

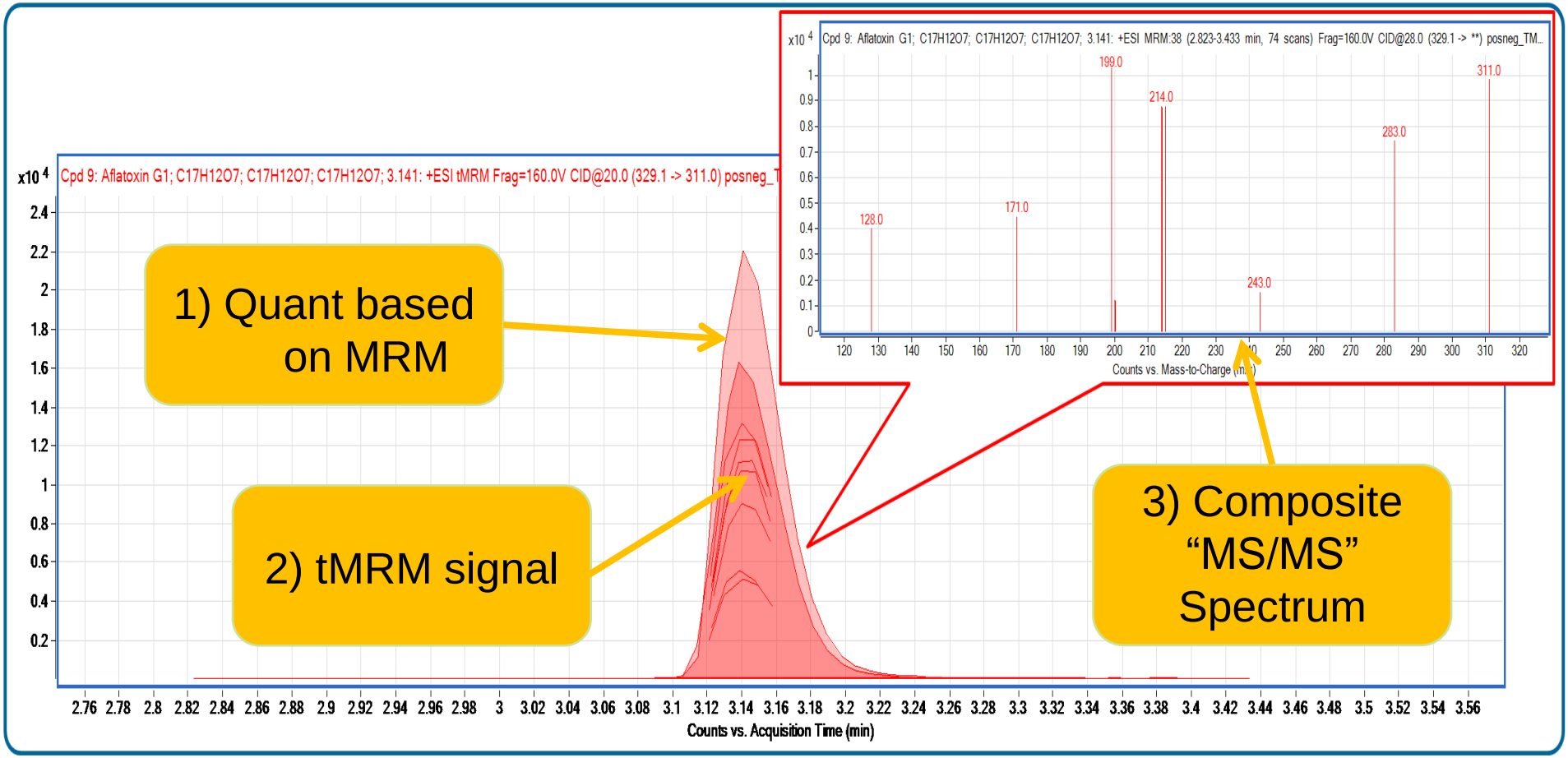
Compound Name	ISTD?	Precursor Ion	MS1 Res	Product Ion	MS2 Res	Primary	Threshold	Fragmentor	Collision Energy	Cell Accelerator Voltage
Deoxynivalenol	☐	297.1	Unit	249.1	Unit	☑	100	95	4	3
Deoxynivalenol	☐	297.1	Unit	203.1	Unit	☑	100	95	8	4

tMRM Product Ion Spectrum

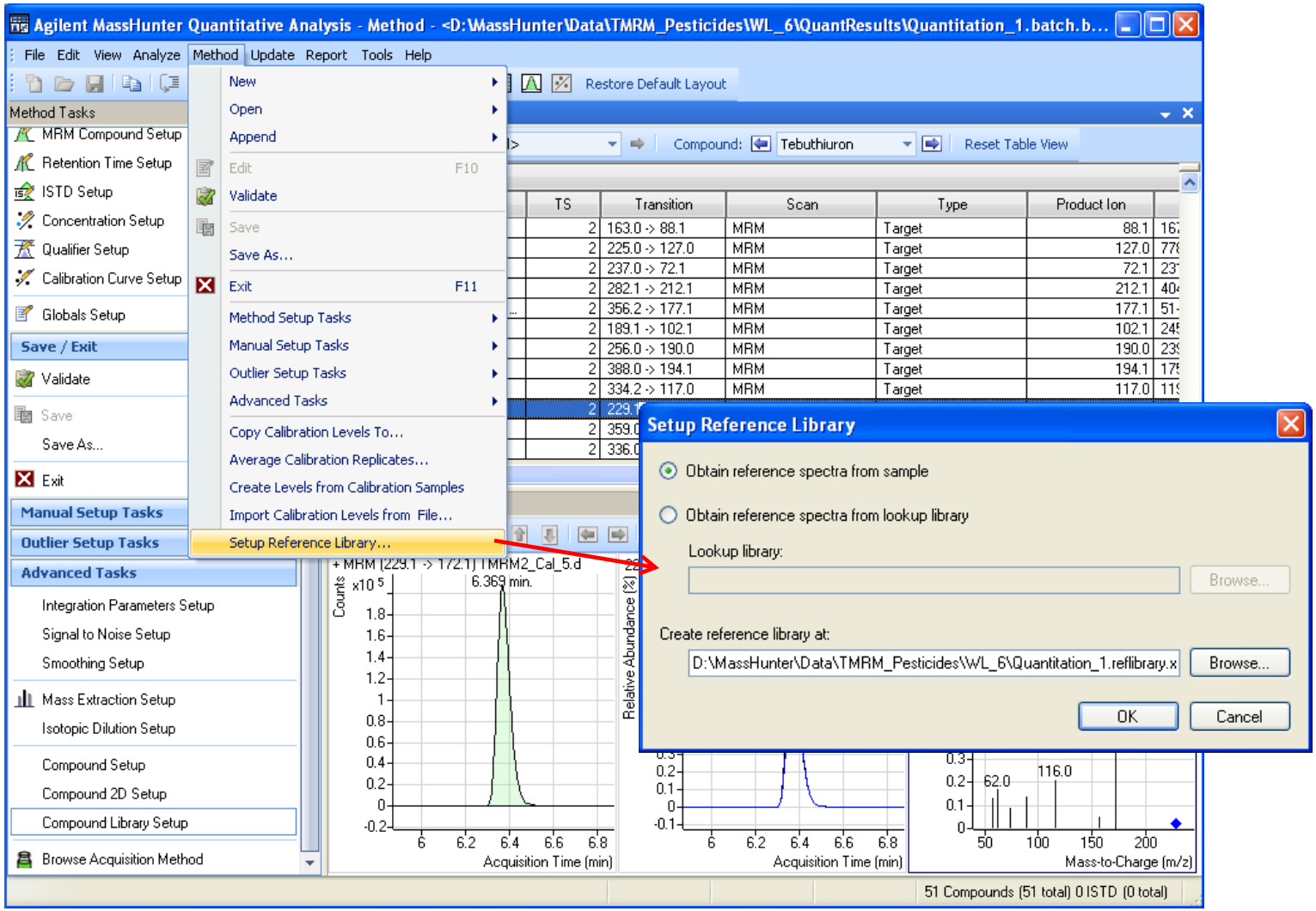


MRM and tMRM Signal

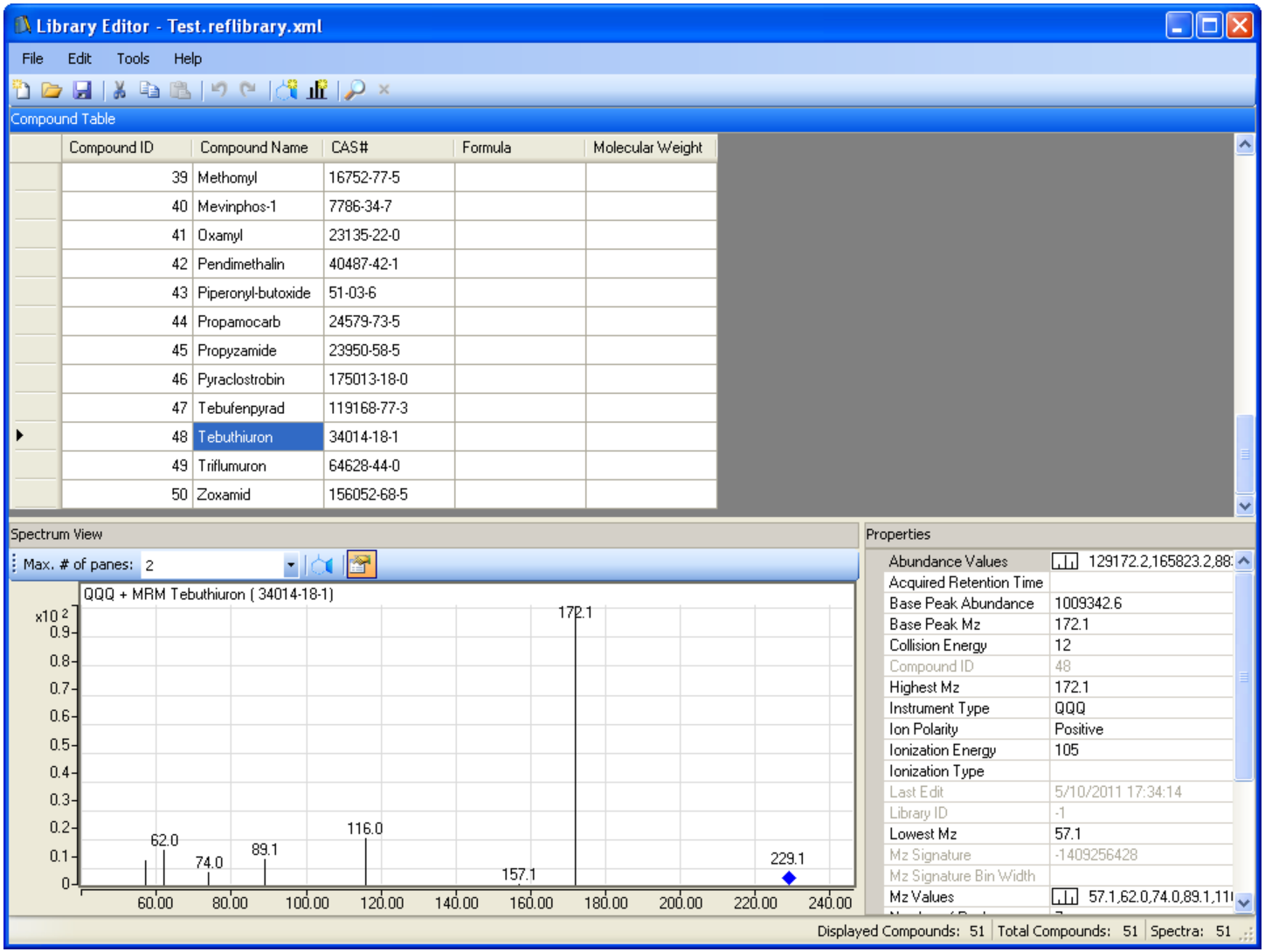
Primary transitions (integrated), triggered MRM transitions (5 repeats), and resulting MRM spectrum for aflatoxin G1.



Automatic tMRM library creation

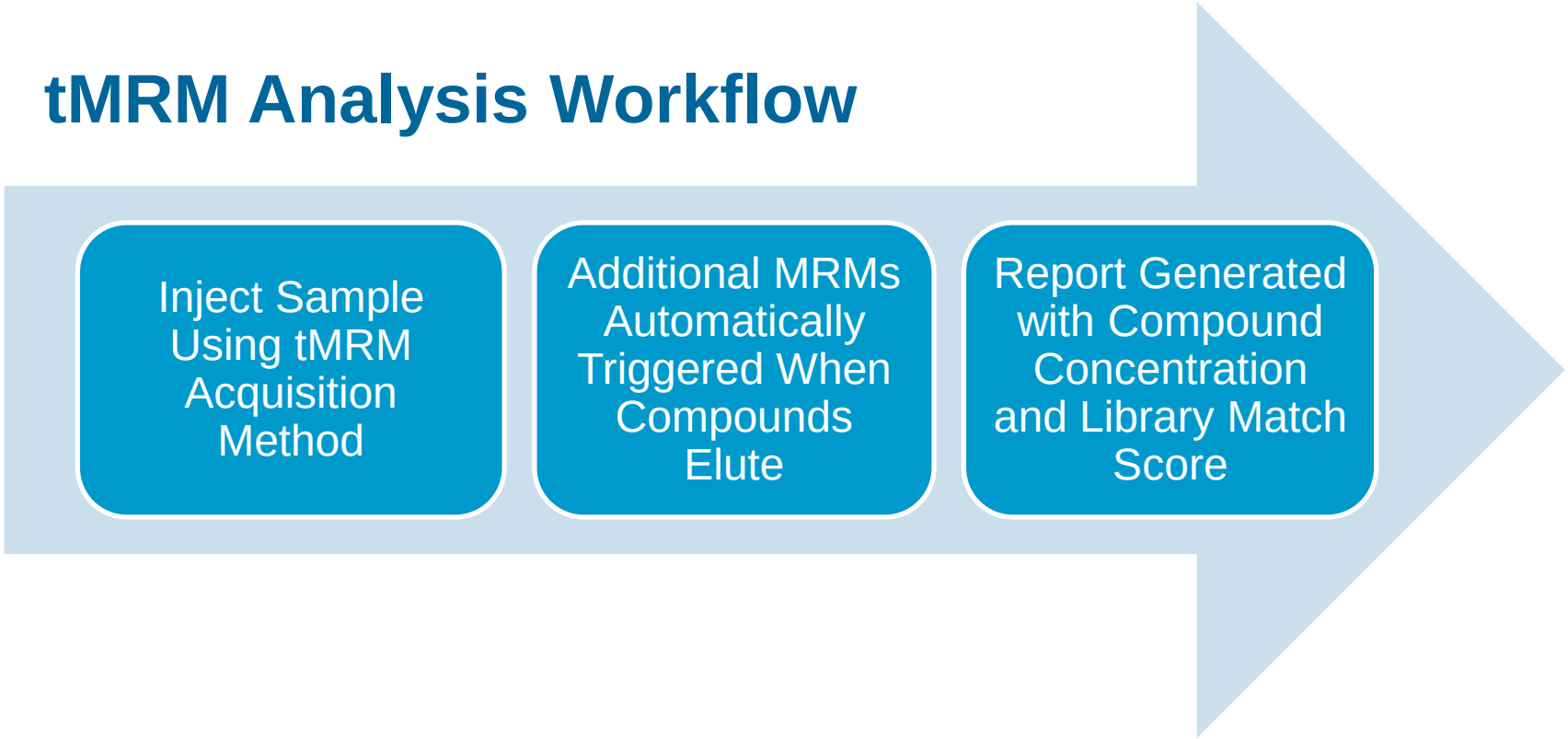


MH Quant Library editor



Triggered MRM (tMRM) Analysis

tMRM Analysis Workflow

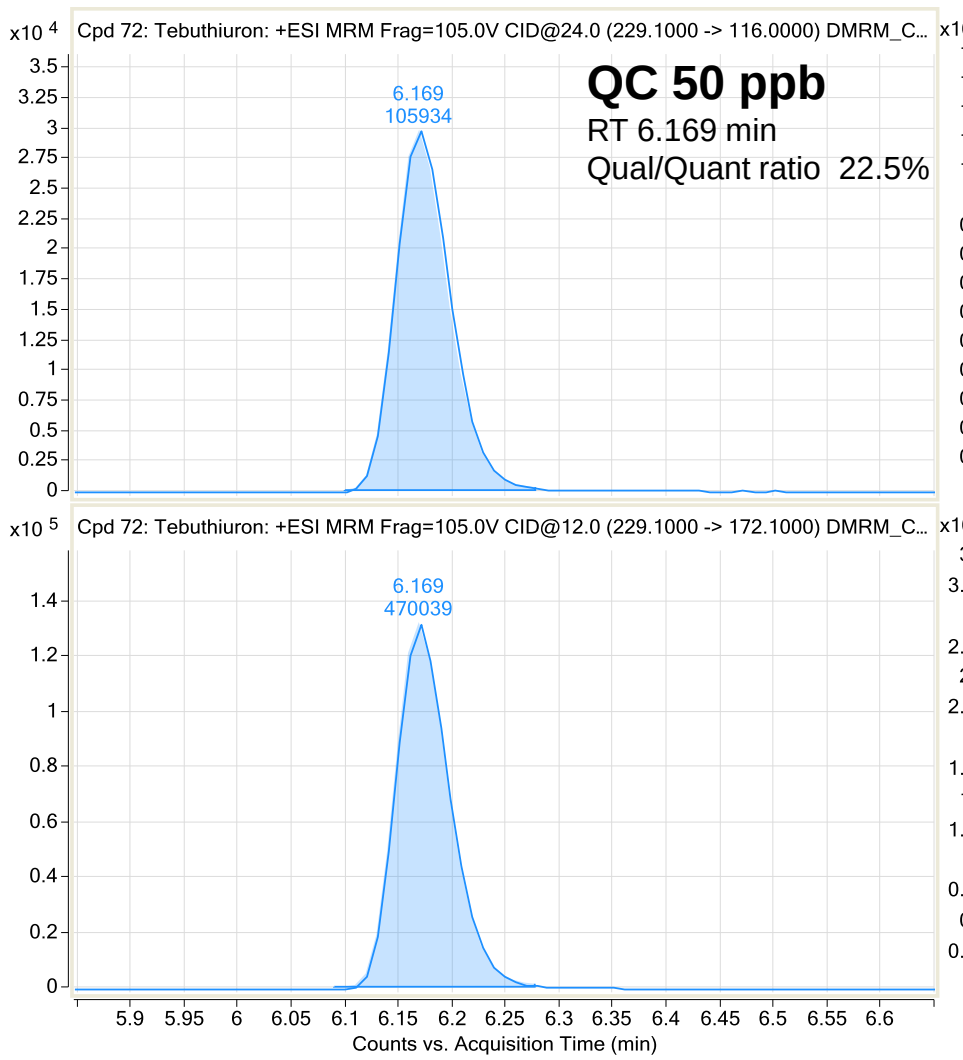


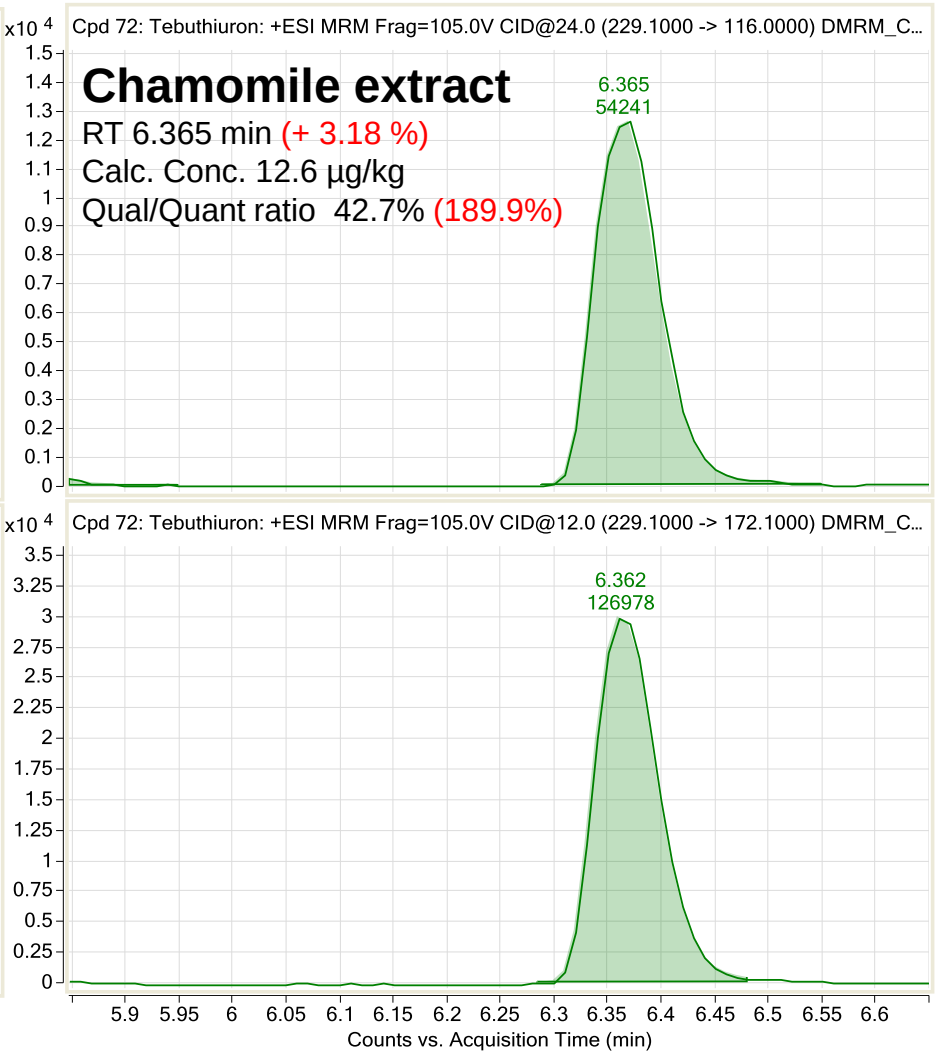
Background information
Chamomile

- Chamomile (*Matricaria chamomilla*)
- Typically the flowers are used as medicine or tea
- Main production areas are Argentina, Egypt, Bulgaria, Hungary, Spain and Germany
- In Germany no use of herbicides is allowed for chamomile production
- In 2009 a contract laboratory has identified a compound in chamomile as tebuthiuron in high concentrations based on the two major transitions and a similar qualifier ratio
- <u>But:</u>
  - retention time was slightly different to standard (due to matrix?)
  - use of tebuthiuron on chamomille production is not likely

Quantitative analysis of pesticides

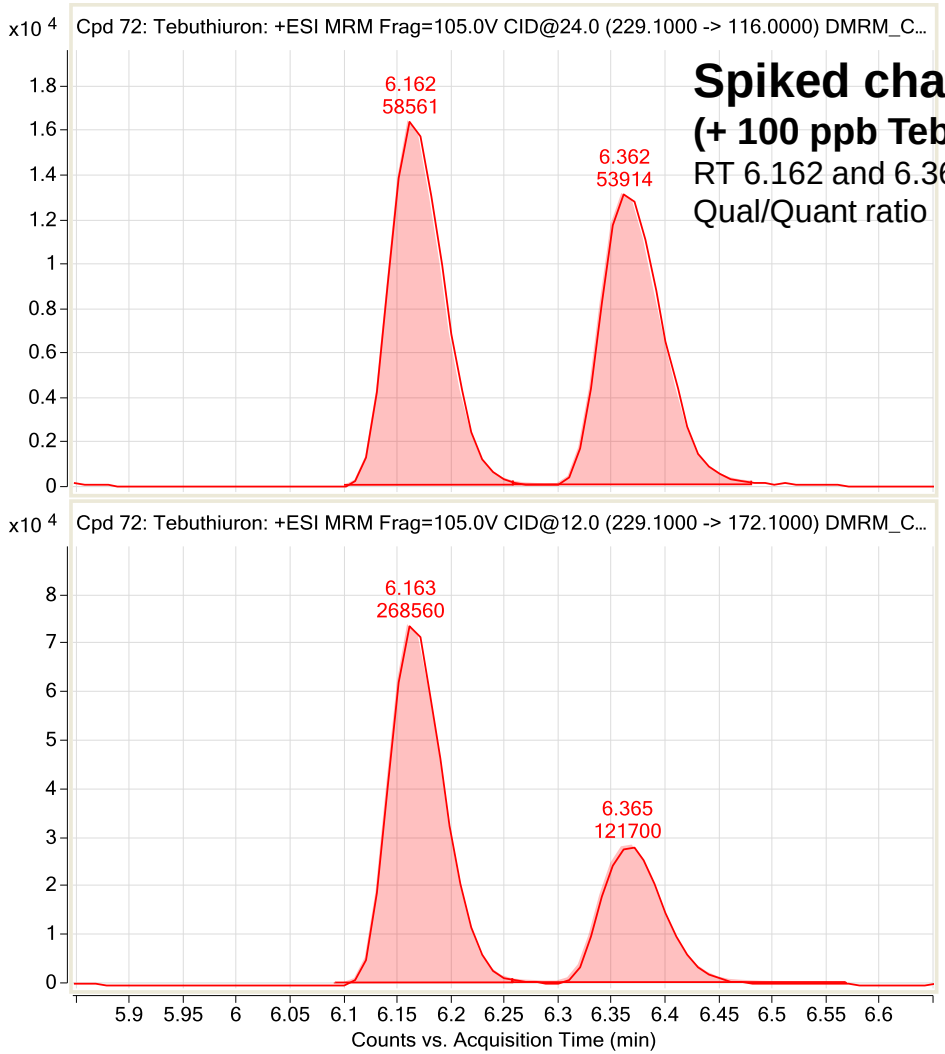
MRM traces of tebuthiuron in QC sample and chamomile extract





Quantitative analysis of pesticides

MRM traces of tebuthiuron in spiked chamomile extract



Spiked chamomile extract
(+ 100 ppb Tebuthiuron)
RT 6.162 and 6.362 min (+ 3.25%)
Qual/Quant ratio 21.8 and 44.3% (95.2 and 195.5%)

- In non-spiked chamomile extract both MRM traces for tebuthiuron show up with higher RT than in reference standard (slightly above criteria of SANCO guidelines)
- For less resolving HPLC separations co-elution of compounds is very likely
- Qualifier/quantifier ratio in non-spiked ginger extract is significantly higher than tolerance allowed in SANCO guidelines
- Estimated concentration exceeds default MRL of 0.01 mg/kg)

Quantitative analysis of pesticides

Triggered MRM traces of tebuthiuron in chamomile extract

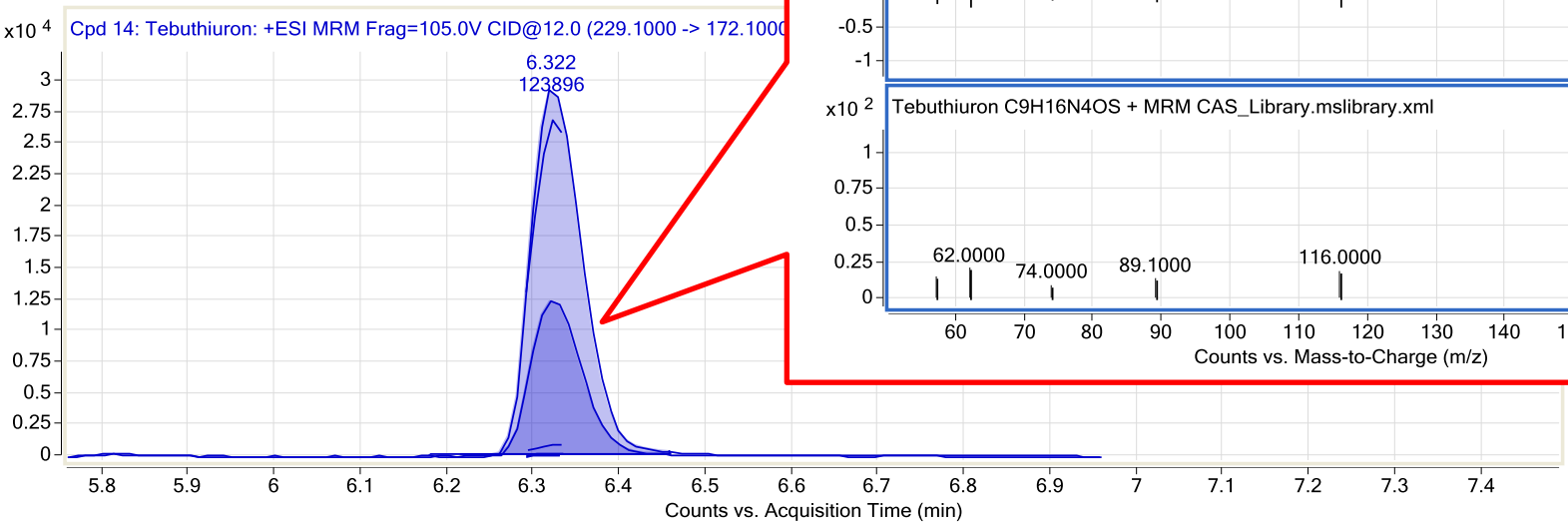
Show/Hide	Label	Polarity	Cpd	Name	Score	Start	RT	End	Width	m/z	Mass (DB)
☑	Cpd 14: Tebuthiuron	Positive	14	Tebuthiuron	69.57	6.216	6.322	6.459	0.067	229.1	228.1045

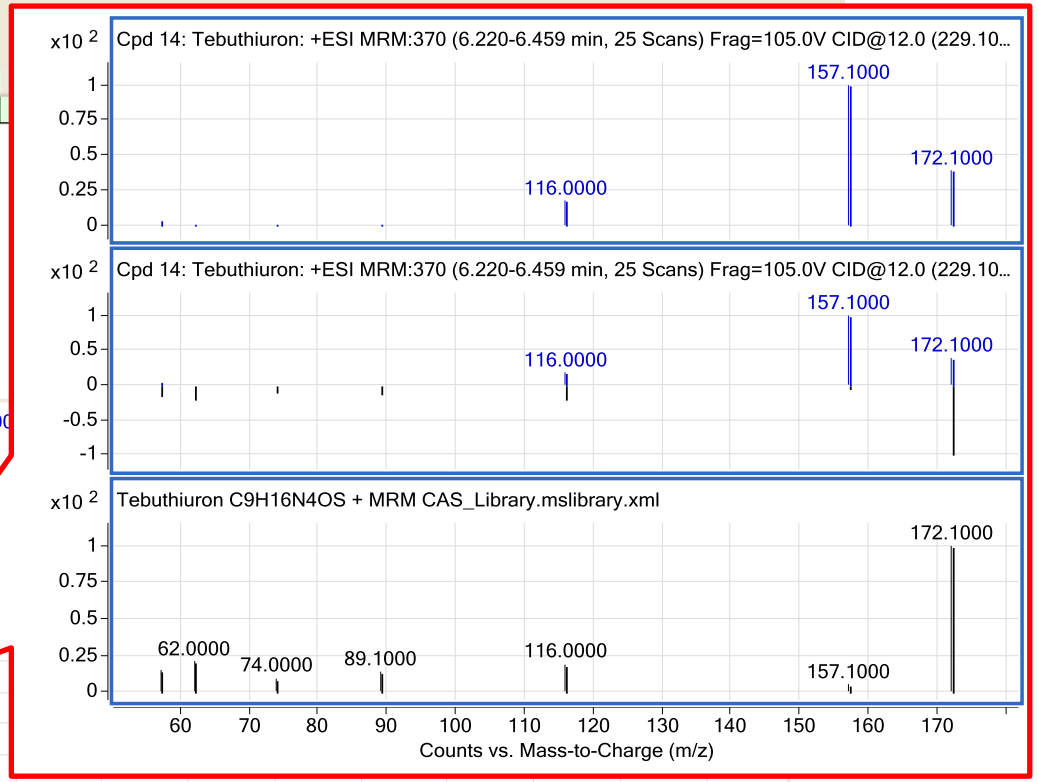
Best	Name	Formula	CAS	Score	Mass (DB)	RT	Score (Lib)	Precursor	Find by MRM	Score (Acq)	ID Source
◉	Tebuthiuron	C9H16N4OS	34014-18-1	69.57	228.1045	6.322	69.57				LibSearch

Name	Num Peaks	m/z (prec.)	Score (Lib)
Tebuthiuron	7	229.1	69.57

Best	Name	Formula	CAS	Score
○	Tebuthiuron			100

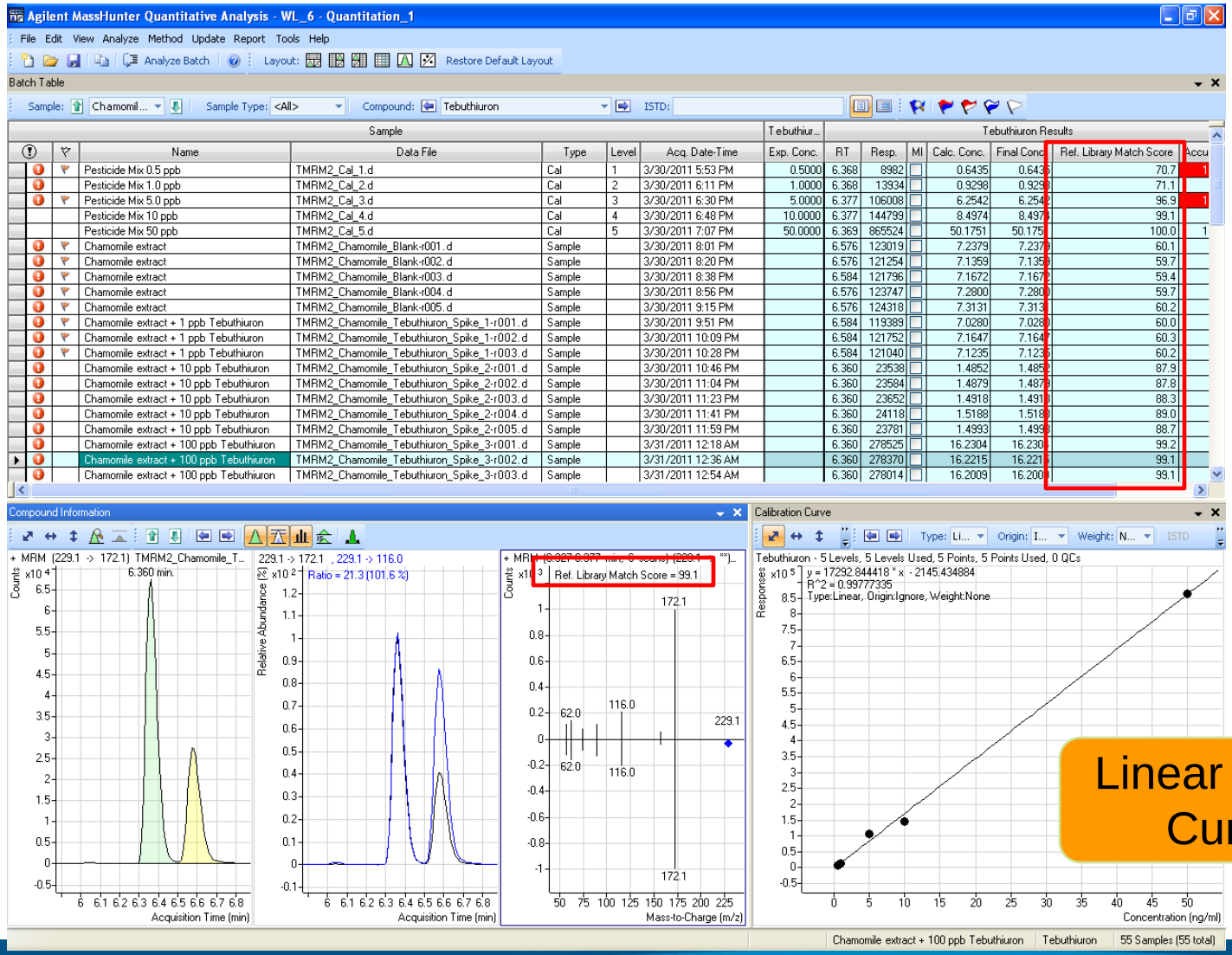
Library match score: 69.57





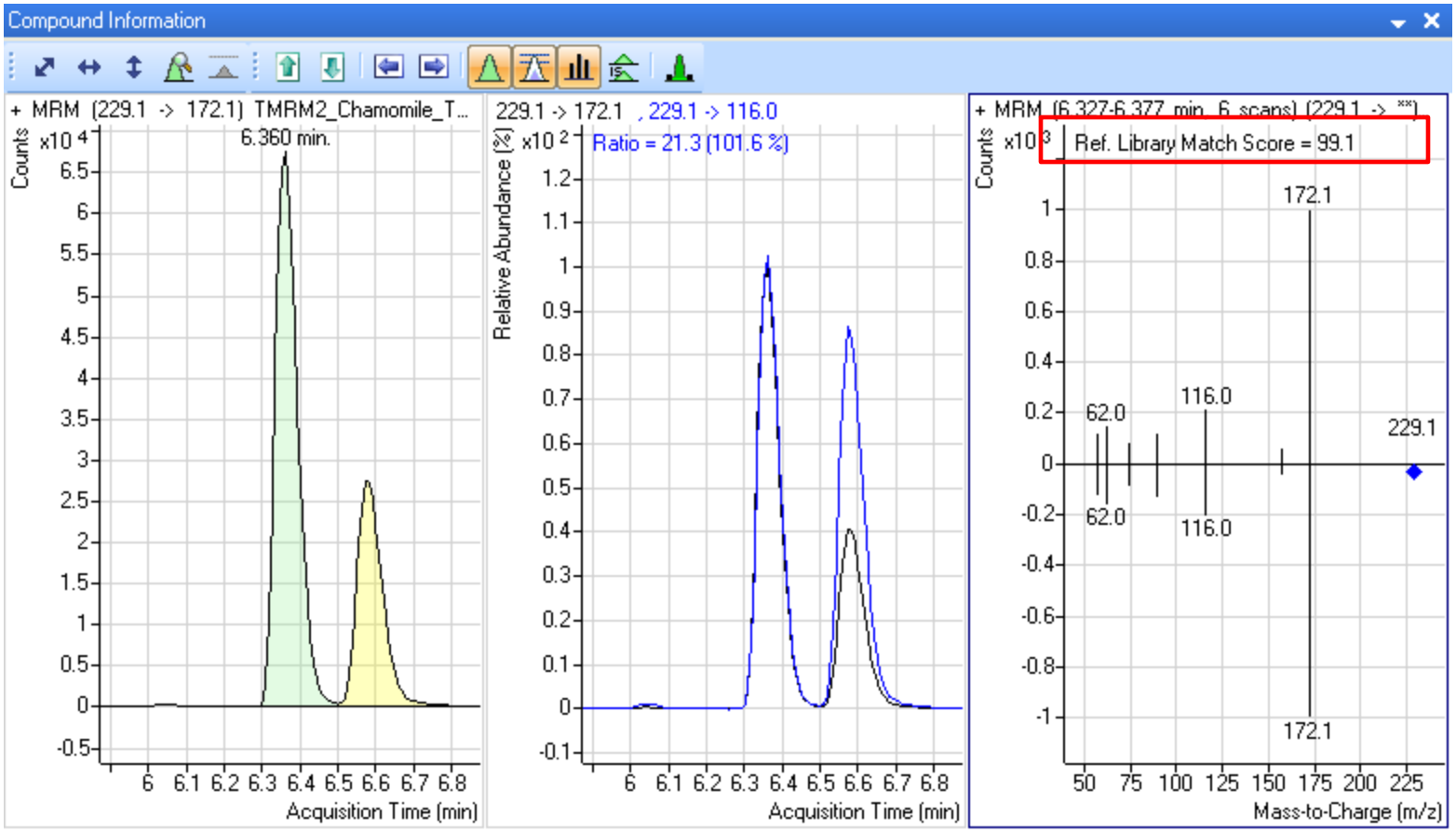
Quantitative analysis of pesticides

Library Searchable Spectrum Confirms ID



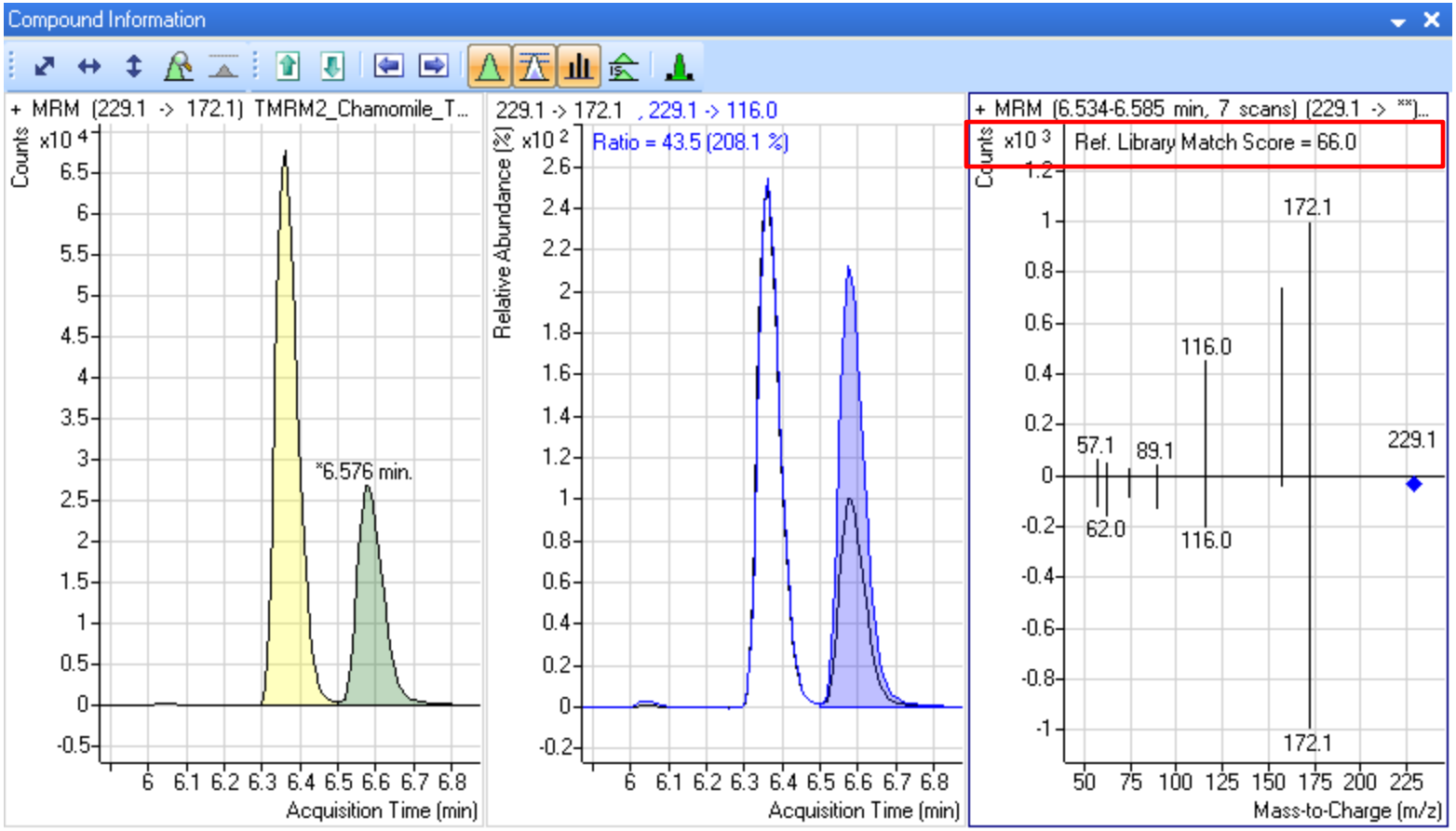
Quantitative analysis of pesticides

Library match for tebuthiuron in spiked chamomile extract



Quantitative analysis of pesticides

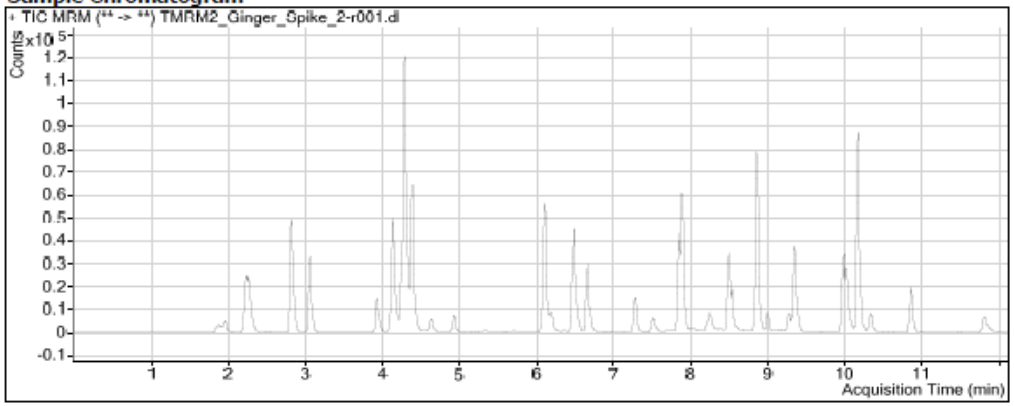
Library match for matrix compound in spiked chamomile extract



Value of tMRM Acquisition

tMRM provides fast, accurate quantitation and rigorous qualitative MS/MS confirmation in a single injection

Sample Chromatogram



Quantitation Results

Compound	RT	Response	Conc	Library match score	Accuracy
Acephat	1.960	14138	9.0141	97.11	
Propamocarb	2.261	88978	16.6692	99.31	
Oxamyl	2.820	115494	12.8257	94.68	
Methomyl	3.063	38286	12.5201	94.42	
Imidacloprid	3.929	17931	18.8245	95.47	
Carbendazim	4.143	100584	12.3491	99.05	
Metamitron	4.242	12077	10.7746	96.57	
Carbofuran	6.111	108542	9.1272	94.97	
Demethon-S-Methyl	6.192	17909	3.7191	93.80	
Tebufenpyrad	10.004	56283	61.2709	69.15	
Furathiocarb	10.024	13827	3.1689	98.72	
Piperonyl-butoxide	10.175	132656	7.6780	96.89	
Hexythiazox	10.334	5642	4.2567	97.80	
Pendimethalin	10.365	4432	5.5085	71.37	
Fenazaquin	10.858	29566	3.0815	97.83	
Fenbutatinoxid	11.818	18629	6.5292	89.17	

Triggered MRM data acquisition

New acquisition mode for enhanced confirmation

- Triggered MRM is new data dependant acquisition mode for the confirmation of target compounds
- When the signal heights of the primary MRMs exceed a given threshold up to 9 additional MRM transitions are triggered
- Triggered MRM makes use of the well established Dynamic MRM functionality
- Triggered MRM has advantages over data dependant product ion scans because:
  - It is more sensitive due to longer dwell times per transition and due to the ideal collision energies for each transition
  - Peak shapes of the primary transitions are not compromised due to constant cycle times
  - In spectra fragment ratios are very constant due to relatively long dwell times per transition
- Triggered MRM spectra can be saved in an user defined library and can be searched from the qualitative and quantitative software.

Questions .....

?

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Identification and Quantitation of Pesticides in Chamomile and Ginger Extracts Using an Agilent 6460 Triple Quadrupole LC/MS system with Triggered MRM

Application Note

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Abstract

This application note describes the use of triggered MRM (tMRM) for the analysis of pesticide residues applied to chamomile and ginger extracts. The analysis is performed using the Agilent 1290 LC system coupled to a 6460 Triple Quadrupole LC/MS with tMRM acquisition. Two examples of false positive identifications were explored: tebuthiuron in chamomile and tebufenpyrad in ginger. Both compounds were quantitated and confirmed with library matching in a single analytical run. False positive identification was avoided by using library matching and tMRM acquisition.

Agilent Technologies

App. No. 5990-8460EN