Direct aqueous analysis of pesticides and PPCPs in drinking and bottled water at parts per trillion levels

SCIEX Triple Quad 7500 system

RUO-MKT-11-12103-A

SCIEX
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Importance of water testing

- Water suppliers and utility companies need to ensure that the final water product they send out for bottling or into supply networks is safe and complies with state and country regulations
- Drinking water analysis is subjected to extremely low and rigid prescribed consent values (PCV) for determinands
- Water can be a challenging matrix, in particular if it is sourced from a river, lake or reservoir before entering the water treatment process
- Labs must have highly sensitive instrumentation to quantify beyond PCV limits with precision and confidence and also handle all the matrix challenges

Enabling new levels of quantification

SCIEX 7500 System

NEW SOFTWARE, NEW ION OPTICS, NEW SOURCE

- SCIEX Triple Quad 7500 LC-MS/MS system enables new levels of quantification across a large suite of sample types and workflows
- SCIEX OS software is the modern mass spectrometry software platform that transforms your samples into meaningful analytical answers

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Samples

- Pesticides and PPCP in water
- Compounds: positive mode 370, negative mode 61 (46 internal stds)
- The calibration standard concentrations were 0.1, 0.2, 0.5, 1, 2, 5, 10, 20, 50, 100, 200 and 500 ng/L. A calibration blank was also prepared.
- MilliQ water, yap water (drinking water), Evian, FIJI

Methods

SCIEX 7500 System

- LC system: ExionLC system
- Column: Luna Omega C18 1.6 µm, 100 × 2.1 mm
- Mobile phase:
  - A : Water + 0.1% formic acid + 5mM NH_4 formate
  - B : MeOH + 0.1 % formic acid + 5mM NH_4 formate
- Temperature: 40 ºC
- Injection volume: 500 µL
- MS: fast pos/neg switching with Scheduled MRM algorithm

Total Time (min)	Flow Rate (µL/min)	A (%)	B(%)
0.00	500	99	1
0.50	500	99	1
16.00	500	1	99
21.00	500	1	99
21.10	500	99	1
25.00	500	99	1

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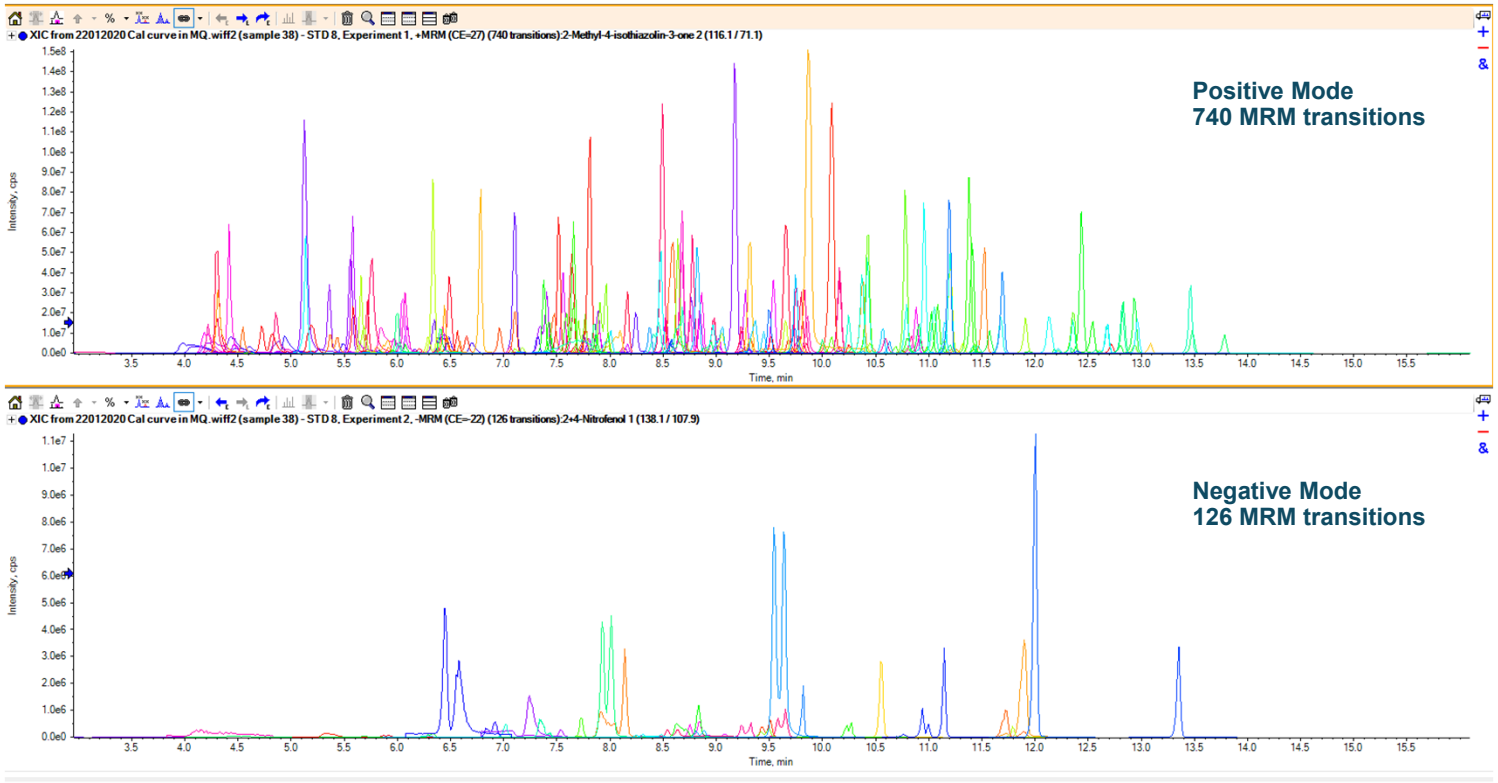
XIC of positive and negative ionization

SCIEX 7500 System

ALL QUANTIFIER IONS IN MILLIQ WATER



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XIC data points - positive

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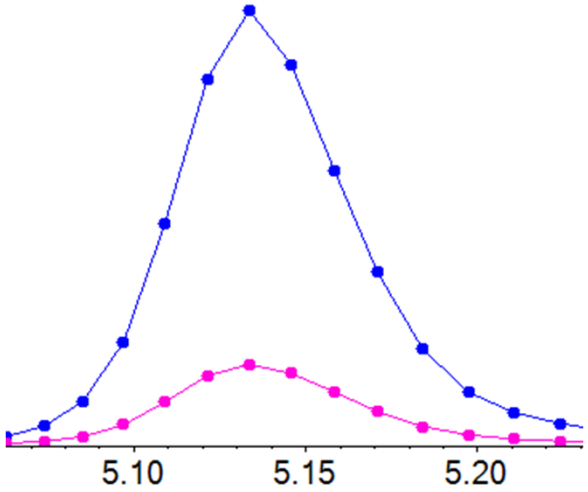
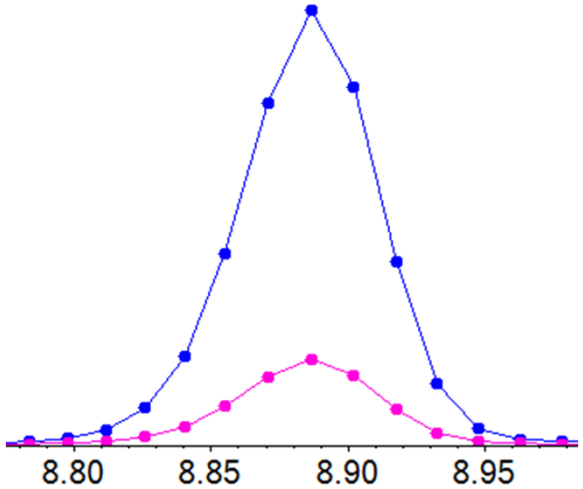
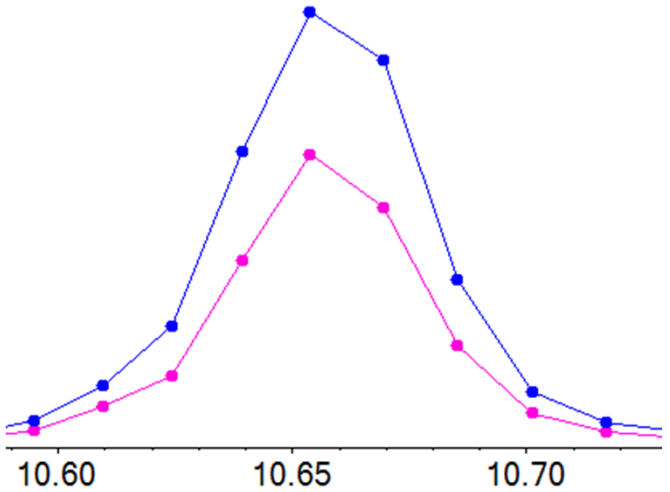


Carbendazim



Atrazine



Cyprodinil

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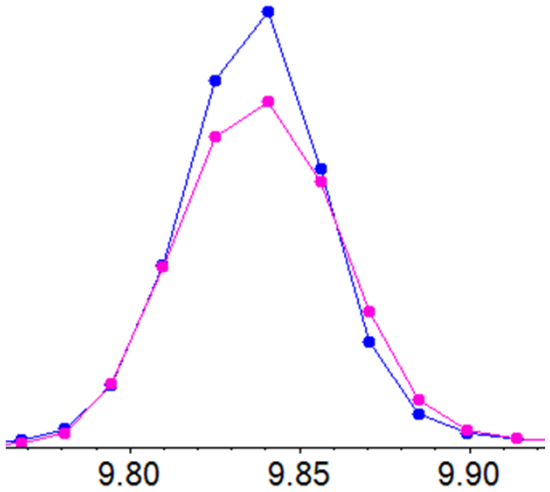
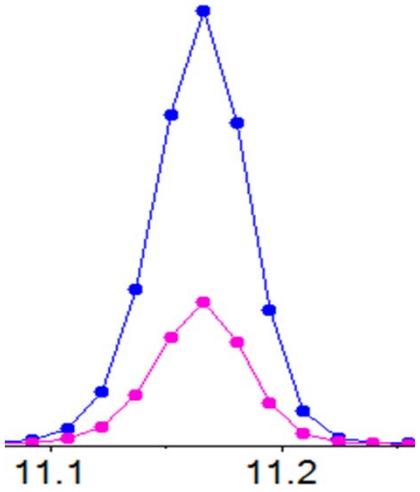
XIC data points - negative

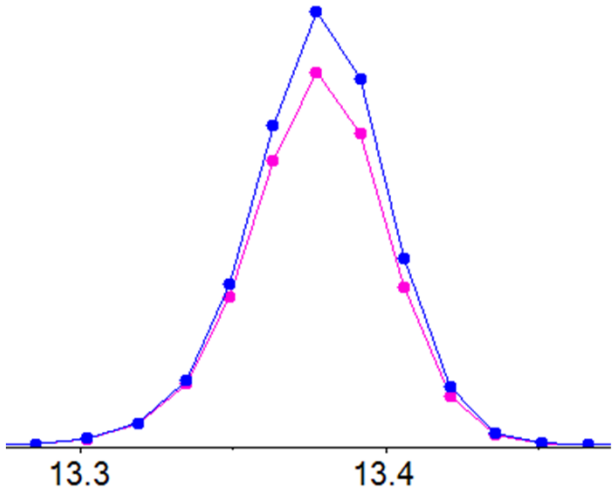
SCIEX 7500 System



PFOA



PFOS



Fluazinam

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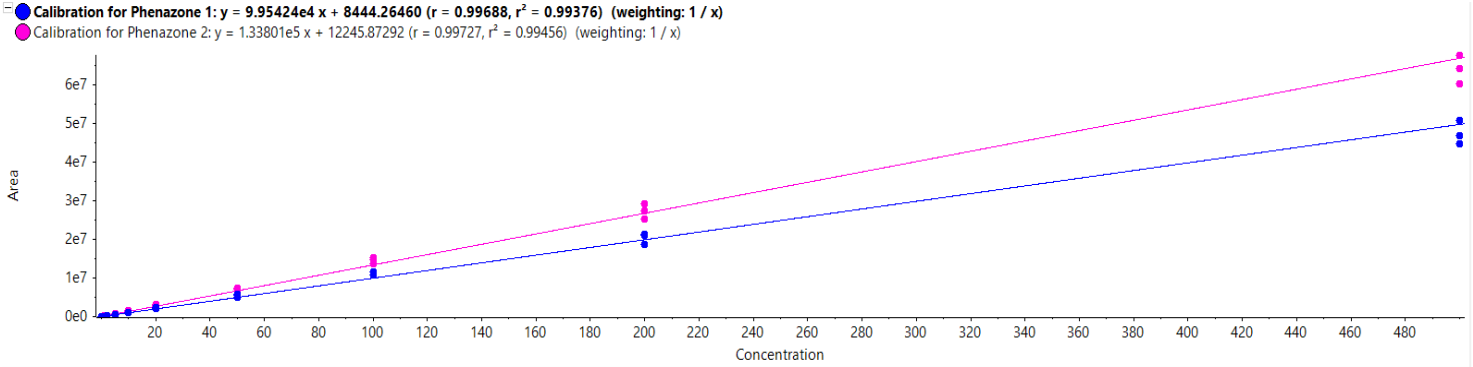
Phenazone (+ve)

SCIEX 7500 System



Index	Sample Name	Sample Type	Component Name	Component Type	Component Group Name	Actual Concentration	Area	Retention Time	Signal / Noise	Used	Calculated Concentration	Ion Ratio	Ion Ratio Confidence
923	STD 16	Standard	Phenazone 1	Quantifiers	Phenazone	0.10	21275.8	6.16	11.3	☑	4.565e-2	0.89	✔
17...	STD 15	Standard	Phenazone 1	Quantifiers	Phenazone	0.20	37733.9	6.15	28.2	☑	1.687e-1	0.67	✔
26...	STD 14	Standard	Phenazone 1	Quantifiers	Phenazone	0.50	67716.0	6.17	27.3	☑	3.928e-1	0.88	✔
35...	STD 13	Standard	Phenazone 1	Quantifiers	Phenazone	1.00	154528.1	6.17	44.9	☑	1.042e0	0.77	✔
43...	STD 12	Standard	Phenazone 1	Quantifiers	Phenazone	2.00	335476.6	6.17	118.5	☑	2.395e0	0.67	✔
52...	STD 11	Standard	Phenazone 1	Quantifiers	Phenazone	5.00	725149.5	6.17	438.0	☑	5.308e0	0.73	✔
61...	STD 10	Standard	Phenazone 1	Quantifiers	Phenazone	10.00	1573538.9	6.17	295.3	☑	1.165e1	0.71	✔
69...	STD9	Standard	Phenazone 1	Quantifiers	Phenazone	20.00	2957920.5	6.18	627.1	☑	2.200e1	0.70	✔
78...	STD 8	Standard	Phenazone 1	Quantifiers	Phenazone	50.00	7441689.9	6.15	1533.3	☑	5.552e1	0.76	✔
87...	STD 7	Standard	Phenazone 1	Quantifiers	Phenazone	100.00	14790475.2	6.18	2688.3	☑	1.105e2	0.72	✔
95...	STD 6	Standard	Phenazone 1	Quantifiers	Phenazone	200.00	27399055.8	6.17	5610.4	☑	2.047e2	0.77	✔
10...	STD 5	Standard	Phenazone 1	Quantifiers	Phenazone	500.00	64296556.3	6.16	10642.9	☑	4.805e2	0.73	✔

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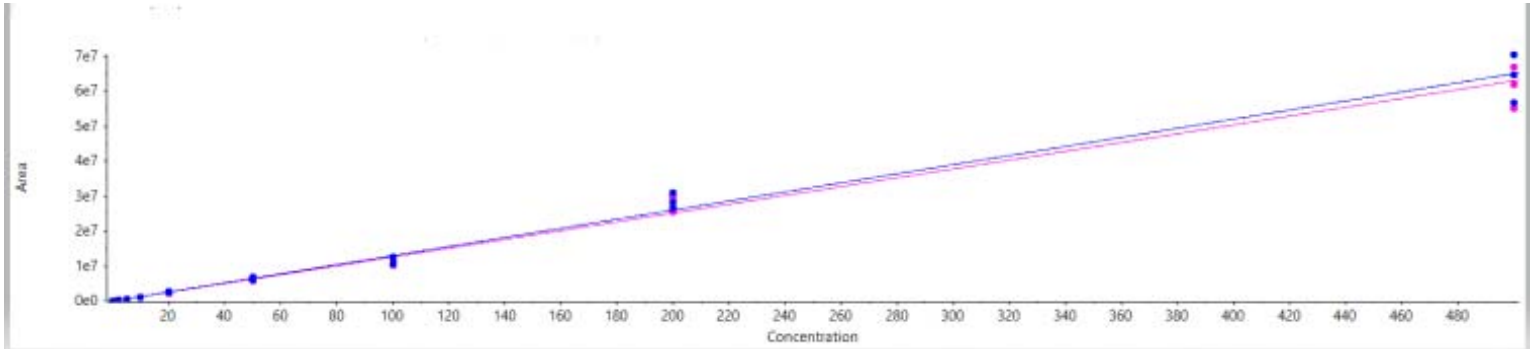
Fluazinam (-ve)

SCIEX 7500 System



Index	Sample Name	Sample Type	Component Name	Component Type	Component Group Name	Actual Concentration	Area	Retention Time	Signal / Noise	Used	Calculated Concentration	Ion Ratio	Ion Ratio Confidence
17...	STD 16	Standard	Fluazinam 1	Quantifiers	Fluazinam	0.10	10828.6	13.35	60.8	☑	1.587e-1	0.93	✓
25...	STD 15	Standard	Fluazinam 1	Quantifiers	Fluazinam	0.20	24399.6	13.34	98.8	☑	2.630e-1	1.01	✓
34...	STD 14	Standard	Fluazinam 1	Quantifiers	Fluazinam	0.50	50224.7	13.35	406.8	☑	4.615e-1	0.99	✓
43...	STD 13	Standard	Fluazinam 1	Quantifiers	Fluazinam	1.00	97459.0	13.36	1174.9	☑	8.246e-1	0.92	✓
51...	STD 12	Standard	Fluazinam 1	Quantifiers	Fluazinam	2.00	244137.1	13.37	2714.3	☑	1.952e0	0.90	✓
60...	STD 11	Standard	Fluazinam 1	Quantifiers	Fluazinam	5.00	572460.2	13.36	7434.7	☑	4.476e0	0.89	✓
69...	STD 10	Standard	Fluazinam 1	Quantifiers	Fluazinam	10.00	1202552.8	13.35	9328.0	☑	9.320e0	0.91	✓
77...	STD9	Standard	Fluazinam 1	Quantifiers	Fluazinam	20.00	2785341.8	13.36	14319.1	☑	2.149e1	0.94	✓
86...	STD 8	Standard	Fluazinam 1	Quantifiers	Fluazinam	50.00	6745866.4	13.34	23155.2	☑	5.193e1	0.99	✓
95...	STD 7	Standard	Fluazinam 1	Quantifiers	Fluazinam	100.00	12697634.5	13.37	46072.0	☑	9.768e1	0.97	✓
10...	STD 6	Standard	Fluazinam 1	Quantifiers	Fluazinam	200.00	31008866.0	13.37	49666.8	☑	2.384e2	0.98	✓
11...	STD 5	Standard	Fluazinam 1	Quantifiers	Fluazinam	500.00	70438403.0	13.36	145466.6	☑	5.415e2	0.95	✓

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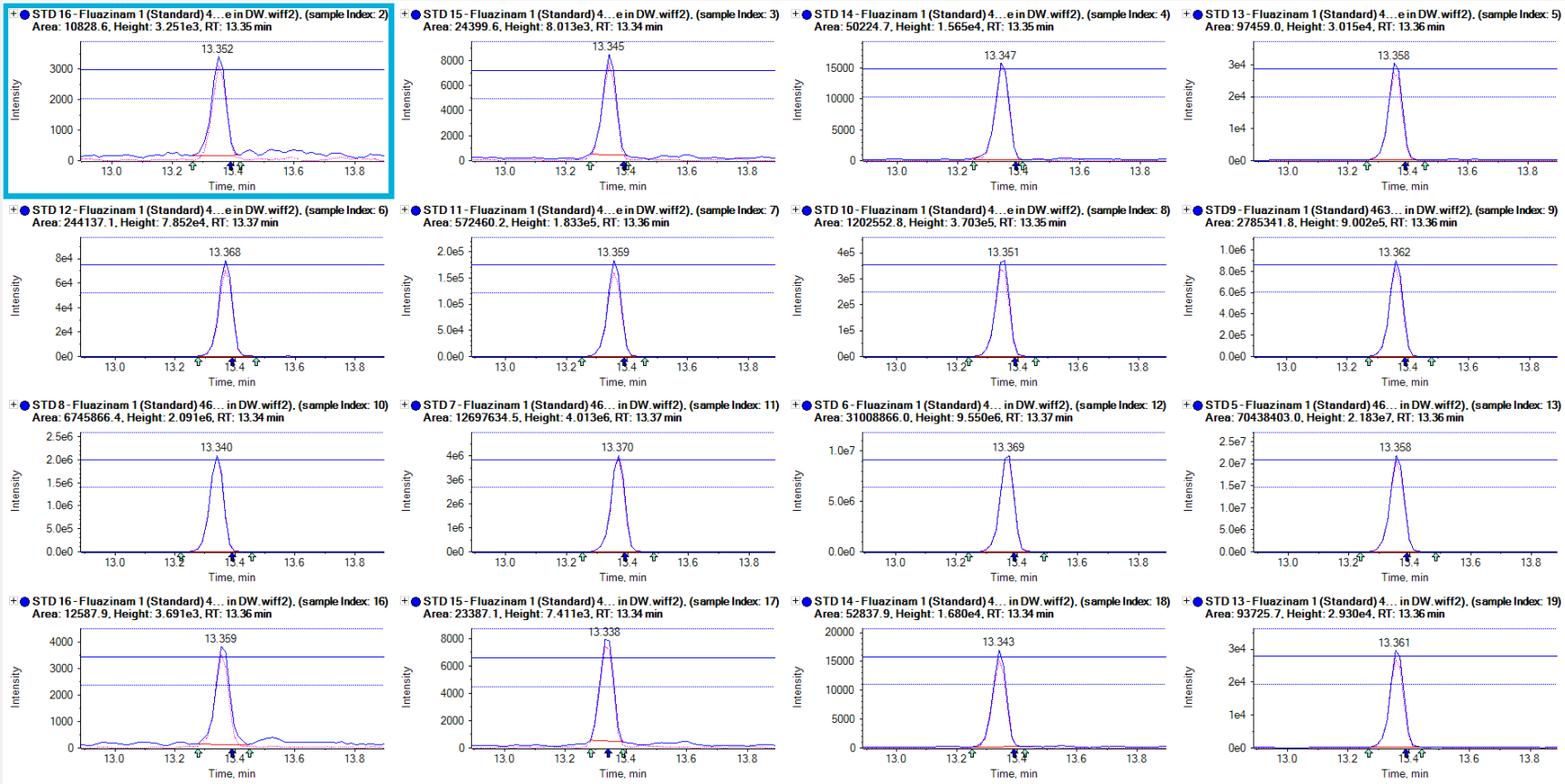
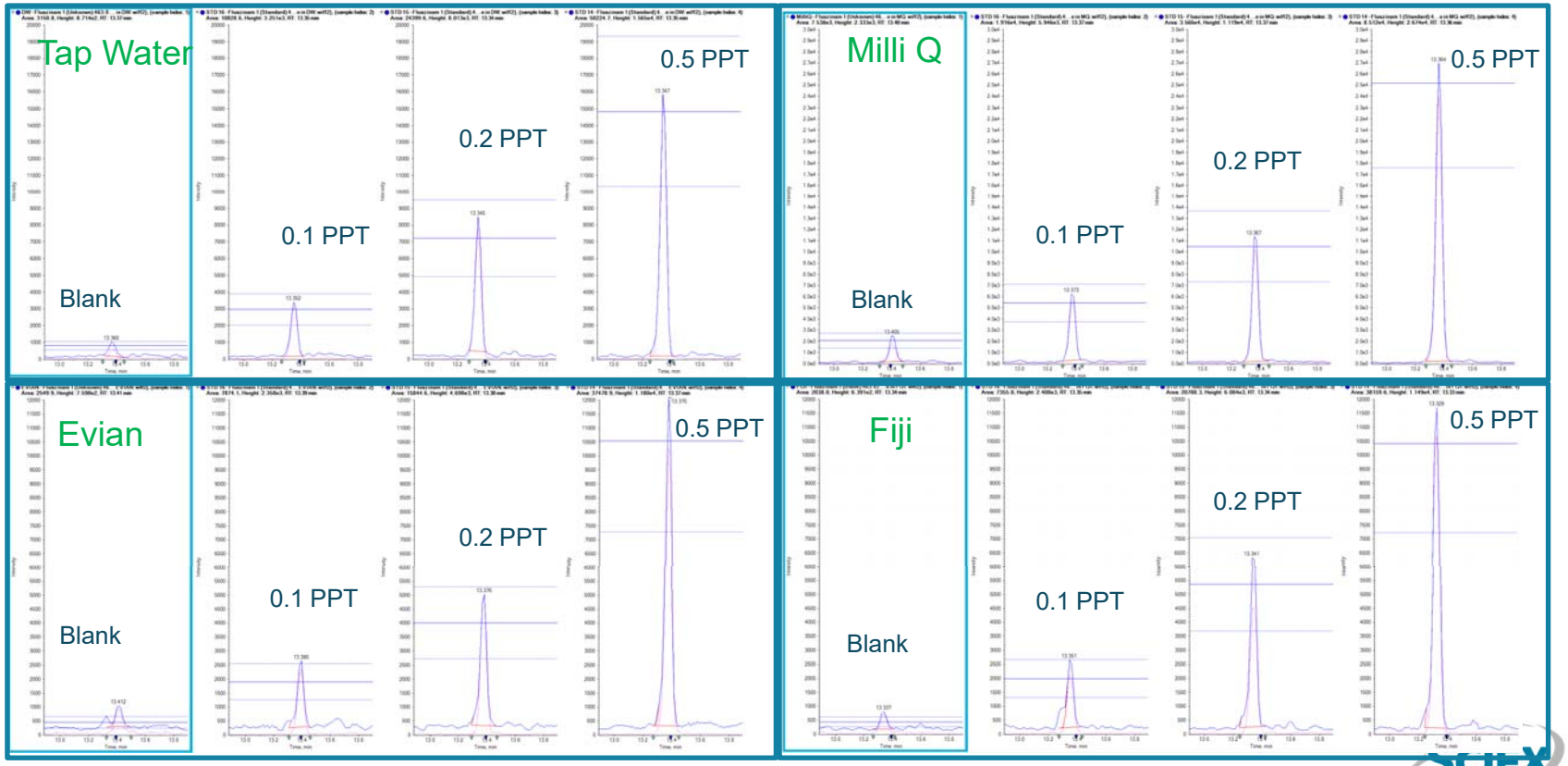
Fluazinam (–ve)

SCIEX 7500 System



Fluazinam (-ve)

SCIEX 7500 System



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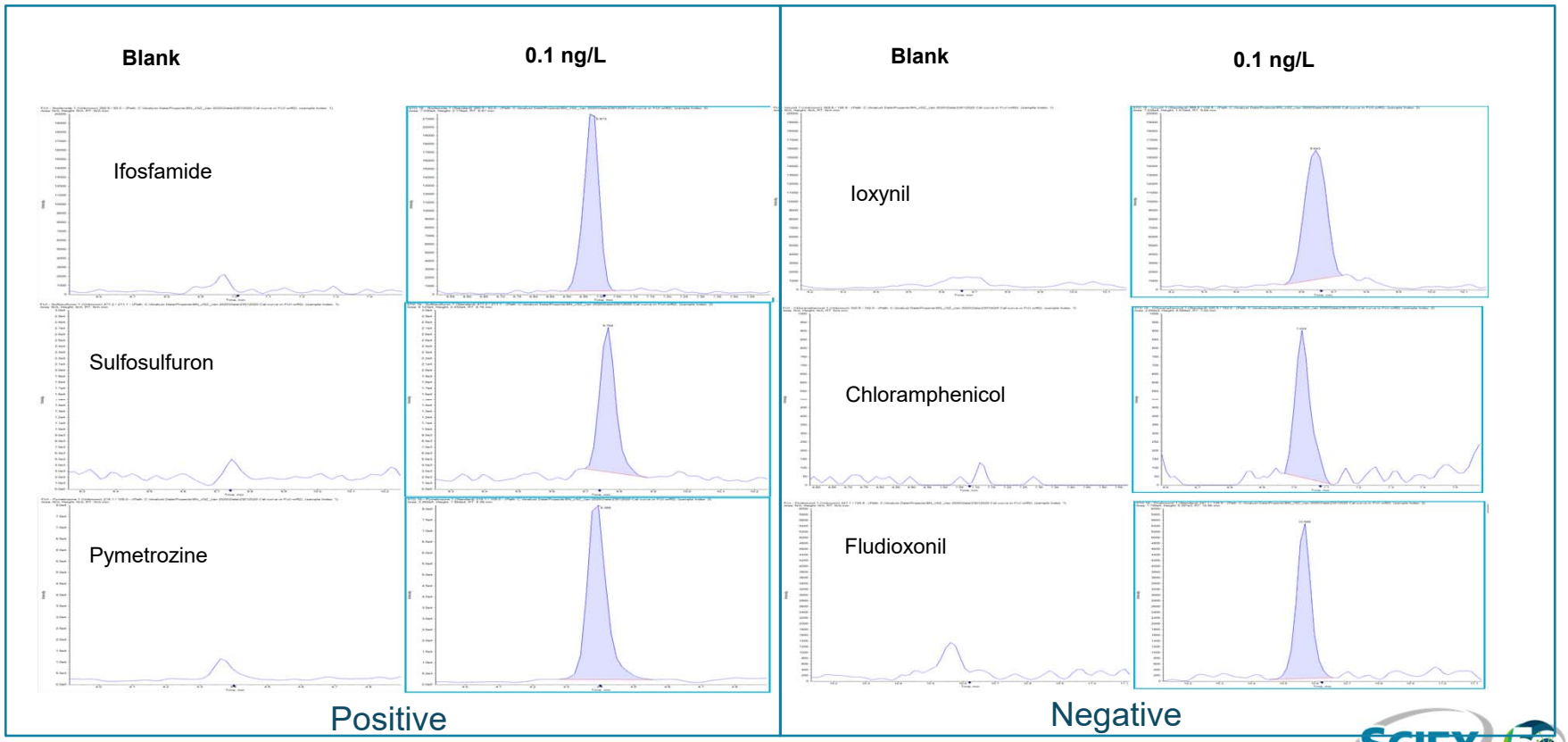
Lower limits of quantification

SCIEX 7500 System



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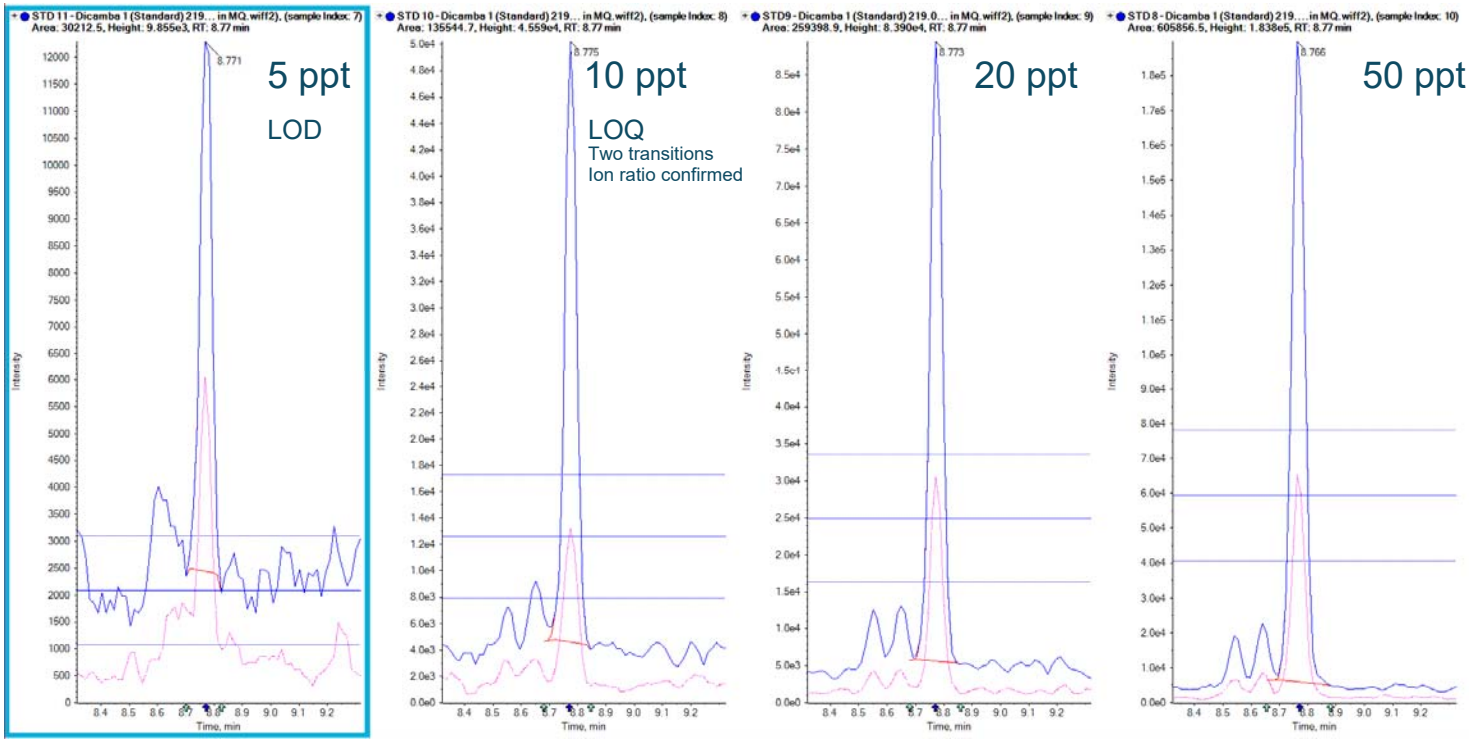
Dicamba

SCIEX 7500 System



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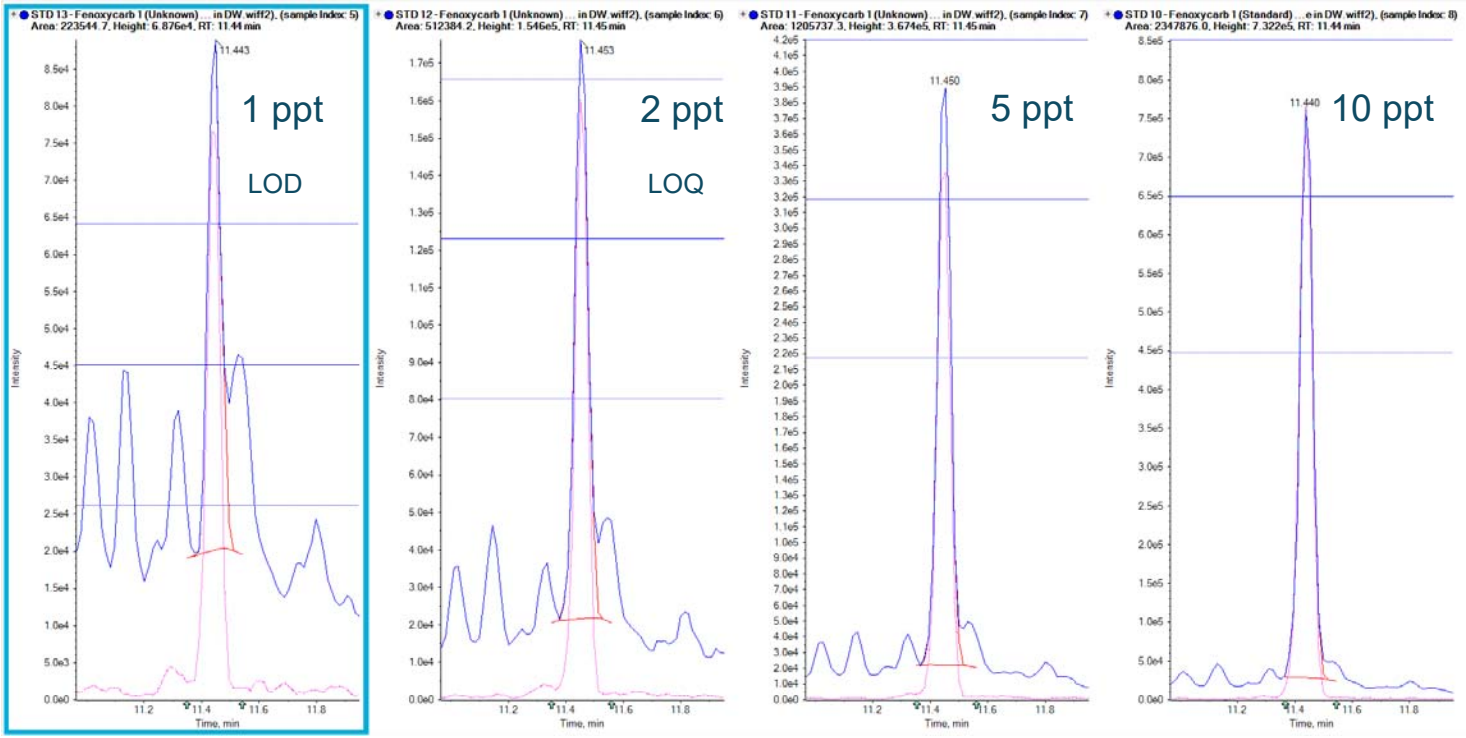
Fenoxycarb

SCIEX 7500 System



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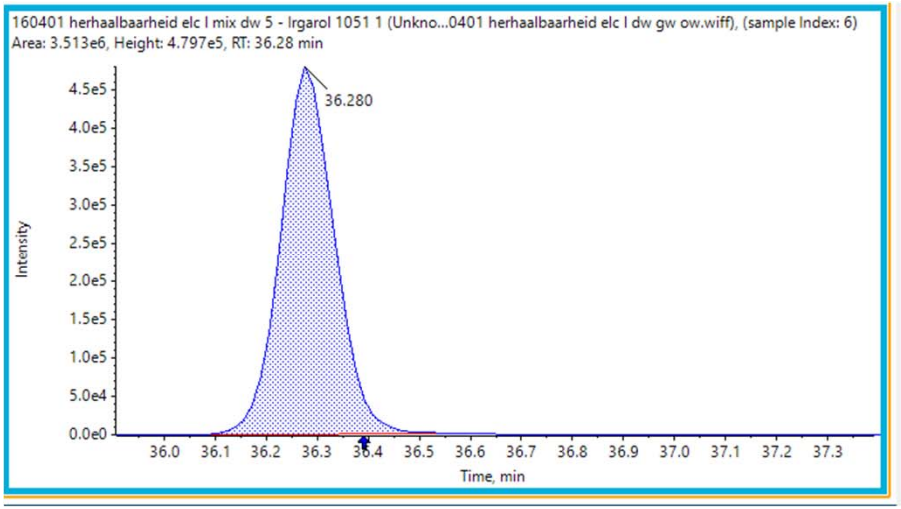
Irgarol 1051(+ve) (tap water)

SCIEX 7500 System

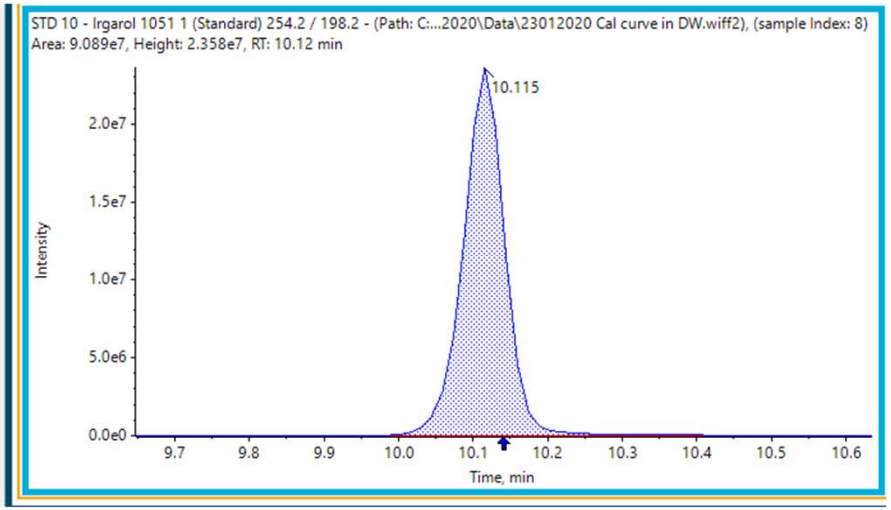
QTRAP 6500+ system



Measured 20 ppt

Calculated LOQ 1 ppt

SCIEX 7500 system



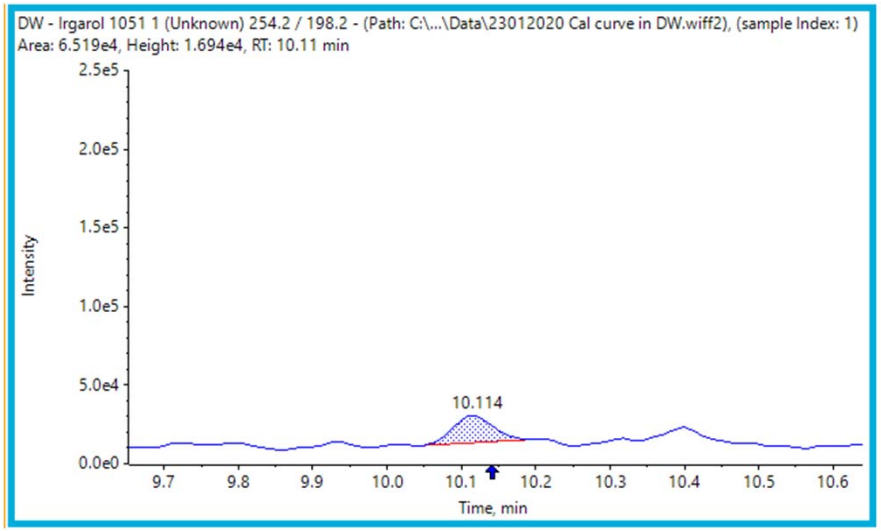
Measured 20 ppt

SCIEX The Power of Precision

Irgarol 1051 (+ve) (tap water)

SCIEX 7500 System

SCIEX 7500 system



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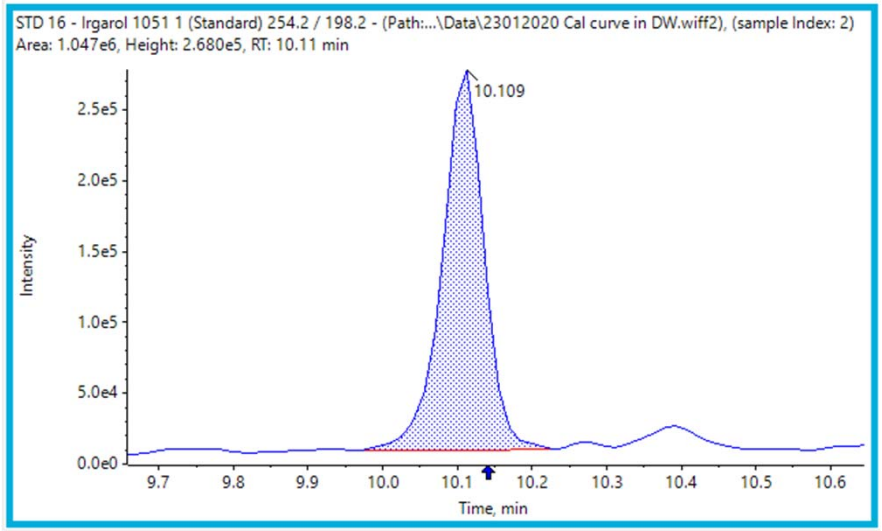

Measured 0.1 ppt

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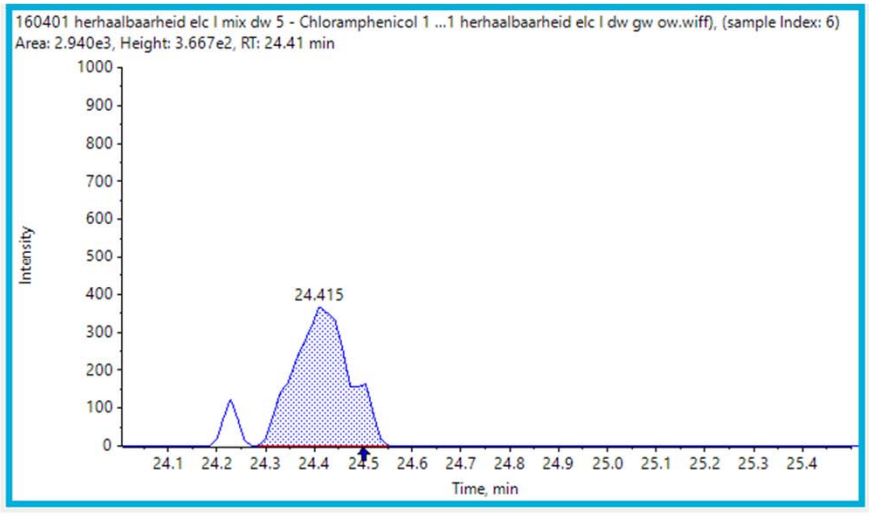
Chloramphenicol (-ve) (tap water)

SCIEX 7500 System

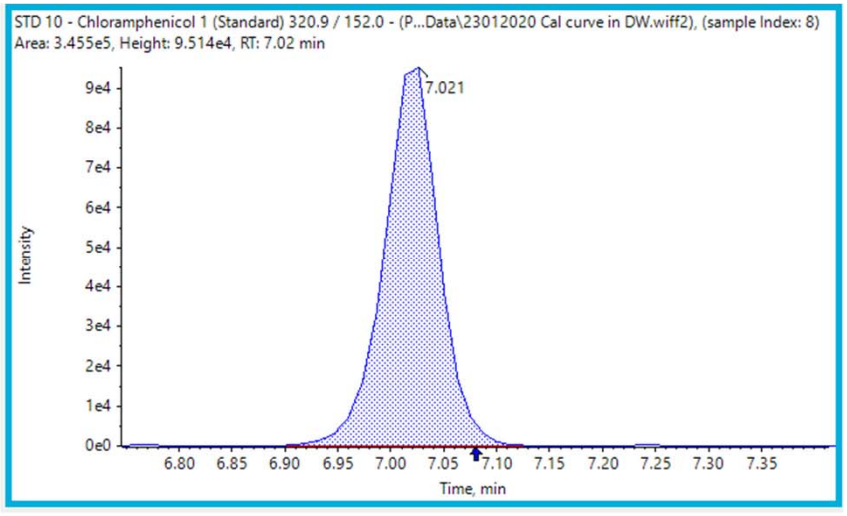
QTRAP 6500+ system



Measured 10 ppt

Calculated LOQ 2 ppt

SCIEX 7500 system



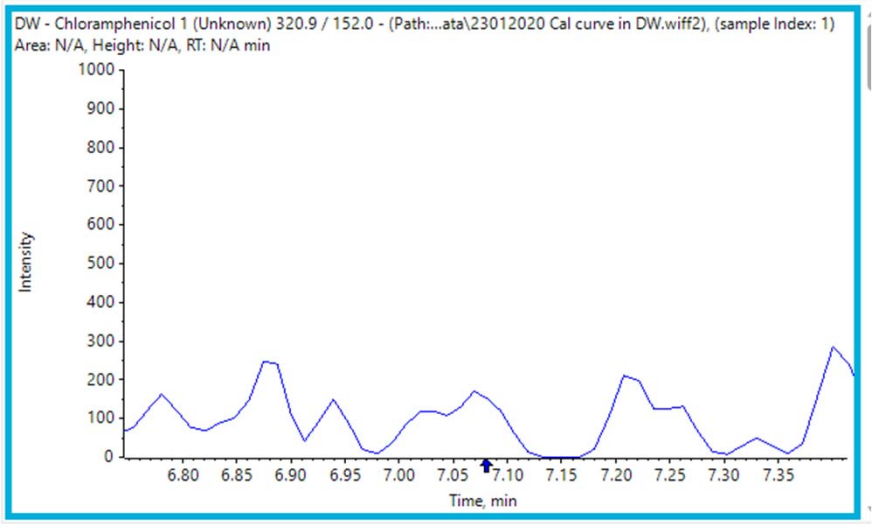
Measured 10 ppt

SCIEX The Power of Precision

Chloramphenicol (-ve) (tap water)

SCIEX 7500 System

SCIEX 7500 system



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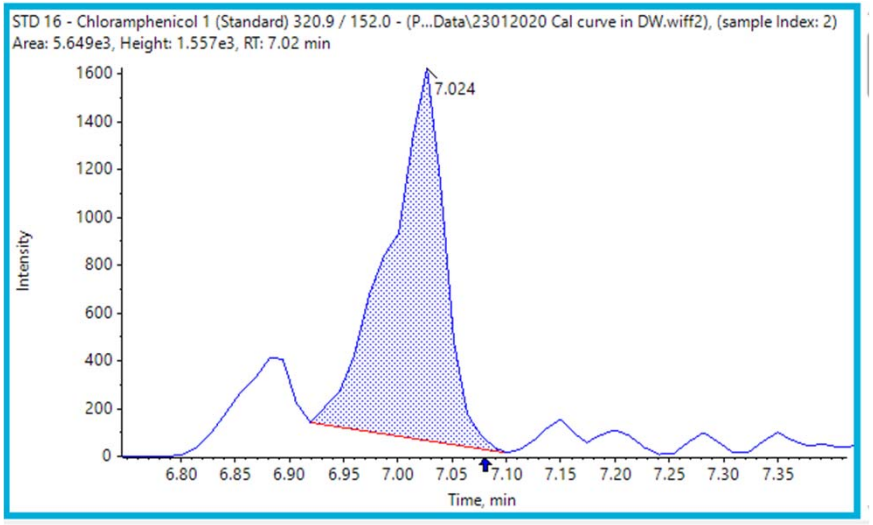
SCIEX 7500 system



Measured 0.1 ppt

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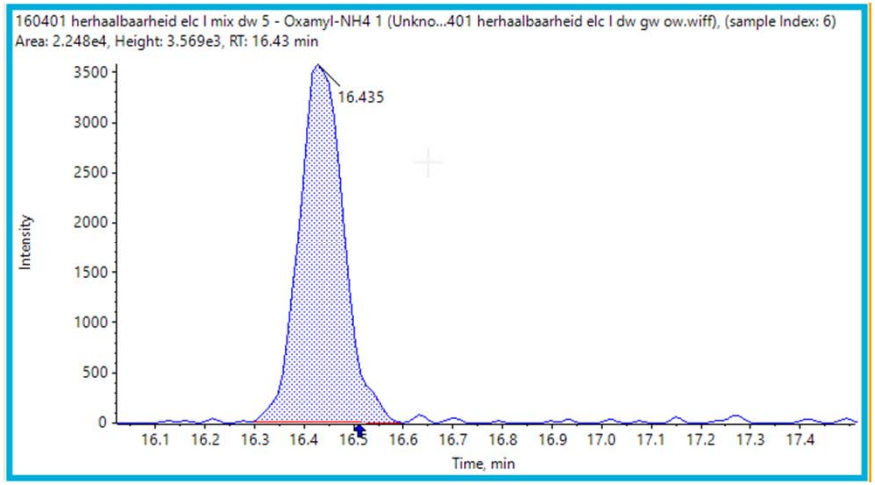
Oxamyl NH4 (+ve)

SCIEX 7500 System

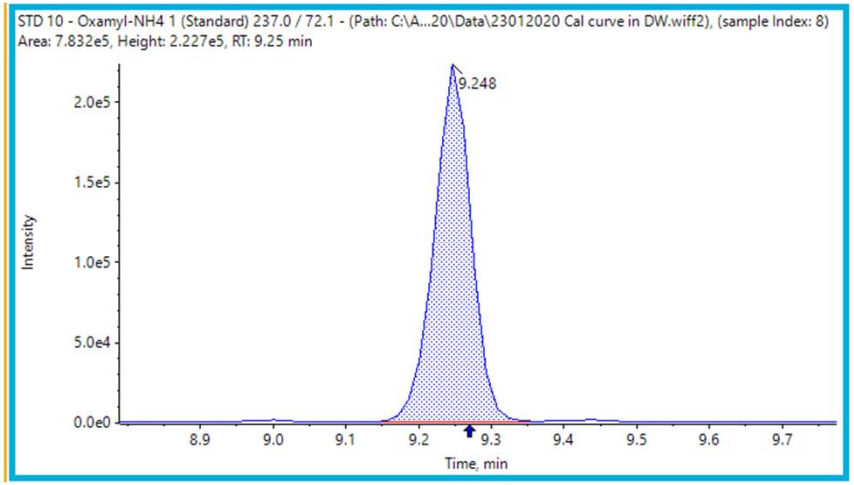
QTRAP 6500+ system



Conc 10 ng/L

Calculated LOQ 1 ng/L

SCIEX 7500 system



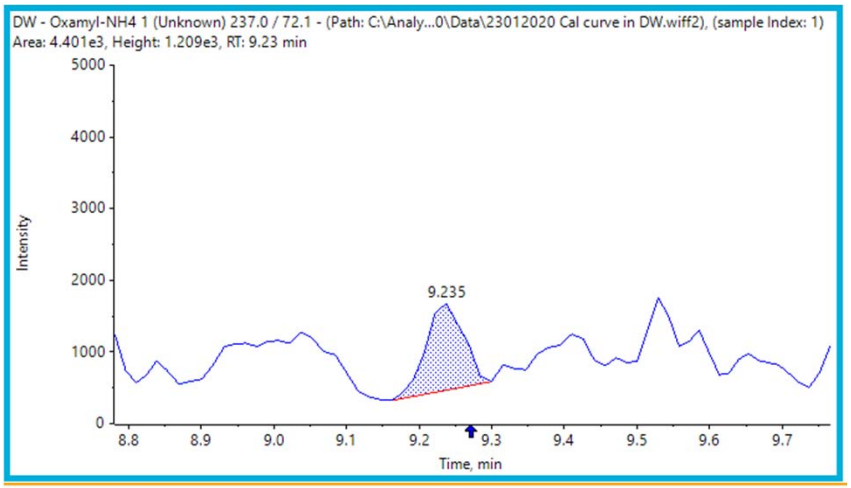
Conc 10 ng/L

SCIEX The Power of Precision

Oxamyl NH_4

SCIEX 7500 System

SCIEX 7500 system



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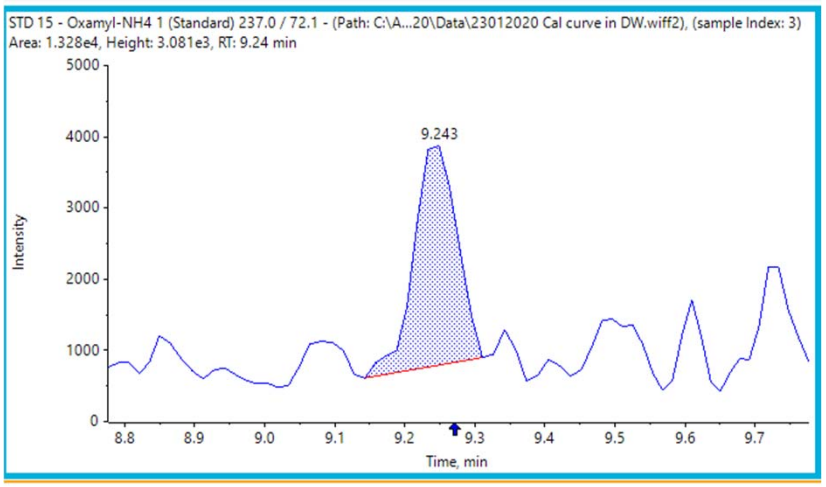

Conc 0.2 ng/L

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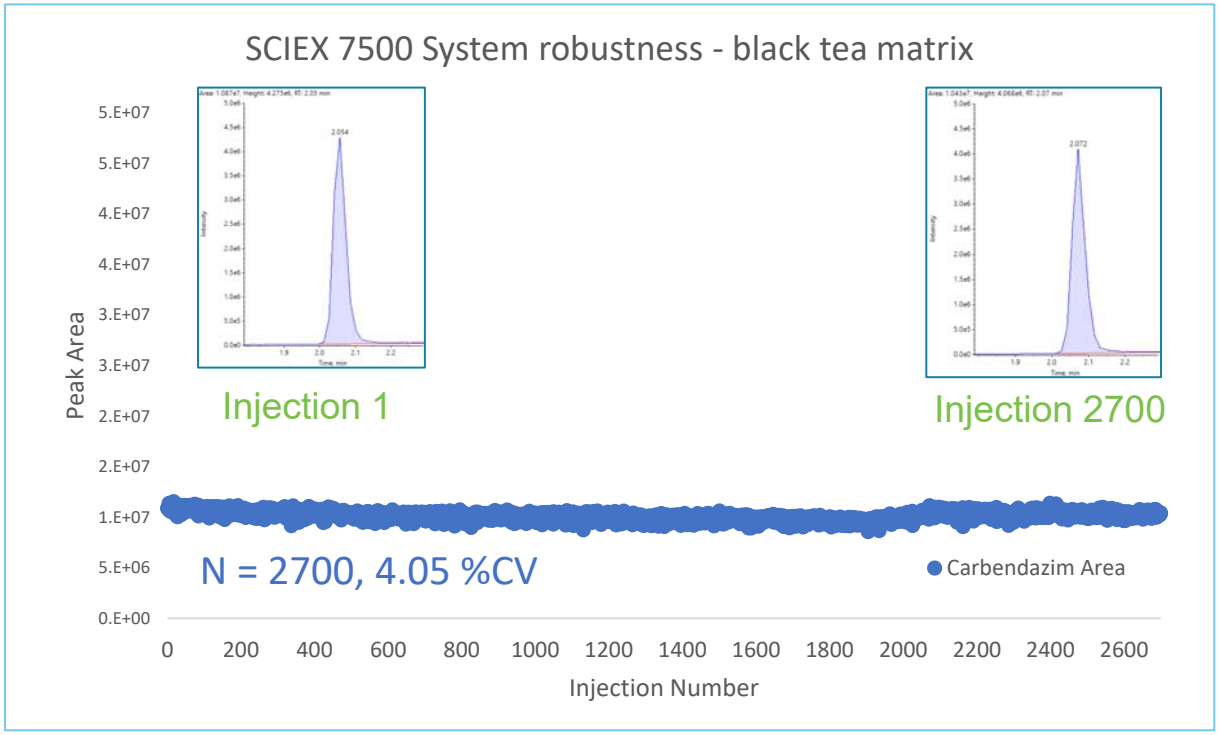
Robustness – tea matrix

SCIEX 7500 System

- Short LC-MS run was performed (4 min gradient at 400 µL/min flow rate)
- Raw peak area plotted
- S/N remained constant across injections
- 1 ppb carbendazim
- 2 µL injection volume



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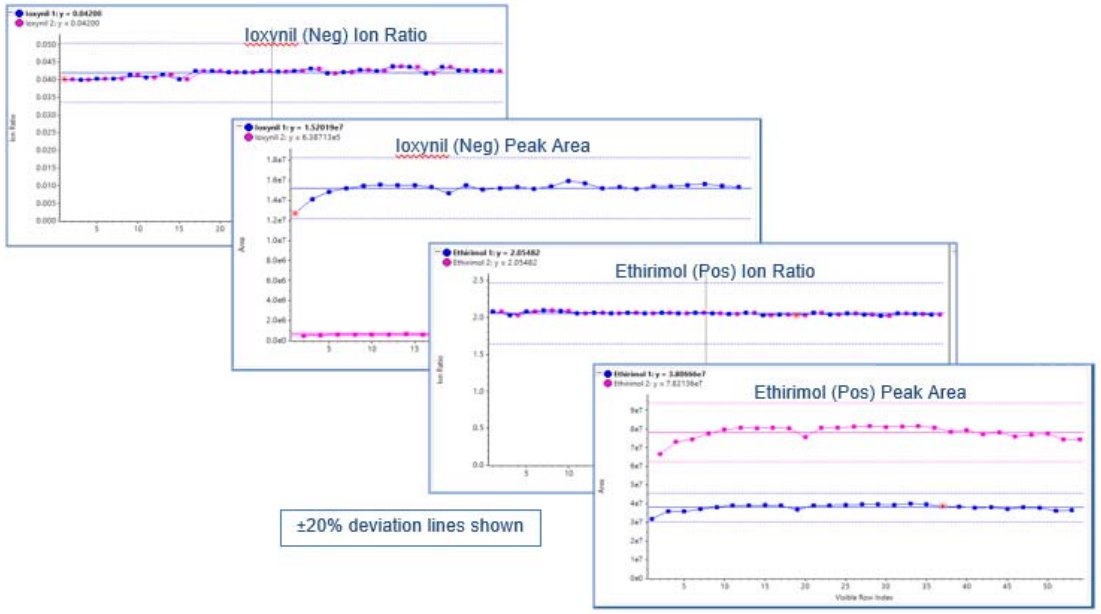
Robustness

SCIEX 7500 System

0 ppb	10 ppb
0.2 ppb	Meat 0
1 ppb	Meat 5
5 ppb	Meat 15
10 ppb	Meat 50
20 ppb	10 ppb
Fruit and Vegetable 0	Animal Oil/Fat 0
Fruit and Vegetable 5	Animal Oil/Fat 5
Fruit and Vegetable 15	Animal Oil/Fat 15
Fruit and Vegetable 50	Animal Oil/Fat 50
10 ppb	10 ppb
Oil Seeds 0	Eggs and products 0
Oil Seeds 5	Eggs and products 5
Oil Seeds 15	Eggs and products 15
Oil Seeds 50	Eggs and products 50
10 ppb	10 ppb
Vegetable Oil 0	Milk and products 0
Vegetable Oil 5	Milk and products 5
Vegetable Oil 15	Milk and products 15
Vegetable Oil 50	Milk and products 50
10 ppb	10 ppb
Grain 0	Fatty Acids 0
Grain 5	Fatty Acids 5
Grain 15	Fatty Acids 15
Grain 50	Fatty Acids 50
10 ppb	10 ppb
Herbs and Spices 0	Herbs and Spices 0 dil 5
Herbs and Spices 5	Herbs and Spices 5 dil 5
Herbs and Spices 15	Herbs and Spices 15 dil 5
Herbs and Spices 50	Herbs and Spices 50 dil 5
	10 ppb



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Conclusions

SCIEX 7500 System

- The SCIEX Triple Quad 7500 system provides impressive levels of sensitivity, robustness and accuracy
- Fast polarity switching functionality and the powerful Scheduled MRM algorithm allow over 1400 MRM transitions for 700 compounds analyzed in a single analysis, example of food
- Fast polarity switching functionality and the powerful Scheduled MRM algorithm allow over 850 MRM transitions for 430 compounds analyzed in a single analysis, example of water
- Multiple MRMs per analyte enabled ion ratio monitoring to ensure confident detection
- The ability to analyze this many compounds with high sensitivity without the need for extensive sample preparation improves operational efficiencies

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Acknowledgements

- Vitens, Netherlands
  - Ronny Bosch
  - Bernard Bajema
- SCIEX
  - Jianru Stahl-Zeng
  - Bertram Nieland
  - Phil Taylor
  - Jack Steed
  - Ian Moore

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