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Application Note

Improvements in Robustness in Multiresidue Pesticide Analysis with Xevo TQ Absolute XR Mass Spectrometer

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Abstract

Typical LC-MS/MS pesticide multiresidue methods can contain more than 200 analytes acquired via multiple reaction monitoring (MRM) methods, with switching between positive and negative ionization modes. When analyzing challenging matrices with high *m/z* ions that can contaminate the quadrupoles of the mass spectrometer, charging can occur, resulting in a loss of signal. This charging can become more pronounced under fast acquisition rates, such as short dwell times and polarity switching. This can affect ion ratios and signal response leading to unplanned instrument downtime. The new StepWave™ XR ion guide within the Xevo™ TQ Absolute XR Mass Spectrometer showed improved robustness over the course of more than 18,000 injections for a single sample derived from a challenging matrix.

Benefits

- Acquired under accelerated method conditions and over a 14 week period of continuous operation, this study demonstrates superior system robustness, enabling improved lab productivity through reduced system maintenance and no unscheduled downtime

- Improved robustness of upto 6x longer for ion ratios, giving laboratories confidence in consistency
- Seamless batch review using waters_connect™ for Quantitation Software's accelerated data validation workflows

Introduction

Technological advancements have enabled testing laboratories to optimize workflows and reduce the analysis cost per sample. High-sensitivity mass spectrometry (MS) systems, featuring larger sampling cone orifices, now allow food testing labs to analyze crude extracts using a simple extract-and-dilute method—saving time, labor, and consumables. However, this approach can burden the MS system, as it often introduces large amounts of complex matrix ions, leading to increased chemical noise and the need for more frequent system maintenance.

Chemical noise is a common challenge in LC-MS/MS, particularly under electrospray ionization (ESI) conditions, where high solvent content can generate solvent-induced ions alongside matrix-derived ions from crude samples. This interference may stem from interactions between solvents and food components, leading to the formation of large molecular clusters such as protein complexes or oligosaccharide aggregates.

In targeted MRM mode, the impact of matrix loading may not be immediately evident during the chromatographic run, as many of these high-mass clusters exceed the mass range of a tandem quadrupole MS. However, they can still contaminate critical MS components—including the ion optics, quadrupoles, and detectors—resulting in unplanned maintenance and servicing requirements.

Fish feed is considered a challenging sample matrix, as it contains high levels of fatty acids, amino acids, phospholipids, carbohydrates, pigments, organic polymers (e.g. lignins), water insoluble content (e.g. cell walls), sugars, and vitamins.

In this application note, an accelerated LC-MS/MS method for more than 200 pesticides in less than 6 minutes runtime was developed and a crude extract of fish feed was generated by QuEChERS extraction, without sample clean-up. These conditions were chosen to best challenge and demonstrate the StepWave XR performance, a novel slotted bandpass ion guide, within the Xevo TQ Absolute XR Tandem Quadrupole Mass Spectrometer. This study demonstrates maintained method performance with improved system robustness and thus gains in laboratory operation achievable, by acquiring more than 14,000 injections, without lengthy or unscheduled user interaction with the system.

Experimental

Sample Preparation

Briefly, 2 g of fish feed (Figure 1) was weighed, rehydrated and extracted using DisQuE QuEChERS CEN pouch (p/n: 186006813 <https://www.waters.com/nextgen/global/shop/sample-preparation--filtration/186006813-disque-1-g-trisodium-citrate-dihydrate-05-g-disodium-hydrogencit.html>) with 10 mL of acetonitrile. Following centrifugation, the sample extracts were collected, spiked with 204 pesticides, and diluted 1 in 10 with acetonitrile to give a final in vial concentration of 0.01 µg/mL. This solution was then aliquoted into 80 samples vials (4 plates of 20 vials) for the robustness study. 1 µL of sample was injected onto a reversed phase column using an LC method that had been accelerated from 20 minutes to 6 minutes on the new Xevo TQ Absolute XR Tandem Quadrupole Mass Spectrometer, acquiring data for 204 pesticides. To maximally challenge the analytical system, the waste divert valve was not used during this study.

Figure 1. Fish feed and the extract before dilution.

Each analysis batch was divided into two sections. 45 injections of the batch acquired 204 pesticides, each with at least 2 transitions. These were used to monitor the ion ratio, calculated as identifier to quantifier ions. A pesticide standard in solvent was injected prior to analysis to obtain an average reference ion ratio value for each analyte. The remaining 5 injections of each batch were used to assess contamination on the quadrupole, referred to as the charging test. The ratio between 2 transitions of the same analyte should be ~1.

Charging may be most pronounced in heavy matrix and during fast MS acquisition rates, for example during polarity switching. Fluazinam was chosen as a representative analyte, with time windowed MRMs overlapping with ESI positive analytes.

LC Conditions

LC system:	ACQUITY™ Premier System with Binary Solvent Manager and Flow-Through Needle
Analytical column:	ACQUITY UPLC™ HSS T3, 2.1 x 30 mm, 1.8 µm

	Column (p/n: 186003944)
Column temperature:	40 °C
Sample temperature:	10 °C
Injection volume:	1 µL using 50 µL extension loop fitted post injector (p/n: 430002012)
Flow rate:	0.5 mL/min
Mobile phase A:	5 mM ammonium acetate, 0.1% formic acid (aq)
Mobile phase B:	5 mM ammonium acetate, 0.1% formic acid in MeCN/MeOH (1/1)

Gradient Table

Time (min)	%A	%B	Curve
0	99	1	Initial
0.15	99	1	6
1.05	60	40	6
3.75	15	85	6
3.78	1	99	6
4.50	1	99	6
4.53	99	1	6
5.70	99	1	6

MS Conditions

MS system:	Xevo TQ Absolute XR Mass Spectrometer

Ionization mode:	ESI+ & ESI-
Capillary voltage:	2 kV
Source temperature:	150 °C
Desolvation temperature:	550 °C
Desolvation flow:	1000 L/hr
Cone flow:	150 L/hr
MRM method:	See appendix for full MRM details

Data Management

Software:	waters_connect for Quantitation Software

Results and Discussion

Quadrupole Charging Test

Fluazinam was chosen to represent a negative ion compound being monitored in the same retention time window as a positive ion compound. Figure 2 shows the Xevo TQ Absolute XR Mass Spectrometer lasted more than 6 times longer than its predecessor.

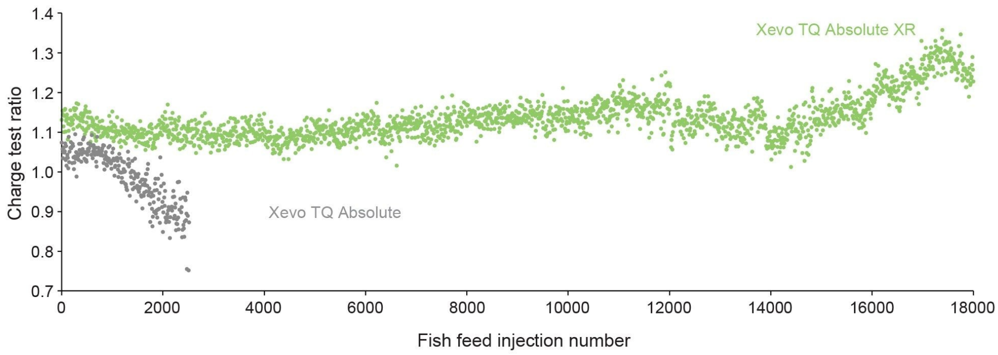

Figure 2. Plot of charge ratio comparison for fluazinam.

Robustness Tests

Thirty solvent injections of the pesticide standard provided average values for each confirmation/quantitation ion ratio, which were used to set a ±30% tolerance for the ion ratio plot of the matrix injections. When fluazinam was measured on the Xevo TQ Absolute Mass Spectrometer (Figure 3), the ion ratio consistently exceeds this tolerance from 1,500 injections onwards, which is where the charge test plot (Figure 2) also began to show evidence of charging. On the Xevo TQ Absolute XR Mass Spectrometer (Figure 3), however, the ion ratio plot reached more than 18,000 injections without ever approaching the ±30% tolerance.

The point of this study is not to denigrate the Xevo TQ Absolute in any way. At the point of failure there were 2000 back-to-back injections on an accelerated LC method. This took 2 weeks, on the standard method that would be closer to 8 weeks and in a real-world lab that isn't constantly injecting it would be most likely be 3 to 4 months before seeing affects like this.

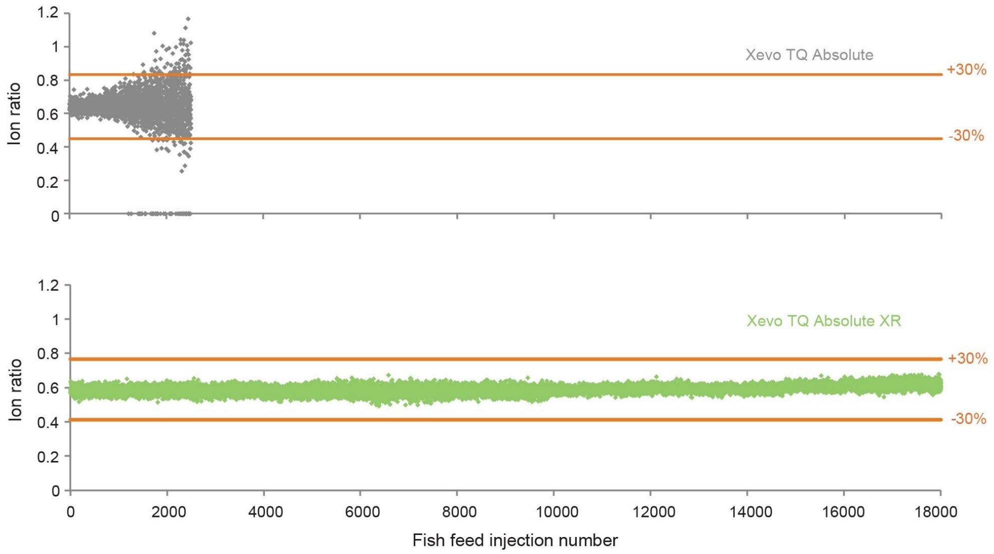

Figure 3. Ion ratio plot comparison for fluazinam.

During polarity switching, negative ion compounds tend to be affected more readily by charging due to the generally lower ion current in negative ion mode. Examples in Figure 4 and Figure 5 of ion ratio comparisons of negative compounds on each instrument show the robustness of the Xevo TQ Absolute XR Mass Spectrometer.

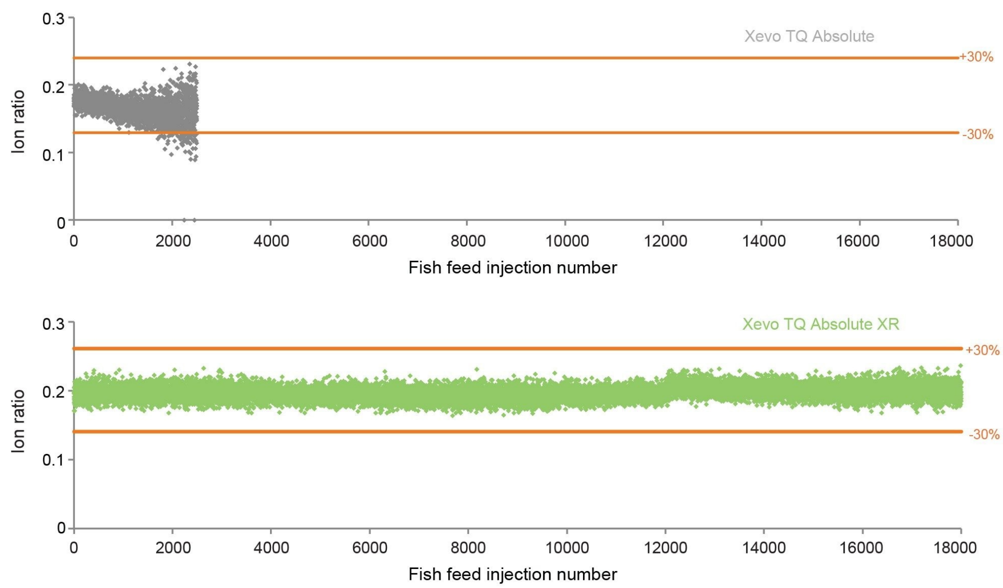

Figure 4. Ion ratio plot comparison for fipronil desulfinyl.

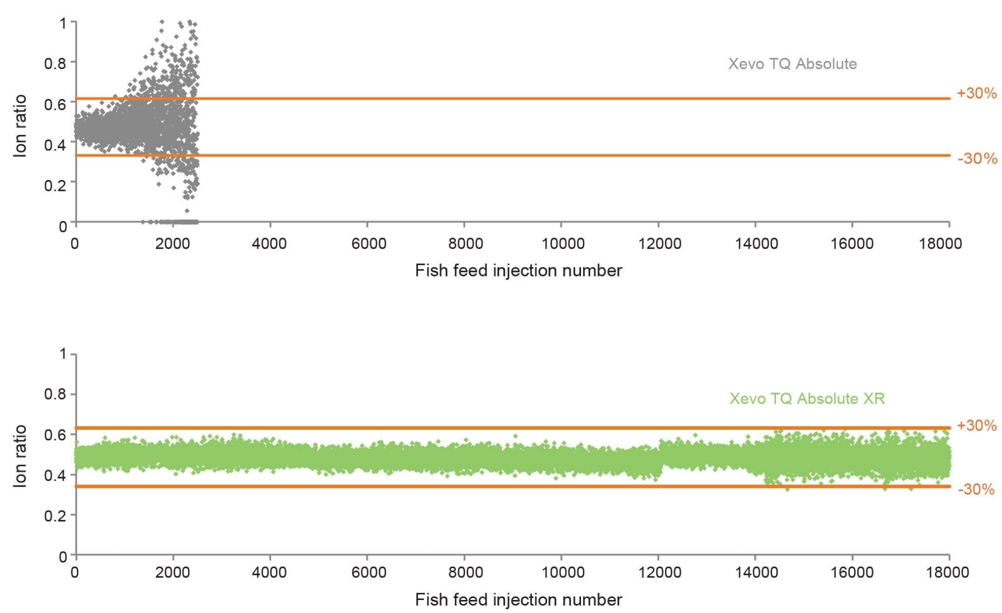

Figure 5. Ion ratio plot comparison for hexaflumuron.

Multiresidue Pesticide	Representing	Ion Ratio %RSD
Dicrotophos	Early RT: 1.31 min	3.76
Pyridaben	Late RT: 4.23 min	2.47
Methomyl	Low response: <1 × 107	6.03
Furalaxyl	High response: >1 × 108	4.34
Azoxystrobin	Low ion ratio: ~0.25	3.85
Imazalil	High ion ratio: ~1	4.60
Fenuron	Low *m/z*: 165	3.59
Spinetoram (L)	High *m/z*: 761	5.05
Fipronil desulfinyl	Negative	4.77
Fluazinam	Negative	3.53
Hexaflumuron	Negative	6.29
Lufenuron	Negative	7.48

Table 1. Compounds and their ion ratio RSD%.

Table 1 shows a selection of compounds from the 204 analytes, selected to represent a wide cross section of parameters like retention time (RT), peak response, ion ratio, *m/z,* and negative ionization. Their calculated RSD% over 18,000 injections is displayed. Of the 204 analytes detected, 79% returned RSD% for ion ratio of less than 10%.

The StepWave XR ion guide was shown to prevent charging on the quadrupoles over a duration of 14 weeks in which >18,000 injections were made of a challenging matrix without prior sample cleanup. The StepWave XR ion guide is capable of effectively removing contaminant ions, preventing fouling of the quadrupoles. This results in improved system robustness- consistent ion ratios, and minimal intervention on the MS system.

Conclusion

This study can give testing laboratories confidence the Xevo TQ Absolute XR Mass Spectrometer will provide maximum uptime while delivering consistent performance.

References

1. Feed Tables webpage, available at https://www.feedtables.com/content/fish-meal-protein-65 (last accessed May 2025)

APPENDIX

Analyte Name	Precursor (m/z)	Product (m/z)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Abamectin	890.6	305.3	Positive	30	25	TRUE	4.33
Abamectin	890.6	567.4	Positive	30	15	FALSE	4.33
Acephate	183.93	94.93	Positive	5	21	FALSE	0.93
Acephate	183.93	142.92	Positive	5	8	TRUE	0.93
Acetamiprid	223	56.1	Positive	30	15	FALSE	1.53
Acetamiprid	223	126	Positive	30	20	TRUE	1.53
Acibenzolar-s-methyl	210.9	69	Positive	25	35	FALSE	2.6
Acibenzolar-s-methyl	210.9	91	Positive	25	20	FALSE	2.6
Acibenzolar-s-methyl	210.9	135.9	Positive	25	30	TRUE	2.6
Aldicarb	213.1	47	Positive	35	25	FALSE	1.73
Aldicarb	213.1	89	Positive	35	20	TRUE	1.73
Aldicarb	213.1	116	Positive	35	11	FALSE	1.73
Aldicarb sulfone	223	86	Positive	35	14	TRUE	1.17
Aldicarb sulfone	223	148	Positive	35	10	FALSE	1.17
Aldicarb sulfoxide	207	69	Positive	20	14	FALSE	1.06
Aldicarb sulfoxide	207	89	Positive	20	15	TRUE	1.06
Ametryn	228.1	68.1	Positive	25	35	FALSE	2.34
Ametryn	228.1	186.1	Positive	25	20	TRUE	2.34
Aminocarb	209	137	Positive	25	25	TRUE	1.04
Aminocarb	209	152	Positive	25	15	FALSE	1.04
Azoxystrobin	404.02	328.9	Positive	10	29	FALSE	2.8
Azoxystrobin	404.02	372	Positive	10	11	TRUE	2.8
Benalaxyl	326.1	91	Positive	25	30	FALSE	3.41
Benalaxyl	326.1	148	Positive	25	20	TRUE	3.41
Bendiocarb	224.11	109	Positive	15	15	TRUE	1.97
Bendiocarb	224.11	167	Positive	15	10	FALSE	1.97
Benzoximate	364	105	Positive	5	25	FALSE	3.6
Benzoximate	364	199.1	Positive	5	10	TRUE	3.6
Bifenazate	301.1	170	Positive	30	20	FALSE	2.97
Bifenazate	301.1	198	Positive	30	5	TRUE	2.97
Bitertanol	338.2	69.97	Positive	6	6	FALSE	3.3
Bitertanol	338.2	99.1	Positive	6	12	TRUE	3.3
Bitertanol	338.2	269.3	Positive	6	8	FALSE	3.3
Bromuconazole I	376	70.1	Positive	15	20	FALSE	2.87
Bromuconazole I	376	158.9	Positive	15	30	TRUE	2.87
Bupirimate	317.11	108.09	Positive	35	27	TRUE	3.15
Bupirimate	317.11	166.03	Positive	35	24	FALSE	3.15
Buprofezin	306.1	115.9	Positive	20	16	FALSE	3.94
Buprofezin	306.1	201	Positive	20	12	TRUE	3.94
Butafenacil	492	180	Positive	25	35	FALSE	3.21
Butafenacil	492	331	Positive	25	25	TRUE	3.21
Butocarboxim	213	75	Positive	30	15	TRUE	1.68
Butocarboxim	213	156	Positive	30	10	FALSE	1.68
Carbaryl	202	117	Positive	25	25	FALSE	2.09
Carbaryl	202	145	Positive	25	10	TRUE	2.09
Carbendazim	192.1	132.1	Positive	10	30	FALSE	1.22

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Carbendazim	192.1	160.1	Positive	10	15	TRUE	1.22
Carbetamide	237	118	Positive	5	15	TRUE	1.78
Carbetamide	237	192	Positive	5	10	FALSE	1.78
Carbofuran	222.11	123	Positive	5	20	FALSE	2.01
Carbofuran	222.11	165.1	Positive	5	10	TRUE	2.01
Carbofuran-3-hydroxyl	238	163	Positive	34	16	FALSE	1.48
Carbofuran-3-hydroxyl	238	181	Positive	34	10	TRUE	1.48
Carboxin	236	87	Positive	5	25	FALSE	2.13
Carboxin	236	143	Positive	5	15	TRUE	2.13
Carfentrazone-ethyl	412	346	Positive	55	24	TRUE	3.31
Carfentrazone-ethyl	412	366	Positive	55	18	FALSE	3.31
Chlorantraniliprole	481.6	283.9	Positive	15	23	TRUE	2.6
Chlorantraniliprole	481.6	450.9	Positive	15	25	FALSE	2.6
Chlorfluazuron	539.8	158	Positive	35	15	FALSE	4.18
Chlorfluazuron	539.8	382.9	Positive	35	20	TRUE	4.18
Chloroxuron	291.11	72.02	Positive	25	20	TRUE	2.81
Chloroxuron	291.11	164.1	Positive	25	15	FALSE	2.81
Clethodim	360.1	164	Positive	38	24	TRUE	3.77
Clethodim	360.1	268.1	Positive	38	16	FALSE	3.77
Clofentezine	303	102	Positive	20	35	FALSE	3.45
Clofentezine	303	138	Positive	20	15	TRUE	3.45
Clothianidin	250	132	Positive	25	15	FALSE	1.43
Clothianidin	250	169	Positive	25	10	TRUE	1.43
Cyazofamid	325	107.9	Positive	25	15	TRUE	3.21
Cyazofamid	325	261	Positive	25	10	FALSE	3.21
Cycluron	199	69.2	Positive	15	20	FALSE	2.3
Cycluron	199	89.1	Positive	15	15	TRUE	2.3
Cymoxanil	199.032	110.896	Positive	15	14	FALSE	1.63
Cymoxanil	199.032	127.875	Positive	15	10	TRUE	1.63
Cyproconazole I	292.2	70.2	Positive	5	20	TRUE	2.85
Cyproconazole I	292.2	125.1	Positive	5	30	FALSE	2.85
Cyprodinil	226.06	93	Positive	20	29	TRUE	3.05
Cyprodinil	226.06	108	Positive	20	24	FALSE	3.05
Cyromazine	167	60.2	Positive	40	20	TRUE	0.83
Cyromazine	167	84.896	Positive	40	12	FALSE	0.83
Demeton-S-methyl-sulfon	263	121	Positive	20	15	FALSE	1.3
Demeton-S-methyl-sulfon	263	169	Positive	20	15	TRUE	1.3
Diclobutrazol	328	70	Positive	15	20	TRUE	3.14
Diclobutrazol	328	158.9	Positive	15	38	FALSE	3.14
Dicrotophos	238	112	Positive	30	10	TRUE	1.33
Dicrotophos	238	193	Positive	30	10	FALSE	1.33
Diethofencarb	268	124	Positive	10	30	FALSE	2.69
Diethofencarb	268	226	Positive	10	10	TRUE	2.69
Difenoconazole	406.16	111.01	Positive	8	58	FALSE	3.49
Difenoconazole	406.16	251.02	Positive	8	24	TRUE	3.49
Diflubenzuron	311.03	141.1	Positive	25	30	FALSE	3.06
Diflubenzuron	311.03	158.15	Positive	25	15	TRUE	3.06

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Dimethoate	230.07	125.02	Positive	15	20	FALSE	1.51
Dimethoate	230.07	198.89	Positive	15	10	TRUE	1.51
Dimethomorph I	388.1	165	Positive	15	30	FALSE	2.77
Dimethomorph I	388.1	300.9	Positive	15	20	TRUE	2.77
Dimoxystrobin	327.1	116.1	Positive	20	20	TRUE	3.19
Dimoxystrobin	327.1	205.2	Positive	20	20	FALSE	3.19
Diniconazole	326.1	70.2	Positive	10	25	TRUE	3.36
Diniconazole	326.1	159	Positive	10	30	FALSE	3.36
Dinotefuran	203	113	Positive	15	10	FALSE	1.08
Dinotefuran	203	129	Positive	15	10	TRUE	1.08
Dioxacarb	224.1	123.1	Positive	10	16	FALSE	1.52
Dioxacarb	224.1	167.1	Positive	10	8	TRUE	1.52
Disulfoton sulphoxide	291	97	Positive	25	30	FALSE	2.23
Disulfoton sulphoxide	291	185	Positive	25	15	TRUE	2.23
Diuron	233	72	Positive	25	18	TRUE	2.15
Diuron	233	159.9	Positive	25	25	FALSE	2.15
Doramectin	916.6	331.2	Positive	15	23	TRUE	4.38
Doramectin	916.6	593.4	Positive	15	14	FALSE	4.38
Emamectin benzoate	886.6	82	Positive	20	72	FALSE	3.89
Emamectin benzoate	886.6	126	Positive	20	30	FALSE	3.89
Emamectin benzoate	886.6	158	Positive	20	35	TRUE	3.89
Epoxiconazole	330	101	Positive	40	40	FALSE	2.99
Epoxiconazole	330	121.04	Positive	40	20	TRUE	2.99
Eprinomectin	915.6	144	Positive	10	41	FALSE	4.29
Eprinomectin	915.6	186	Positive	10	35	TRUE	4.29
Etaconazole I	327.93	158.97	Positive	65	32	TRUE	2.97
Etaconazole I	327.93	204.81	Positive	65	17	FALSE	2.97
Ethiofencarb	226.1	107	Positive	10	15	TRUE	2.18
Ethiofencarb	226.1	164	Positive	10	10	FALSE	2.18
Ethiprole	414.1	350.9	Positive	10	25	FALSE	2.76
Ethiprole	414.1	396.9	Positive	10	9	TRUE	2.76
Ethirimol	210.1	98	Positive	5	25	FALSE	1.56
Ethirimol	210.1	140	Positive	5	20	TRUE	1.56
Ethofumesate	287.1	121.1	Positive	25	15	TRUE	2.83
Ethofumesate	287.1	259.1	Positive	25	10	FALSE	2.83
Etoxazole	360.2	57.2	Positive	60	25	FALSE	4.12
Etoxazole	360.2	141.1	Positive	60	25	TRUE	4.12
Famoxadone	392.2	238	Positive	5	15	FALSE	3.44
Famoxadone	392.2	331.1	Positive	5	10	TRUE	3.44
Fenamidone	312.1	92	Positive	5	25	TRUE	2.8
Fenamidone	312.1	236.1	Positive	5	14	FALSE	2.8
Fenarimol	331	81	Positive	40	30	TRUE	2.88
Fenarimol	331	268	Positive	40	25	FALSE	2.88
Fenazaquin	307.2	57.2	Positive	5	20	TRUE	4.16
Fenazaquin	307.2	161	Positive	5	15	FALSE	4.16
Fenbuconazole	337	70.1	Positive	15	20	TRUE	3.11

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Fenbuconazole	337	125	Positive	15	30	FALSE	3.11
Fenhexamid	301.986	55.181	Positive	35	35	FALSE	3
Fenhexamid	301.986	97.117	Positive	35	25	TRUE	3
Fenobucarb	207.89	95.07	Positive	15	15	TRUE	2.6
Fenobucarb	207.89	152	Positive	30	15	FALSE	2.6
Fenoxycarb	302.1	88	Positive	10	20	TRUE	3.12
Fenoxycarb	302.1	116.1	Positive	10	11	FALSE	3.12
Fenpropimorph	304.2	57.2	Positive	25	30	FALSE	2.6
Fenpropimorph	304.2	147.1	Positive	25	30	TRUE	2.6
Fenpyroximate	422.1	138.05	Positive	30	32	FALSE	4.16
Fenpyroximate	422.1	366.1	Positive	30	15	TRUE	4.16
Fenuron	165	45.9	Positive	15	15	FALSE	1.47
Fenuron	165	71.9	Positive	15	15	TRUE	1.47
Fipronil	435.1	249.81	Negative	50	27	FALSE	3.28
Fipronil	435.1	329.75	Negative	50	15	TRUE	3.28
Fipronil desulfinyl	386.9	282	Negative	35	30	FALSE	3.29
Fipronil desulfinyl	386.9	351	Negative	35	15	TRUE	3.29
Fipronil sulfide	418.9	262	Negative	10	25	TRUE	3.44
Fipronil sulfide	418.9	383	Negative	10	20	FALSE	3.44
Fipronil sulfone	451	282	Negative	30	27	FALSE	3.5
Fipronil sulfone	451	415	Negative	30	16	TRUE	3.5
Flonicamid	230.1	174	Positive	45	16	FALSE	1.31
Flonicamid	230.1	203	Positive	45	16	TRUE	1.31
Fluazinam	462.81	397.8	Negative	50	16	FALSE	3.89
Fluazinam	462.81	415.7	Negative	50	19	TRUE	3.89
Flubendiamide	680.84	253.974	Negative	28	30	TRUE	3.38
Flubendiamide	680.84	273.996	Negative	28	18	FALSE	3.38
Fludioxonil	246.7	126	Negative	40	32	TRUE	2.67
Fludioxonil	246.7	179.9	Negative	40	32	FALSE	2.67
Flufenacet	364	152.1	Positive	5	20	TRUE	3.13
Flufenacet	364	194.1	Positive	5	11	FALSE	3.13
Flufenoxuron	489	141	Positive	30	40	FALSE	4.07
Flufenoxuron	489	158	Positive	30	20	TRUE	4.07
Fluometuron	233	46.4	Positive	30	15	FALSE	2.15
Fluometuron	233	72.2	Positive	30	15	TRUE	2.15
Fluoxastrobin	459	188	Positive	40	35	FALSE	3.13
Fluoxastrobin	459	427	Positive	40	15	TRUE	3.13
Fluquinconazole	376	306.9	Positive	25	25	FALSE	2.95
Fluquinconazole	376	348.8	Positive	25	20	TRUE	2.95
Flusilazole	316	165	Positive	5	25	TRUE	3.1
Flusilazole	316	247	Positive	5	20	FALSE	3.1
Flutolanil	324.1	65	Positive	25	35	FALSE	2.97
Flutolanil	324.1	262.1	Positive	25	20	TRUE	2.97
Flutriafol	302.1	70.1	Positive	30	15	TRUE	2.24
Flutriafol	302.1	122.9	Positive	30	25	FALSE	2.24
Fonofos	247	109	Positive	20	20	FALSE	3.41

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Fonofos	247	137	Positive	20	10	TRUE	3.41
Forchlorfenuron	248.1	93	Positive	25	35	FALSE	2.24
Forchlorfenuron	248.1	129	Positive	25	15	TRUE	2.24
Formetanate	222.01	46	Positive	30	26	FALSE	1.01
Formetanate	222.01	165	Positive	30	15	TRUE	1.01
Fuberidazole	185	156	Positive	10	26	FALSE	1.35
Fuberidazole	185	157	Positive	10	21	TRUE	1.35
Furalaxyl	302.1	95	Positive	10	25	TRUE	2.72
Furalaxyl	302.1	242.1	Positive	10	15	FALSE	2.72
Furathiocarb	383.2	194.9	Positive	20	15	TRUE	3.91
Furathiocarb	383.2	252	Positive	20	10	FALSE	3.91
Halofenozide	331.1	104.9	Positive	10	15	TRUE	2.75
Halofenozide	331.1	275	Positive	10	5	FALSE	2.75
Haloxyfop	360	288	Negative	15	15	TRUE	3.13
Haloxyfop	362	290	Negative	15	15	FALSE	3.13
Hexaconazole	314.1	70.1	Positive	30	20	TRUE	3.26
Hexaconazole	314.1	158.8	Positive	30	40	FALSE	3.26
Hexaflumuron	459.1	175	Negative	5	30	TRUE	3.65
Hexaflumuron	459.1	276.1	Negative	5	15	FALSE	3.65
Hexythiazox	353	168.1	Positive	10	25	FALSE	4.01
Hexythiazox	353	228.1	Positive	10	15	TRUE	4.01
Imazalil	297.01	69.08	Positive	23	18	TRUE	2.15
Imazalil	297.01	158.88	Positive	23	22	FALSE	2.15
Imidacloprid	256.1	174.9	Positive	25	20	FALSE	1.45
Imidacloprid	256.1	209	Positive	25	12	TRUE	1.45
Indoxacarb	528.1	202.9	Positive	30	40	TRUE	3.68
Indoxacarb	528.1	217.9	Positive	30	20	FALSE	3.68
Ipconazole	334.2	70	Positive	50	25	TRUE	3.56
Ipconazole	334.2	125	Positive	50	25	FALSE	3.56
Iprovalicarb	321.1	119.1	Positive	20	20	TRUE	2.94
Iprovalicarb	321.1	203.1	Positive	20	10	FALSE	2.94
Isocarbofos	291.2	121	Positive	16	30	FALSE	2.51
Isocarbofos	291.2	215.1	Positive	16	8	FALSE	2.51
Isocarbofos	291.2	231	Positive	16	12	TRUE	2.51
Isoprocarb	193.99	95.09	Positive	15	13	TRUE	2.29
Isoprocarb	193.99	136.91	Positive	15	8	FALSE	2.29
Isoproturon	207	46	Positive	20	15	FALSE	2.29
Isoproturon	207	72	Positive	20	20	TRUE	2.29
Ivermectin	892.6	307.2	Positive	15	24	TRUE	4.45
Ivermectin	892.6	551.4	Positive	15	25	FALSE	4.45
Ivermectin	892.6	569.4	Positive	15	14	FALSE	4.45
Linuron	249	159.9	Positive	20	20	TRUE	2.64
Linuron	249	181.9	Positive	20	16	FALSE	2.64
Lufenuron	509	325.89	Negative	2	20	TRUE	3.96
Lufenuron	509	338.96	Negative	2	12	FALSE	3.96
Mandipropamid	411.8	125	Positive	35	35	FALSE	2.9

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Mandipropamid	411.8	328.1	Positive	35	15	TRUE	2.9
Mefenacet	299	120	Positive	5	25	FALSE	2.91
Mefenacet	299	148	Positive	5	15	TRUE	2.91
Mepanipyrim	224.1	77	Positive	15	35	FALSE	2.92
Mepanipyrim	224.1	106	Positive	15	25	TRUE	2.92
Mepronil	270.1	91	Positive	15	35	FALSE	2.94
Mepronil	270.1	119	Positive	15	25	TRUE	2.94
Mesotrione	340.1	104	Positive	30	30	FALSE	1.77
Mesotrione	340.1	228.1	Positive	30	15	TRUE	1.77
Metaflumizone	507.13	178	Positive	40	28	TRUE	3.89
Metaflumizone	507.13	287.1	Positive	45	22	FALSE	3.89
Metalaxyl	280.1	192.1	Positive	30	15	FALSE	2.39
Metalaxyl	280.1	220.1	Positive	30	15	TRUE	2.39
Metconazole	320	70	Positive	10	20	TRUE	3.31
Metconazole	320	125	Positive	10	35	FALSE	3.31
Methabenzthiazuron	222	150	Positive	10	30	FALSE	2.13
Methabenzthiazuron	222	165	Positive	10	15	TRUE	2.13
Methamidophos	141.9	93.9	Positive	30	12	TRUE	0.7
Methamidophos	141.9	124.8	Positive	30	14	FALSE	0.7
Methiocarb	226	121	Positive	25	20	FALSE	2.62
Methiocarb	226	169	Positive	25	10	TRUE	2.62
Methiocarb sulfone	258.07	107.1	Positive	40	35	FALSE	1.59
Methiocarb sulfone	258.07	122.1	Positive	40	20	TRUE	1.59
Methomyl	162.9	88	Positive	15	15	TRUE	1.24
Methomyl	162.9	105.9	Positive	15	15	FALSE	1.24
Methoprotryne	272.07	197.98	Positive	13	22	TRUE	2.37
Methoprotryne	272.07	240.05	Positive	13	18	FALSE	2.37
Methoxyfenozide	369.2	149.1	Positive	15	15	TRUE	2.99
Methoxyfenozide	369.2	313.23	Positive	5	10	FALSE	2.99
Metobromuron	259.1	148.1	Positive	25	15	TRUE	2.28
Metobromuron	259.1	170	Positive	25	20	FALSE	2.28
Metribuzin	215	89	Positive	5	20	FALSE	1.92
Metribuzin	215	131	Positive	5	20	TRUE	1.92
Mevinphos I	225.1	127.1	Positive	15	15	TRUE	1.48
Mevinphos I	225.1	193.1	Positive	15	10	FALSE	1.48
Mexacarbate	223.2	151	Positive	40	25	FALSE	1.59
Mexacarbate	223.2	166.1	Positive	40	15	TRUE	1.59
Monocrotophos	224.1	98	Positive	20	10	FALSE	1.25
Monocrotophos	224.1	109	Positive	20	30	FALSE	1.25
Monocrotophos	224.1	127	Positive	20	15	TRUE	1.25
Monolinuron	215.04	99	Positive	25	30	FALSE	2.17
Monolinuron	215.04	126	Positive	25	15	TRUE	2.17
Moxidectin	640.5	199	Positive	5	25	FALSE	4.36
Moxidectin	640.5	498.3	Positive	5	14	FALSE	4.36
Moxidectin	640.5	528.4	Positive	5	10	TRUE	4.36
Myclobutanil	289.1	70.2	Positive	25	15	TRUE	2.88

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Myclobutanil	289.1	125.1	Positive	25	30	FALSE	2.88
Neburon	275	57	Positive	15	20	FALSE	3.18
Neburon	275	88	Positive	15	15	TRUE	3.18
Nitenpyram	271.1	125.9	Positive	30	30	FALSE	1.21
Nitenpyram	271.1	225	Positive	30	10	TRUE	1.21
Novaluron	493.02	141	Positive	5	30	FALSE	3.75
Novaluron	493.02	158.03	Positive	5	15	TRUE	3.75
Nuarimol	315	81.1	Positive	25	15	FALSE	2.55
Nuarimol	315	252	Positive	25	20	TRUE	2.55
Omethoate	214	124.8	Positive	25	22	FALSE	1.01
Omethoate	214	182.8	Positive	25	10	TRUE	1.01
Oxadixyl	279.1	132.3	Positive	20	25	FALSE	1.86
Oxadixyl	279.1	219	Positive	20	12	TRUE	1.86
Oxamyl	237	72	Positive	15	10	TRUE	1.19
Oxamyl	237	90	Positive	15	10	FALSE	1.19
Paclobutrazol	294.1	70.2	Positive	10	20	TRUE	2.71
Paclobutrazol	294.1	125.1	Positive	10	35	FALSE	2.71
Penconazole	284	70.1	Positive	15	15	TRUE	3.18
Penconazole	284	159	Positive	15	25	FALSE	3.18
Pencycuron	329.1	124.9	Positive	30	30	TRUE	3.56
Pencycuron	329.1	218	Positive	30	16	FALSE	3.56
Phenmedipham	301	136	Positive	45	20	FALSE	2.58
Phenmedipham	301	168	Positive	45	10	TRUE	2.58
Picoxystrobin	368.01	145.07	Positive	13	24	TRUE	3.31
Picoxystrobin	368.01	205.06	Positive	13	8	FALSE	3.31
Piperonyl butoxide	356.3	119	Positive	20	35	FALSE	3.92
Piperonyl butoxide	356.3	176.9	Positive	20	10	TRUE	3.92
Pirimicarb	239.1	72	Positive	25	20	TRUE	1.81
Pirimicarb	239.1	182.1	Positive	25	15	FALSE	1.81
Pirimiphos Methyl	306.3	108.1	Positive	35	30	TRUE	3.57
Pirimiphos Methyl	306.3	164.1	Positive	35	20	FALSE	3.57
Prochloraz	376.03	70.1	Positive	25	25	FALSE	3.31
Prochloraz	376.03	307.9	Positive	25	10	TRUE	3.31
Promecarb	208.1	109	Positive	25	15	TRUE	2.72
Promecarb	208.1	151	Positive	25	10	FALSE	2.72
Prometon	226	86.3	Positive	15	30	FALSE	2.06
Prometon	226	184.3	Positive	15	20	TRUE	2.06
Prometryn	242	158	Positive	25	25	TRUE	2.73
Prometryn	242	200.1	Positive	25	18	FALSE	2.73
Propamocarb	189.1	102	Positive	15	15	TRUE	1.04
Propamocarb	189.1	144	Positive	15	10	FALSE	1.04
Propargite	368	57	Positive	15	15	FALSE	4.13
Propargite	368	175	Positive	15	15	FALSE	4.13
Propargite	368	231	Positive	15	10	TRUE	4.13
Propetamphos	282.09	138	Positive	45	20	TRUE	3.03
Propetamphos	282.09	156	Positive	45	15	FALSE	3.03

Analyte Name	Precursor (m/z)	Product (m/z)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Propiconazole	342.1	69.1	Positive	35	30	FALSE	3.3
Propiconazole	342.1	158.9	Positive	35	20	TRUE	3.3
Propoxur	210.1	92.9	Positive	15	25	FALSE	1.98
Propoxur	210.1	110.9	Positive	15	12	TRUE	1.98
Pymetrozine	218.1	79	Positive	25	25	FALSE	0.99
Pymetrozine	218.1	105	Positive	25	15	TRUE	0.99
Pyracarbolid	218.1	97.1	Positive	10	30	FALSE	2.05
Pyracarbolid	218.1	125.1	Positive	10	20	TRUE	2.05
Pyraclostrobin	388.17	163.1	Positive	18	24	FALSE	3.49
Pyraclostrobin	388.17	194.1	Positive	18	12	TRUE	3.49
Pyridaben	365.1	147.1	Positive	20	25	TRUE	4.25
Pyridaben	365.1	309.1	Positive	20	10	FALSE	4.25
Pyrimethanil	199.99	82.05	Positive	45	26	FALSE	2.46
Pyrimethanil	199.99	107.06	Positive	45	24	TRUE	2.46
Pyriproxyfen	322.2	95.9	Positive	15	15	TRUE	3.91
Pyriproxyfen	322.2	184.9	Positive	15	20	FALSE	3.91
Quinoxyfen	308	161.9	Positive	35	45	FALSE	3.84
Quinoxyfen	308	197	Positive	35	30	TRUE	3.84
Rotenone	395	192.1	Positive	10	20	FALSE	3.16
Rotenone	395	213.1	Positive	10	24	TRUE	3.16
Secbumeton	226.2	100.2	Positive	5	25	FALSE	2.04
Secbumeton	226.2	170.2	Positive	5	20	TRUE	2.04
Siduron	233.01	94.06	Positive	23	20	TRUE	2.62
Siduron	233.01	137.06	Positive	23	17	FALSE	2.62
Simetryn	214	95.9	Positive	15	25	FALSE	1.96
Simetryn	214	124	Positive	15	20	TRUE	1.96
Spinetoram (J)	748.53	98.07	Positive	60	35	FALSE	3.7
Spinetoram (J)	748.53	142.16	Positive	60	30	TRUE	3.7
Spinetoram (L)	760.53	98.07	Positive	34	66	FALSE	3.83
Spinetoram (L)	760.53	142.09	Positive	34	30	TRUE	3.83
Spinosad A	732.6	98.1	Positive	35	50	FALSE	3.43
Spinosad A	732.6	142	Positive	35	30	TRUE	3.43
Spinosad D	746.52	98.1	Positive	40	35	FALSE	3.6
Spinosad D	746.52	142	Positive	40	31	TRUE	3.6
Spirodiclofen	411.14	71.6	Positive	35	15	FALSE	4.26
Spirodiclofen	411.14	313.1	Positive	35	10	TRUE	4.26
Spiromesifen	371.1	255.1	Positive	35	25	FALSE	4.22
Spiromesifen	371.1	273.1	Positive	35	5	TRUE	4.22
Spirotetramat	374	302	Positive	20	30	FALSE	2.97
Spirotetramat	374	330	Positive	20	15	TRUE	2.97
Sulfentrazone	387	145.8	Positive	60	35	TRUE	2.15
Sulfentrazone	387	307	Positive	60	30	FALSE	2.15
Tebuconazole	308.2	70.1	Positive	30	30	TRUE	3.17
Tebuconazole	308.2	124.9	Positive	30	30	FALSE	3.17
Tebufenozide	353.3	133.07	Positive	2	16	TRUE	3.26
Tebufenozide	353.3	297.2	Positive	2	4	FALSE	3.26

Analyte Name	Precursor (*m/z*)	Product (*m/z*)	Polarity	Cone Voltage (V)	Collision Energy (V)	Quan	Retention Time (min)
Tebufenpyrad	334	117	Positive	15	25	FALSE	3.8
Tebufenpyrad	334	145	Positive	15	25	TRUE	3.8
Tebuthiuron	229	116	Positive	5	25	FALSE	1.85
Tebuthiuron	229	172	Positive	5	15	TRUE	1.85
Teflubenzuron	381	113	Positive	25	60	FALSE	3.71
Teflubenzuron	381	141	Positive	25	30	FALSE	3.71
Teflubenzuron	381	158	Positive	25	15	TRUE	3.71
Temephos	466.8	125	Positive	50	30	TRUE	3.95
Temephos	466.8	418.9	Positive	50	20	FALSE	3.95
Terbumeton	226.1	114.1	Positive	35	25	FALSE	2.04
Terbumeton	226.1	170.1	Positive	35	15	TRUE	2.04
Terbutryn	242.1	91	Positive	5	25	FALSE	2.79
Terbutryn	242.1	186.1	Positive	5	20	TRUE	2.79
Tetraconazole	372	70.1	Positive	15	20	FALSE	3
Tetraconazole	372	159	Positive	15	25	TRUE	3
Tetradifon	294	197.2	Positive	56	21	TRUE	2.89
Tetradifon	294	225	Positive	56	19	FALSE	2.89
Thiabendazole	202	130.9	Positive	45	30	FALSE	1.3
Thiabendazole	202	174.9	Positive	45	25	TRUE	1.3
Thiacloprid	253	90	Positive	35	40	FALSE	1.66
Thiacloprid	253	125.8	Positive	35	20	TRUE	1.66
Thiamethoxam	292	132	Positive	25	20	FALSE	1.31
Thiamethoxam	292	211.2	Positive	25	10	TRUE	1.31
Thidiazuron	221	102	Positive	10	15	TRUE	1.85
Thidiazuron	221	128	Positive	10	15	FALSE	1.85
Thiobencarb	258.1	89.1	Positive	25	45	FALSE	3.48
Thiobencarb	258.1	125.1	Positive	25	15	TRUE	3.48
Thiophanate methyl	343	151	Positive	25	20	TRUE	1.96
Thiophanate methyl	343	311	Positive	25	15	FALSE	1.96
Triadimefon	294.1	69.1	Positive	30	20	TRUE	2.89
Triadimefon	294.1	196.9	Positive	30	16	FALSE	2.89
Triadimenol	296.1	70	Positive	30	10	TRUE	2.78
Triadimenol	296.1	98.9	Positive	30	15	FALSE	2.78
Trichlorfon	256.9	79	Positive	25	30	FALSE	1.44
Trichlorfon	256.9	108.8	Positive	25	20	TRUE	1.44
Tricyclazole	190	136	Positive	10	25	FALSE	1.61
Tricyclazole	190	163	Positive	10	20	TRUE	1.61
Trifloxystrobin	409.2	145	Positive	25	40	FALSE	3.71
Trifloxystrobin	409.2	185.9	Positive	25	14	TRUE	3.71
Triflumizole	346.1	73.1	Positive	15	18	FALSE	3.56
Triflumizole	346.1	278	Positive	15	10	TRUE	3.56
Triflumuron	359	139.1	Positive	5	30	FALSE	3.4
Triflumuron	359	156.1	Positive	5	20	TRUE	3.4
Triticonazole	318.1	70.1	Positive	5	20	TRUE	2.91
Triticonazole	318.1	124.9	Positive	5	30	FALSE	2.91
Vamidothion	288	118	Positive	20	25	FALSE	1.45
Vamidothion	288	146	Positive	20	20	TRUE	1.45
Zoxamide	336.05	158.97	Positive	13	42	FALSE	3.4
Zoxamide	336.05	186.91	Positive	13	20	TRUE	3.4

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