

A generic approach for simultaneous detection and quantification of pesticides, veterinary drugs, and aflatoxin M1 in milk using LC-MS/MS

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Goal

This study is aimed to simultaneously detect and quantify multi-class pesticides, veterinary drugs, and aflatoxin M1 in milk using liquid chromatography-tandem mass spectrometry. The optimized method performance was verified following SANTE 12682/2019, 2002/657/EC, and EC 1881/2006 guidelines.

Introduction

India is the second largest milk producer in the world with 187 million tons produced in 2018–2019.¹ The health of the animals and good quality feed are equally important for good milk production. Veterinary medicines are used to treat bacterial infections, fungal infections, and parasites in the animals and to increase milk yields. Overuse of veterinary medicines in food-producing animals is a potential cause for an increase in antimicrobial resistance and their residues in the food chain.



On the other hand, pesticides are chemicals used to control pests, fungi, and weeds to protect crops, including those used as animal feed. The most frequently detected residues in milk according to the literature are organochlorine pesticides, organophosphorus pesticides, and synthetic pyrethroids.^{2,3} Most of these compounds are GC-amenable, whereas very few (ethion, malathion, and profenofos) are LC-amenable. Bedi et al reported animal feed and water to be the most prevalent source of pesticide residues in milk.² The Food Safety and Standards Authority of India (FSSAI) and the European Union have set the maximum residue limits for pesticides and aflatoxins as well as the minimum required performance limit (MRPL) for banned drugs.^{4,5} Therefore, monitoring of these toxic compounds becomes essential. In this study we used liquid chromatography coupled with tandem mass spectrometry to develop a method for LC-amenable compounds enabling laboratories to broaden their analytical scope and more accurately

determine and control the number and levels of residues and contaminants in milk produced in India.⁶ Existing methods for veterinary medicines/drugs are typically class specific, while methods for pesticides and mycotoxins are mostly multi-residue. Each of these three groups of compounds tends to use specific extraction protocols, which require different methods thus increasing analysis time, turn-around time, and cost of analysis. To address these challenges, we set a goal to develop a generic approach for the simultaneous extraction of pesticides, veterinary medicines/drugs, and aflatoxin M1 followed by a single combined LC-MS/MS analysis. The optimized method was validated following the SANTE/12682/2019, 2002/657/EC and EC 1881/2006 guidelines.⁷⁻⁹

Experimental

Chemicals, apparatus, and consumables

- Fisher Scientific™ Acetonitrile, Optima™ LC/MS grade (P/N A955-4)
- Fisher Scientific™ Water, Optima™ LC/MS grade (P/N W6-4)
- Fisher Scientific™ Methanol, Optima™ LC/MS grade (P/N A456-4)
- Fisher Scientific™ Ammonium formate, Optima™ LC/MS grade (P/N A11550)
- Fisher Scientific™ Formic acid, 99% Optima™ LC/MS grade (P/N A117-50)
- Analytical balance (ACZET, CY2202) and precision balance (ACZET, CY205C, San Diego, CA)
- Thermo Scientific™ Vortex mixer
- Thermo Scientific™ Sorvall™ ST 8 refrigerated centrifuge
- Thermo Scientific™ Variable volume micropipettes
- Thermo Fisher™ Ammonium oxalate (P/N A679-500)
- Thermo Fisher™ EDTA (P/N 15576028)
- Thermo Fisher™ Anhydrous sodium sulfate (P/N S421-500)

- Thermo Scientific™ HyperSep™ Dispersive SPE Mylar™ Pouches (QuEChERS), 500 mg CEC18, slim line pouch with 50 mL centrifuge tubes (P/N 60105-367-SP)
- Thermo Scientific™ 50 mL extraction tubes (P/N 339652)
- Nitrogen evaporator, PCI Analytics (P/N 18FVOCT384)

Sample preparation

A fresh milk sample was collected from a farm known to produce little to no amount of incurred aflatoxin M1 as well as antibiotics contamination. Analysis of the control/blank samples verified the absence of targeted pesticides, veterinary medicines/drugs, and aflatoxin M1 from the system itself as well as the solvents and additives. The same sample was utilized for recovery and precision experiments as well as matrix-matched standards preparation (Table 1).

Sample extraction and clean-up

Protocol: Veterinary drug explorer (VDX)⁶

- Weigh 4 g of the milk sample in a 50 mL falcon tube (spiking performed at this step).
- Add 10 mL acidified acetonitrile (1% acetic acid), vortex for 1 min at 2500 rpm.
- Add ammonium oxalate/EDTA solution (1 mL).
- Add 3 g sodium sulfate, shake well, and vortex for 5 min at 2500 rpm.
- Centrifuge at 4500 rpm for 5 min.
- Decant 8 mL of the supernatant into a 15 mL falcon tube.
- Add 500 mg C₁₈ material into the tube.
- Vortex and centrifuge at 4500 rpm for 10 min.
- Evaporate 5 mL of supernatant to dryness using the nitrogen evaporator.
- Reconstitute in 1 mL with water/methanol/acetonitrile (70:15:15)
- Inject into the LC-MS/MS system.
 - A method with procedural standard
 - A method with matrix-matched standards

Table 1. Spiked concentrations for recovery experiment and linearity range for pesticides, veterinary medicines/drugs, and aflatoxin M1

Recovery and linearity	Pesticides (mg/kg)	Sulfonamides, anthelmintic, quinolones-1 (µg/kg)	Tetracyclines, quinolones-2 (µg/kg)	Nitroimidazole, chloramphenicol (µg/kg)	Aflatoxin M1 (µg/kg)
Spike Level-1	0.005	5.0	25.0	0.25	0.025
Spike Level-2	0.010	10.0	50.0	0.5	0.05
Spike Level-3	0.025	25.0	100.0	1.0	0.1
Linearity	0.001 to 0.10	1.0 to 100.0	10.0 to 250.0	0.1 to 10.0	0.01 to 5.0

LC-MS/MS analysis

An ultra-high-performance liquid chromatography system (Thermo Scientific™ Vanquish™ UHPLC Flex system) was coupled with a tandem mass spectrometer (Thermo Scientific™ TSQ Quantis™ mass spectrometer) with heated electrospray ionization (HESI). The optimized LC-MS/MS conditions are given in Table 2. The UHPLC gradient program was from a previously reported application note.⁶

Table 2a. LC instrument conditions

Liquid chromatography method				
Instrumentation	Thermo Scientific™ Vanquish™ Flex Binary UHPLC system (P/N VF-P10-A), consisting of: <ul style="list-style-type: none">• Vanquish Split Sampler FT, P/N VF-A10-A• Vanquish Column Compartment, P/N VH-C10-A• Vanquish Pump Mixer Set, Vanquish F Pumps, P/N 6044.3870			
Column	Thermo Scientific™, Accucore™ aQ column, 100 mm × 2.1 mm, 2.6 μm (P/N 17326-102130)			
Sample compartment temp.	15 °C			
Column oven temp.	40 °C (Still air)			
Injection volume	10 μL			
Needle wash	80% methanol and 20% water			
Mobile phases	A: 1 mM HCOONH ₄ + 0.1% formic acid in H ₂ O B: 1 mM HCOONH ₄ + 0.1% formic acid in CH ₃ OH			
Set inline filter (mixer)	35 μL, VF-P1 (10 μL mixer kit)			
Total run time	17 min			
LC gradient program	<i>Time (min)</i>	<i>Flow rate (mL/min)</i>	<i>%B</i>	<i>Curve</i>
	0.0	0.3	5	5
	1.0	0.3	5	5
	9.0	0.3	100	5
	13.0	0.3	100	5
	13.5	0.3	5	5
17.0	0.3	5	5	

Table 2b. MS/MS instrument conditions

Mass spectrometry method	
Instrumentation	TSQ Quantis triple quadrupole mass spectrometer
Method type	Acquisition-Timed (t-SRM mode)
Ion source type	H-ESI II
Spray voltage	Static Positive: 3,700 V Negative: 2,500 V
Polarity switching	Yes
Sheath gas	50 Arb
Aux gas	10 Arb
Sweep gas	1 Arb
Ion transfer tube temp.	310 °C
Vaporizer temp.	350 °C

Data acquisition and processing

Data acquisition and processing were carried out using Thermo Scientific™ TraceFinder™ software, version 4.1. The data was acquired in in timed selected reaction monitoring (t-SRM) mode with polarity switching, which includes two transitions per analyte. The target list of analytes is given in Appendix 2 with their transitions, collision energies, and retention time (min). For data processing, two transitions per analyte, retention time (±0.1 min), ion ratio (±30%), linearity (>0.99 with residuals ±20%), recovery (70–120%) and precision (±20%) were set as acceptance criteria as per the SANTE guideline, 2002/657/EC, and EC 1881/2006 guideline⁷⁻⁹.

Results and discussion

Sample preparation

As milk is a high-fat food matrix, a 4 g sample size was selected for extraction.⁶ The VDX method was validated using matrix-matched standards and procedural standard (PS) calibration, whereby samples are spiked with known amounts of analytes before extraction. Using PS calibration, 251 (>94% analytes) of the 266 analytes gave recoveries within 70 to 120% maintaining less than 20% RSD. The recovery of analytes using PS calibration was higher compared to the use of matrix-standards because PS calibration will correct for any losses of analytes during extraction and clean-up (Figure 1).

The VDX protocol with the PS calibration approach was selected for further method validation because it yielded the highest number of analytes with acceptable accuracy and precision values. To comply with the stringent regulatory requirement of EU and FSSAI (India) for pesticides, veterinary drugs, and aflatoxin M1, the dSPE (dispersive solid phase extraction) C₁₈ cleaned extract was concentrated by using nitrogen gas and reconstitution to 1 mL to improve the limits of quantitation.

LC-MS/MS analysis

The reversed-phase Accucore aQ column chemistry offered acceptable retention for polar and early eluting analytes with good peak shapes in the highly aqueous phase. The liquid chromatographic method developed for the Thermo Scientific™ VetDrugs Explorer analytical workflow, provides excellent separation and peak shape for a large number of multi-class target veterinary drug residues, with minimal isobaric interferences from matrix³. The extracted ion chromatogram (XIC) is shown for selected compounds (Figure 2).

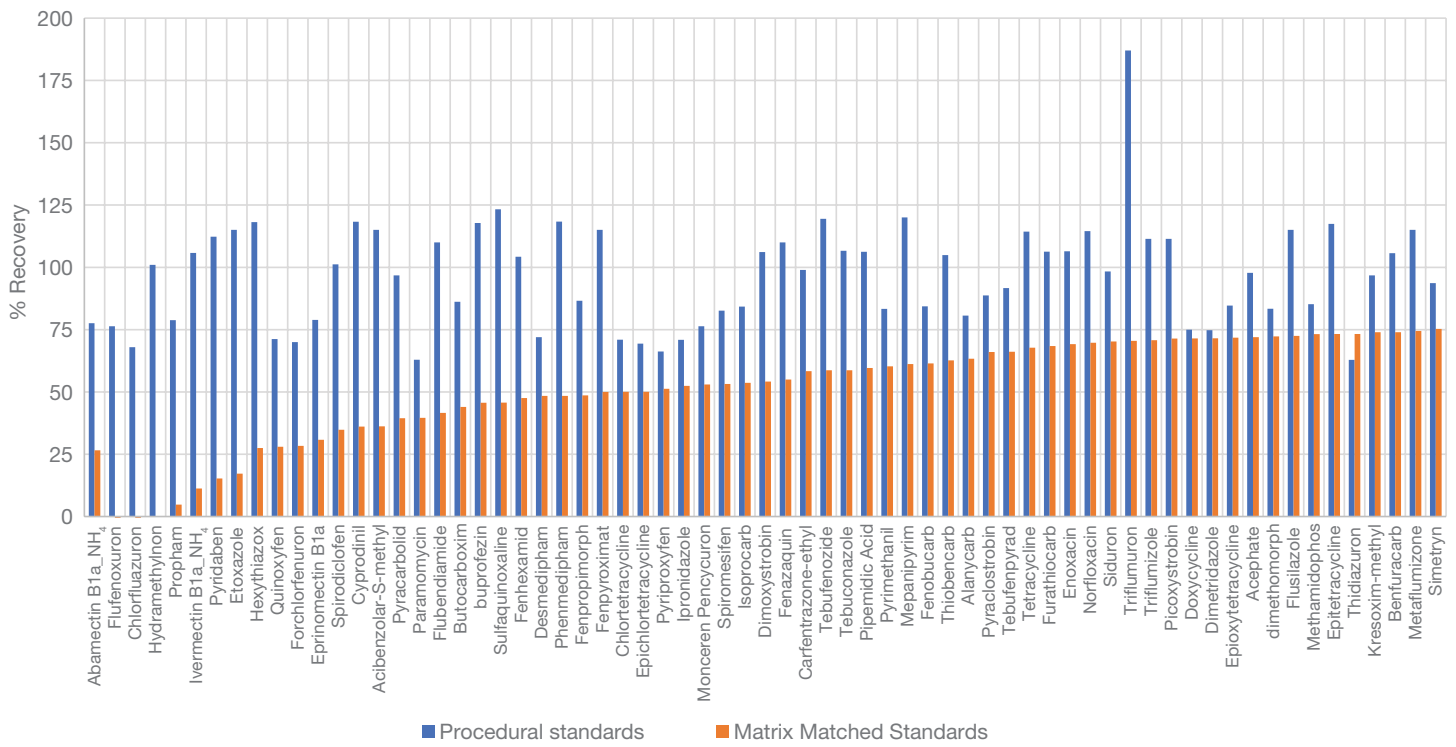


Figure 1. Impact of procedural standards vs matrix-matched standards on recoveries of selected target compounds

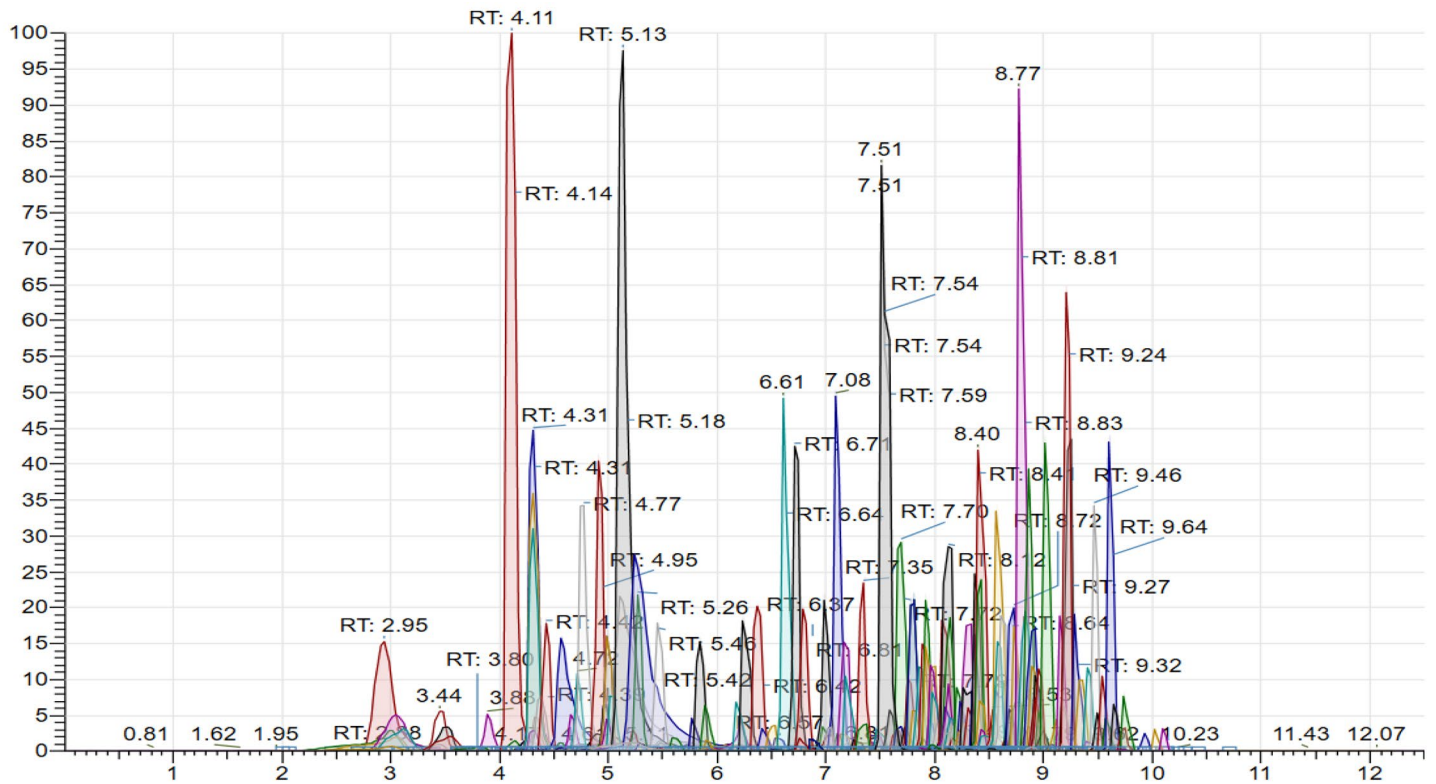


Figure 2. Extracted ion chromatogram of target analytes displayed in TraceFinder software at the recovery level-1

A representation of auto-optimized dwell times with the number of transitions per cycle is shown in Figure 3. The TSQ Quantis instrument control has a provision in t-SRM mode to auto-optimize the dwell time instead of performing it manually. This feature is useful when the laboratory needs to analyze hundreds of analytes in a single method. Cycle times maintain a consistent scan rate, which in addition to water dilution, enable symmetrical and sharp peak shapes with the help of Accucore aQ C18 chemistry. The analytes were distributed predominantly between 4 and 12 min. Automatically optimized dwell times were in the range of 2 to 46 ms per transition and offered more than 12 data points per peak, which allowed for accurate quantitative analysis. A representation of a few compounds with a minimum dwell time of 2.8 ms offered good peak shape even at low concentration levels such as 0.001 mg/kg as shown in Figure 4.

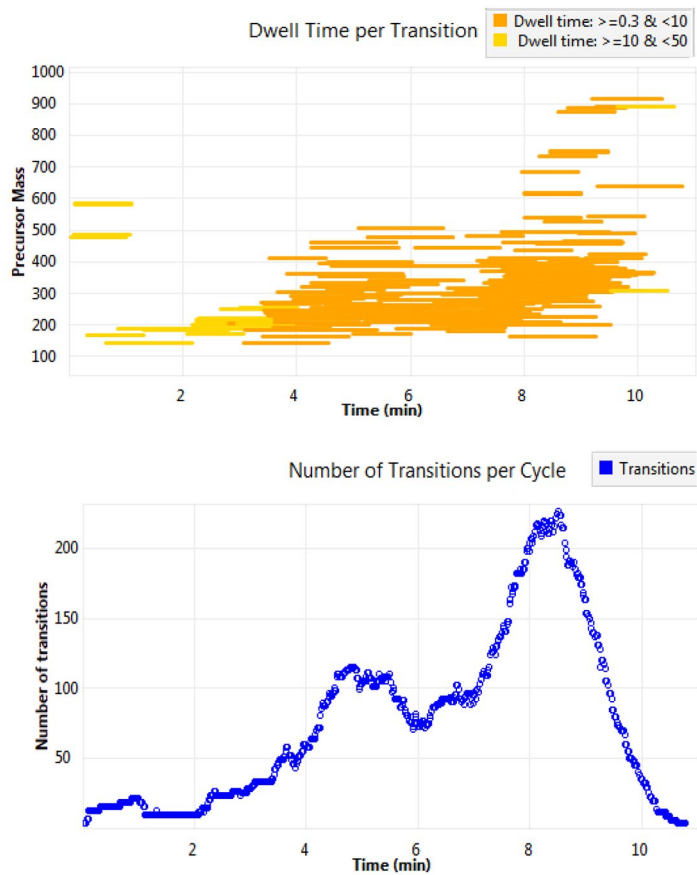
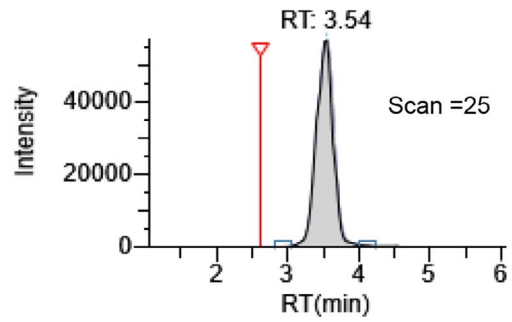
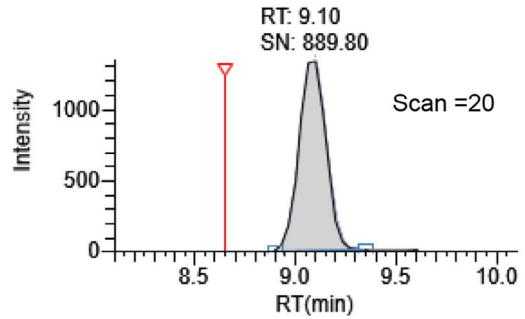


Figure 3. Representation of SRM transitions with auto-optimized dwell times

Milk_Recovery_Level_1_1 Aldicarb Sulfoxide m



Milk_PS_Level_1 Emamectin-benzoate m/z: 158.200



Milk_PS_Level_1 Forchlorfenuron m/z: 128.970

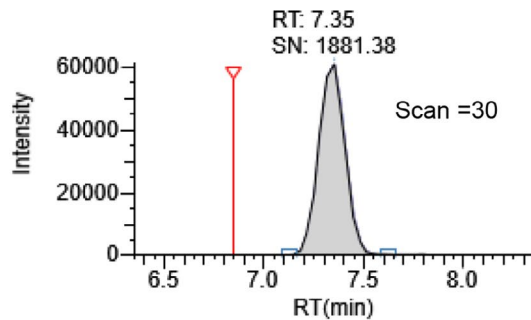


Figure 4. Extracted ion chromatograms (XIC) for representative analytes at the lowest concentration of 0.001 mg/kg

Polarity switching

For this analysis, most analytes perform best in the positive mode, with just a few providing the best response in the negative mode. Instead of requiring a separate analysis, polarity switching was performed in the t-SRM mode. Polarity switching time was <20 ms, and in total 650 MS/MS transitions were included in the acquisition program. Fenbuconazole and fipronil, which eluted very close together (near 8.35 min), were acquired in the positive and negative modes, respectively (Figure 5). The fast polarity switching capability allowing the acquisition of positive mode and negative mode compounds in the same analytical run, instead of two separate runs, increases laboratory throughput.

Identification and quantitation

As per pre-defined parameters, the data was processed with the automatic flagging feature in TraceFinder software. These flags are color-coded, so it is easy to automatically determine whether results pass or fail against the predefined acceptance criteria in the processing method.

Those results passing all the pre-defined criteria are shown with a green flag (Figure 6), which minimizes the time required for manual review of results. Red-colored flags indicate that there is an additional requirement of further investigation based on the reason provided by the flags. The identification and confirmation criteria have been demonstrated for abamectin (Figure 6) with two transitions,

i.e., m/z 890.526→305.238 (quantifier ion), m/z 890.526→567.304 and m/z 890.526→307.238 (qualifier ions), at a retention time of 9.75 ± 0.1 min and ion ratio within 30% in comparison with the procedural standards (Figure 6A and B). Furthermore, the quantitation was performed based on the procedural standards curve plotted in the range of 0.001–0.1 mg/kg. This calibration curve offered excellent linearity ($r^2=0.9959$) with <14% residuals by following $1/x$ weighting function and linear fit equation (Figure 6C).

Method performance

In this method, the procedural calibration standards linearity was plotted for pesticides, veterinary medicines/drugs, and aflatoxin M1 in the range mentioned in Table 1. Excellent correlation coefficients (>0.99) with <20% residuals for all the target analytes were observed in both solvents as well as in matrix, using a $1/x$ weighting factor. The lowest calibration level showed good sensitivity with $\geq 10:1$ signal-to-noise ratio. As per the extraction protocol (VDX with procedural standards), the sample was concentrated (2x), and recovery was calculated using procedural standards. The limit of quantitation (LOQ) for pesticides observed in milk was 0.005 mg/kg with recovery between 70 and 120% and <20% RSD ($n=6$), but different for veterinary drugs and aflatoxin as mentioned in Table 1. Representative extracted ion chromatograms of recovery level-1 (LOQ) are shown in Figure 7.

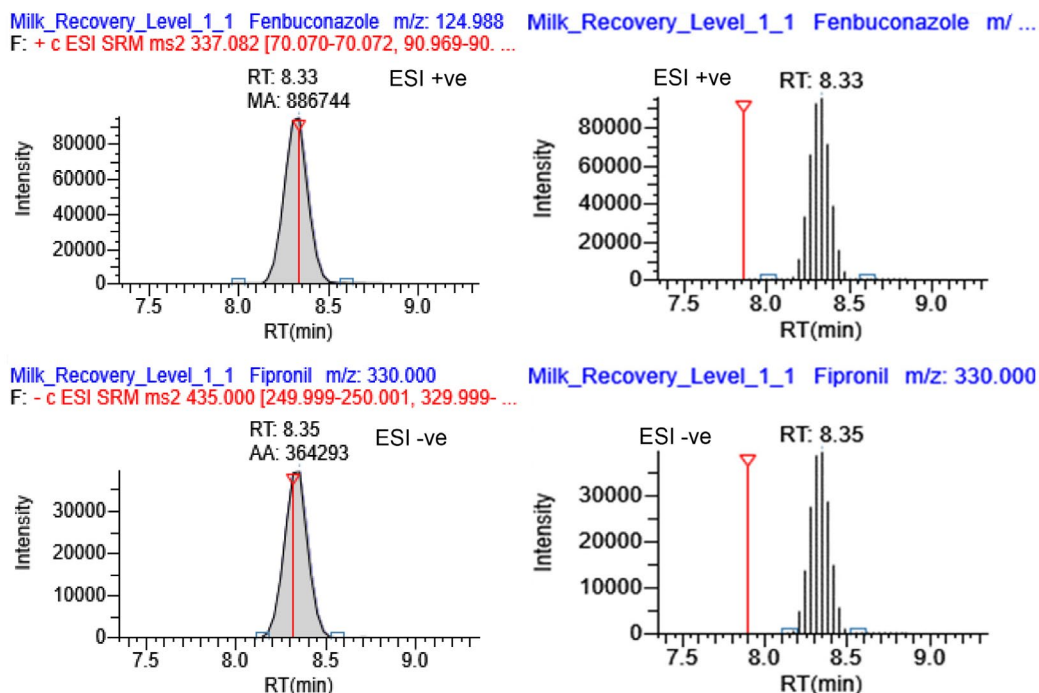


Figure 5. Impact of optimized dwell time and polarity switching on the data points per peak at 0.001 mg/kg

(A)

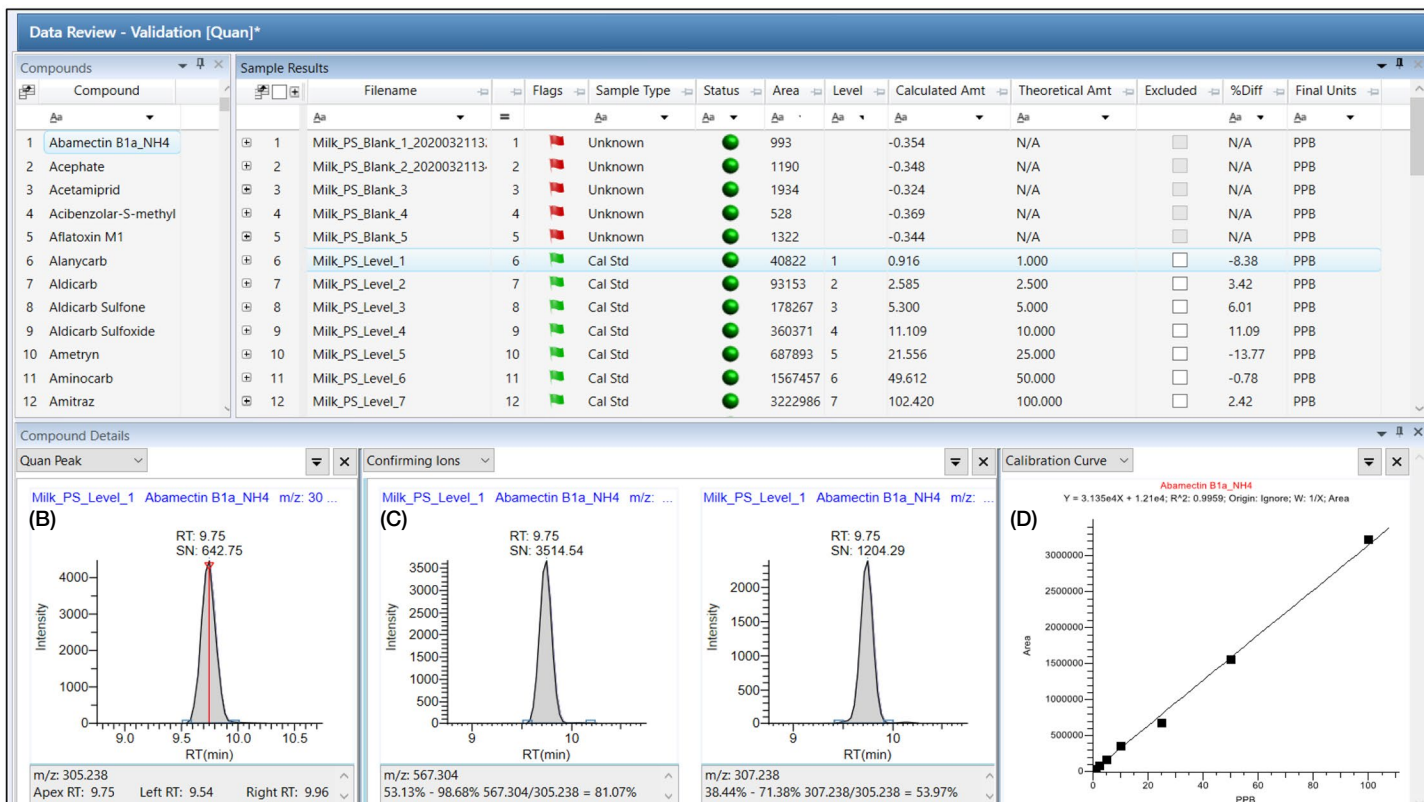


Figure 6. (A) Table showing the processed data with flagging, i.e., red and green flags, (B) Extracted ion chromatogram for quantifier ion of abamectin, (C) identification based on qualifier ions with ion ratio at 0.001 mg/kg, and (D) calibration curve

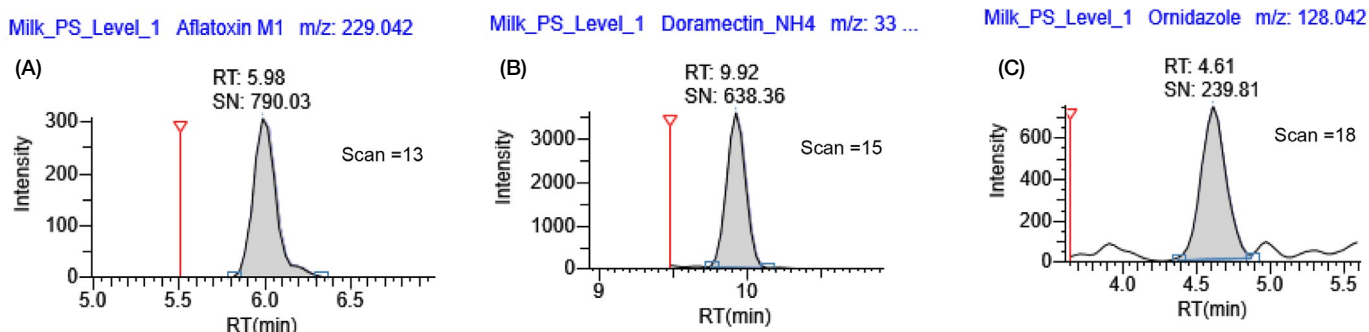


Figure 7. (A) Extracted ion chromatogram (XIC) for quantifier ion of aflatoxin M1 (0.025 µg/kg), (B) doramectin (5.0 µg/kg), and (C) ornidazole (0.25 µg/kg) spiked in the milk sample at LOQ (level 1)

The recovery experiment was carried out for pesticides, veterinary drugs, and aflatoxin M1 at Level 1 (LOQ), Level 2 and Level 3 with six replicates each to demonstrate the performance of the method in terms of accuracy and precision (n=6). The quantitation was performed against the matrix extracted standards (MES)/procedural standard (PS) calibration curve. Average recoveries were observed in the range of 72 to 120% with <15% RSD and ion ratios were within ±30%. A few analytes showed recoveries in the range of 120 to 135% (above the acceptable limit), but the precision and ion ratios were <15% and <±30%, respectively. The accuracy and precision observed

were represented for veterinary drugs, aflatoxin M1, and pesticides (Appendix 1). Overall, the validation data is within the acceptance criteria of validation guidelines.⁷⁻⁹ Also, the robustness of the method was assessed in terms of area precision by injecting 100 injections of spiked milk samples at level 1. The area repeatability was <15% RSD without internal standard correction and <±0.05 min for the retention time in the milk matrix (n=100 injections). This reveals that the optimized method provided excellent repeatability in results. Compound peak area repeatability examples are shown in Figures 8 and 9.

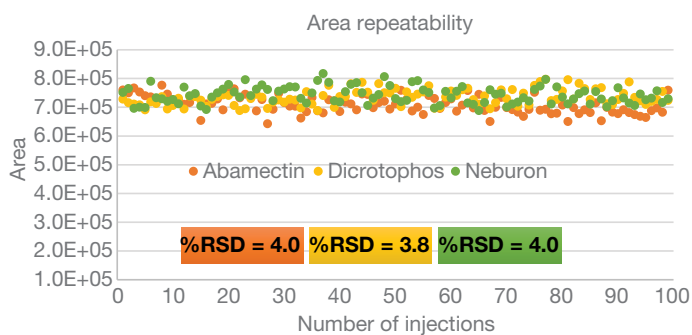


Figure 8. Demonstration of precision in terms of area repeatability presented for abamectin, dicrotophos, and neburon in milk (n=100) at 0.005 mg/kg

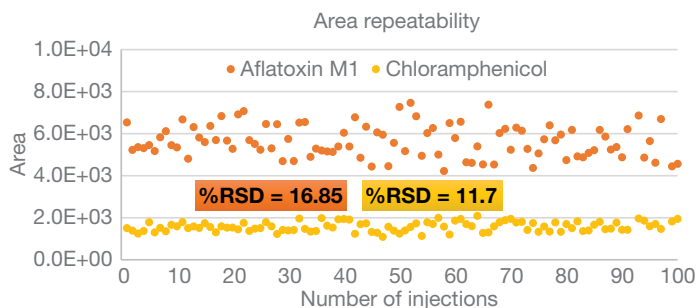


Figure 9. Demonstration of precision in terms of area repeatability presented for aflatoxin M1 (0.025 µg/kg) and chloramphenicol (0.25 µg/kg) in milk (n=100)

Conclusion

This application note describes an analytical solution for simultaneous detection and quantitation of a diverse range of contaminants—pesticide residues (192), veterinary medicine/drugs (54), and aflatoxin M1 in milk—using a simple modified QuEChERS method followed by LC-MS/MS analysis. The optimized method demonstrated good chromatographic separations in combination with the auto-optimized dwell times that allow for many SRM transitions to be monitored in a single injection without compromising data quality. Using this approach, at

least 70 injections (standards, samples, blank) could be completed in a day and increase the overall throughput of a commercial food testing laboratory. Average recoveries and precision data meet the validation guideline criteria.⁷⁻⁹ TraceFinder software was used for data acquisition and processing. The software has flagging options that minimize the user's time required for data review and reporting. Based on the flagging option, the user can make quick decisions on data quality. This approach will help increase the throughput of commercial food testing laboratories up to 50% by integrating multiple class-specific methods into a single generic approach. Also, this method complies with the EU as well as the FSSAI MRLs requirement by achieving excellent lower limits of quantitation (LOQs).

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Appendix 1. Recovery and precision of analytes at three different levels, based on procedural standard calibration

Sr. No.	Name of compound	Level I		Level II		Level III	
		% RSD	% Rec.	% RSD	% Rec	% RSD	% Rec.
Pesticides							
1	Acephate	5.2	89	2.8	85	5.1	87
2	Acetamiprid	7.9	97	1.9	96	3.2	92
3	Acibenzolar-S-methyl	11.2	120	2.9	108	8.3	98
4	Alanycarb	6.9	104	4.8	120	11.6	103
5	Aldicarb	8.3	96	6.0	98	9.8	96
6	Aldicarb sulfone	11.6	92	2.8	94	5.7	98
7	Aldicarb sulfoxide	4.2	92	3.2	88	6.6	87
8	Ametryn	4.1	99	3.3	96	7.0	95
9	Aminocarb	4.8	90	3.8	89	12.5	101
10	Amitraz	3.0	117	5.4	110	5.5	103
11	Azoxystrobin	2.8	118	3.5	109	2.5	104
12	Benalaxyl	4.5	117	6.0	108	4.6	100
13	Bendiocarb	5.2	99	2.8	95	2.7	89
14	Benfuracarb	4.9	114	8.1	86	12.5	79
15	Benzoximate	6.3	120	10.1	109	8.7	99
16	Bitertanol	3.8	113	8.7	112	5.1	102
17	Boscalid	4.7	117	3.6	111	3.0	99
18	Bromuconazole I	12.4	114	2.8	102	6.9	86
19	Bromuconazole II	10.6	105	6.2	94	8.7	91
20	Bupirimate	3.2	105	7.1	93	6.0	88
21	Buprofezin	8.9	99	8.5	85	14.3	77
22	Butafenacil+NH ₄	15.7	117	4.4	119	4.3	99
23	Butocarboxim	9.3	99	3.8	87	3.9	96
24	Butoxycarboxim	11.3	93	2.2	93	5.8	98
25	Carbaryl	7.3	90	5.3	82	4.6	81
26	Carbendazim	6.3	97	2.4	93	5.0	90
27	Carbetamide	5.5	97	3.9	94	3.4	92
28	Carbofuran	7.2	92	2.4	95	3.0	92
29	Carbofuran-3-hydroxy+NH ₄	6.1	103	2.2	94	4.9	88
30	Carboxin	9.3	82	3.8	81	3.3	85
31	Carfentrazone-ethyl	16.1	116	7.4	118	9.4	112
32	Chlorantraniliprole	7.7	112	3.1	112	6.4	105
33	Chlorfluazuron	12.0	116	4.2	104	12.5	85
34	Chlorotoluron	5.5	97	3.9	95	5.7	97
35	Chloroxuron	7.7	119	3.5	106	4.6	96
36	Clethodim	6.6	110	8.2	89	7.2	89
37	Clofentezine	10.7	103	5.2	88	7.9	82
38	Clothianidin	8.9	113	3.3	105	5.5	92
39	Cyazofamid	2.2	110	13.1	99	7.5	96
40	Cycluron	6.5	103	3.7	100	6.9	101
41	Cymoxanil	5.2	116	9.9	97	10.8	91

Appendix 1 (continued). Recovery and precision of analytes at three different levels, based on procedural standard calibration

Sr. No.	Name of compound	Level I		Level II		Level III	
		% RSD	% Rec.	% RSD	% Rec.	% RSD	% Rec.
Pesticides							
42	Cyproconazole	9.0	116	2.6	103	5.0	90
43	Cyprodinil	8.8	99	8.8	87	11.6	89
44	Diclobutrazol	5.7	113	3.8	103	6.6	94
45	Diclotophos	4.3	102	3.6	96	7.4	103
46	Diethofencarb	5.9	117	3.8	106	5.3	95
47	Difenoconazole	4.1	120	9.8	110	9.6	96
48	Diflubenzuron	3.8	114	3.4	116	8.4	97
49	Dimethoate	4.2	97	2.2	87	4.4	82
50	Dimethomorph	3.0	112	3.2	98	8.0	96
51	Dimoxystrobin	3.9	102	4.4	108	3.6	102
52	Diniconazole	10.4	118	5.2	104	7.8	92
53	Dinotefuran	2.7	102	4.3	94	6.0	93
54	Dioxacarb	11.1	89	2.9	92	6.8	100
55	Diuron	4.7	107	2.7	103	8.3	102
56	Epoxiconazole	4.3	116	3.7	110	4.0	98
57	Etaconazol	6.9	109	3.8	103	6.6	94
58	Ethiofencarb	6.8	114	2.2	101	5.1	85
59	Ethiprole	5.6	111	7.3	101	13.6	92
60	Ethirimol	10.3	83	4.0	86	7.0	96
61	Ethofumesate	6.6	110	4.7	107	1.8	91
62	Etoxazole	11.8	98	18.2	79	16.8	79
63	Famoxadone	15.4	102	18.2	100	10.7	74
64	Fenamidone	8.8	118	3.5	102	5.6	91
65	Fenarimol	2.6	120	3.5	104	6.3	96
66	Fenazaquin	17.1	73	1.5	72	8.2	75
67	Fenbuconazole	9.3	118	5.1	104	9.0	97
68	Fenhexamid	10.1	118	3.5	112	5.8	98
69	Fenobucarb	9.6	108	4.9	101	3.7	83
70	Fenoxycarb	9.6	119	7.3	109	9.5	95
71	Fenpropimorph	12.6	90	5.5	92	15.7	105
72	Fenpyroximat	10.9	114	19.7	87	6.6	88
73	Fipronil	9.8	99	7.9	84	10.8	92
74	Flonicamid	9.4	86	3.4	86	4.7	85
75	Fluazinam neg	8.8	102	7.7	79	17.3	79
76	Fludioxinil	7.8	97	11.2	104	2.5	85
77	Flufenacet	4.1	113	1.7	106	2.8	91
78	Flufenoxuron	15.9	119	7.6	113	13.3	101
79	Fluometuron	5.0	104	2.6	102	8.3	104
80	Fluoxastrobin	7.4	119	5.1	113	3.9	103
81	Fluquinconazole	8.2	119	5.6	108	10.3	103
82	Flusilazole	11.1	107	5.3	115	7.0	93
83	Flutolanil	5.1	118	3.8	109	3.5	94
84	Flutriafol	9.0	111	2.8	101	3.6	86
85	Forchlorfenuron	10.4	114	3.0	112	3.4	88

Appendix 1 (continued). Recovery and precision of analytes at three different levels, based on procedural standard calibration

Sr. No.	Name of compound	Level I		Level II		Level III	
		% RSD	% Rec.	% RSD	% Rec.	% RSD	% Rec.
Pesticides							
86	Formetanate	4.4	97	3.9	93	6.6	99
87	Fuberidazole	5.2	98	2.4	95	5.2	94
88	Furalaxyl	4.2	107	5.4	105	2.8	93
89	Furathiocarb	5.6	112	12.6	94	12.9	98
90	Halofenozide	3.4	111	5.9	100	4.5	86
91	Hexaconazole	7.0	107	4.9	116	7.7	98
92	Hexaflumuron_pos	13.2	109	18.8	89	14.9	104
93	Hexythiazox	14.7	92	9.6	85	15.0	79
94	Hydramethylnon	10.0	119	3.7	111	14.5	102
95	Imazalil	5.1	92	5.4	89	7.6	99
96	Imidacloprid	8.4	111	2.8	99	8.3	84
97	indoxacarb	9.7	113	14.7	107	14.9	102
98	Ipconazole	2.4	118	6.0	97	8.6	92
99	Iprovalicarb	4.5	119	2.9	107	4.5	101
100	Isocarbophos	5.5	111	3.7	104	12.6	89
101	Isoprocarb	7.4	112	1.5	109	4.5	92
102	Isoproturon	5.5	101	2.2	98	4.9	102
103	Kresoxim-methyl	6.8	117	7.2	107	4.8	99
104	Linuron	7.5	120	3.1	105	4.1	85
105	Lufenuron_NH ₄ _1	8.1	114	15.1	116	14.3	105
106	Mandipropamid	5.8	116	5.2	98	5.2	97
107	Mefenacet	7.6	119	3.1	112	2.0	101
108	Mepanipyrim	6.5	104	4.9	90	10.9	94
109	Mepronil	8.8	119	2.9	106	6.0	93
110	Mesotrione	4.8	109	3.1	103	5.4	103
111	Metalaxyl	3.5	109	1.9	103	4.0	97
112	Metconazole	10.8	120	4.9	120	4.6	106
113	Methabenzthiazuron	5.8	114	1.2	106	2.1	96
114	Methamidophos	8.2	79	2.7	77	5.8	78
115	Methiocarb	6.8	114	2.2	101	5.1	85
116	Methomyl	14.9	119	2.3	112	4.4	100
117	Methoprotryne	4.3	99	3.7	94	7.4	95
118	Methoxyfenozide	9.9	117	5.8	110	3.0	93
119	Metobromuron	3.8	112	2.8	107	6.2	96
120	Metribuzin	6.8	88	5.7	89	5.0	91
121	Mevinphos-I	6.3	93	5.4	92	5.4	91
122	Mevinphos-II	4.3	97	4.2	98	4.6	96
123	Mexacarbate	11.6	93	2.5	93	5.7	98
124	Monceren pencycuron	5.6	119	6.6	103	8.0	95
125	Monocrotophos	3.2	95	5.3	89	8.3	92
126	Monolinuron	3.7	109	3.2	102	7.8	100
127	Myclobutanil	4.5	114	3.3	99	8.0	93
128	Neburon	9.8	120	5.6	114	8.2	101
129	Nitenpyram	12.3	84	3.9	82	6.0	82

Appendix 1 (continued). Recovery and precision of analytes at three different levels, based on procedural standard calibration

Sr. No.	Name of compound	Level I		Level II		Level III	
		% RSD	% Rec.	% RSD	% Rec.	% RSD	% Rec.
Pesticides							
130	Nuarimol	5.7	95	6.3	92	7.7	85
131	Omethoate	3.8	98	2.6	93	6.7	97
132	Oxadixyl	7.0	97	4.6	91	3.0	92
133	Oxamyl	6.3	93	3.4	90	3.2	88
134	Pacllobutrazol	8.0	118	1.8	101	5.9	89
135	Penconazole	8.0	115	4.3	108	5.3	97
136	Phenmedipham	4.5	92	10.0	97	4.6	91
137	Picoxystrobin	4.1	117	5.8	99	6.5	92
138	Piperonyl butoxide	5.7	113	10.0	99	11.1	95
139	Pirimicarb	5.6	95	2.7	93	5.2	94
140	Prochloraz	6.7	114	7.9	99	12.1	96
141	promecarb	7.1	113	4.1	103	4.4	85
142	Prometon	4.5	94	2.6	92	8.0	92
143	Prometryn	5.0	103	4.5	98	4.0	91
144	Propamocarb	6.3	97	3.7	98	8.8	99
145	Propargite	11.3	116	10.5	102	9.9	94
146	Propham	7.9	119	17.3	95	6.6	73
147	Propiconazole	7.1	116	4.8	107	8.3	96
148	Propoxur	6.9	85	2.8	86	4.4	86
149	Pymetrozine	3.8	102	3.1	95	7.7	96
150	Pyracarbolid	1.9	95	1.7	93	3.6	87
151	Pyraclostrobin	6.6	110	7.4	98	17.2	112
152	Pyridaben	13.2	104	11.9	92	15.7	80
153	Pyrimethanil	6.9	99	3.6	98	4.4	93
154	Pyriproxyfen	12.2	101	11.0	92	16.3	87
155	Quinoxifen	16.7	81	9.9	72	18.8	71
156	Rotenone	11.4	116	7.2	108	5.3	100
157	Secbumeton	3.2	92	3.4	90	5.5	89
158	Siduron	4.3	110	4.5	105	3.1	95
159	Simetryn	3.9	97	2.4	95	4.4	94
160	Spinetoram	3.6	106	12.3	96	13.9	104
161	Spinosad (Spinosyn D)	5.5	98	13.5	92	13.4	103
162	Spinosad A	4.2	107	9.7	101	10.3	107
163	Spiroclufen	5.9	119	16.1	104	17.0	93
164	Spiromesifen	9.3	119	19.3	98	16.8	89
165	Spirotetramat	5.9	120	4.9	107	6.5	102
166	Spiroxamine	5.7	105	6.7	98	7.7	98
167	Sulfentrazone	4.4	119	3.4	107	8.5	106
168	Tebuconazole	10.2	106	5.2	98	7.8	95
169	Tebufenozide	11.1	118	4.7	117	3.2	104
170	Tebufenpyrad	5.2	116	13.0	93	13.6	82
171	Tebuthiuron	6.2	100	2.1	92	2.4	84
172	Teflubenzuron	8.9	120	9.8	94	15.4	95
173	Temephos	3.7	116	9.8	119	15.4	105

Appendix 1 (continued). Recovery and precision of analytes at three different levels, based on procedural standard calibration

Sr. No.	Name of compound	Level I		Level II		Level III	
		% RSD	% Rec.	% RSD	% Rec.	% RSD	% Rec.
Pesticides							
174	Terbumeton	4.2	93	3.2	91	6.7	91
175	Terbutryn	4.3	100	4.3	95	4.6	92
176	Tetraconazole	6.0	106	5.5	91	6.4	86
177	Thiabendazole	3.5	96	3.2	92	5.5	91
178	Thiacloprid	4.3	106	3.0	100	3.8	95
179	Thiamethoxam	3.5	115	1.9	104	3.5	96
180	Thidiazuron	12.7	86	8.2	84	5.2	79
181	Thiobencarb	10.7	117	3.1	119	6.2	90
182	Thiofanox	4.6	97	3.6	92	4.4	94
183	Triadimefon	6.7	117	5.1	104	8.1	92
184	Triadimenol	10.6	120	4.7	103	7.2	89
185	Trichlorfon	9.6	105	1.9	100	5.1	90
186	Tricyclazole	11.4	88	3.8	86	2.6	87
187	Trifloxystrobin	5.8	110	12.3	93	13.9	92
188	Triflumizole	6.4	101	13.6	84	19.0	86
189	Triflumuron	5.9	117	5.3	105	9.9	94
190	Triticonazole	5.1	110	9.7	98	4.9	94
191	Vamidotion	4.7	101	2.7	94	3.2	91
192	Zoxamide	12.3	116	5.1	119	6.5	106
Veterinary medicines/drugs							
193	Abamectin B1a_NH ₄	3.0	112	18.2	99	12.9	97
194	Cardinazole	12.4	72	7.0	75	12.5	70
195	Chloramphenicol	8.8	108	13.9	112	13.2	107
196	Chlortetracycline	8.6	95	7.9	92	2.5	90
197	Cinoxacin	5.5	94	10.8	98	3.9	98
198	Ciprofloxacin	17.3	83	8.2	103	4.6	113
199	Difloxacin	8.7	92	12.0	98	3.5	96
200	Dimetridazole	15.2	77	10.9	88	5.8	91
201	Doramectin_NH ₄	13.1	94	18.0	85	19.1	90
202	Doxycycline	12.4	72	15.1	82	8.1	95
203	Enamectin-benzoate	3.3	102	11.2	99	7.3	97
204	Enoxacin	20.0	87	10.1	109	5.0	119
205	Enrofloxacin	10.7	83	15.1	91	3.4	95
206	Epichlortetracycline	8.8	92	3.9	104	6.6	103
207	Epioxytetracycline	12.0	77	11.6	86	12.4	93
208	Epitetracycline	19.9	90	11.3	104	15.8	105
209	Eprinomectin B1a	9.0	119	16.4	104	14.2	97
210	Flumequine	3.7	112	10.2	108	3.7	98
211	Hydroxyipronidazole	11.2	90	6.2	84	5.5	79
212	Hydroxymetronidazole	10.1	77	10.1	75	6.8	71
213	Ipronidazole	12.6	88	7.9	91	4.1	86
214	Ivermectin B1a_NH ₄	14.7	101	9.2	90	10.6	94
215	Lomefloxacin	10.7	89	12.3	97	3.6	95
216	Marbofloxacin	11.5	81	15.4	91	2.7	94

Appendix 1 (continued). Recovery and precision of analytes at three different levels, based on procedural standard calibration

Sr. No.	Name of compound	Level I		Level II		Level III	
		% RSD	% Rec.	% RSD	% Rec.	% RSD	% Rec.
Veterinary medicines/drugs							
217	Metronidazole_M+H	7.7	87	13.0	94	10.7	83
218	Moxidectin	16.9	99	13.9	79	17.7	76
219	Nalidixic acid	5.2	105	12.4	107	7.8	108
220	Norfloxacin	16.3	89	9.8	109	5.5	121
221	Ofloxacin	11.3	83	14.7	92	2.4	94
222	Orbifloxacin	7.9	95	9.1	99	5.5	97
223	Ornidazole	4.4	72	9.1	69	11.3	64
224	Oxolinic acid	3.6	104	5.8	94	1.4	96
225	Oxytetracycline	11.9	77	11.6	86	12.4	93
226	Pipemidic acid	6.1	88	10.3	100	4.3	118
227	Ronidazole	5.1	79	3.7	78	4.6	76
228	Sarafloxacin	8.7	93	4.2	104	3.0	110
229	Sulfachlorpyridazine	12.5	87	2.3	86	6.6	81
230	Sulfadiazine	6.1	97	2.2	90	8.5	88
231	Sulfadimethoxine	6.8	100	1.6	96	4.5	84
232	Sulfadoxine	6.8	100	1.6	96	4.5	84
233	Sulfaethoxypyridazine	18.2	96	5.6	88	7.7	81
234	Sulfamerazine	12.1	79	1.7	84	7.6	81
235	Sulfamethazine	5.6	104	2.2	94	8.6	87
236	Sulfamethizole	8.3	115	2.6	106	8.5	95
237	Sulfamethoxazole	9.0	104	2.6	97	5.5	85
238	Sulfamethoxypyridazine	5.6	102	2.3	96	9.6	86
239	Sulfamoxole	8.8	104	2.4	101	7.6	85
240	Sulfaquinoxaline	4.7	87	3.0	87	5.2	86
241	Sulfathiazole	5.8	106	2.5	100	7.9	100
242	Sulfisomidine	5.6	104	2.2	94	8.6	87
243	Sulfisoxazole	8.0	106	2.1	101	7.0	86
244	Ternidazole	10.2	72	6.4	73	4.9	75
245	Tetracycline	10.1	87	10.2	102	3.2	103
246	Tinidazole	11.5	94	9.2	79	5.8	82
Mycotoxin							
247	Aflatoxin M1	12.9	98	10.1	82	6.3	106

Appendix 2. MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Abamectin B1a *	Veterinary medicines/drugs	9.75	[M+NH ₄]	890.5	305.2	23.7
Abamectin B1a *	Veterinary medicines/drugs	9.75	[M+NH ₄]	890.5	307.2	19.2
Abamectin B1a *	Veterinary medicines/drugs	9.75	[M+NH ₄]	890.5	567.3	13.0
Acephate	Pesticide	2.06	[M+H]	184.1	95.0	22.1
Acephate	Pesticide	2.06	[M+H]	184.1	124.9	18.3
Acephate	Pesticide	2.06	[M+H]	184.1	142.9	9.4
Acetamiprid	Pesticide	5.47	[M+H]	223.0	99.0	53.0
Acetamiprid	Pesticide	5.47	[M+H]	223.0	126.0	29.0
Acibenzolar-S-methyl	Pesticide	8.07	[M+H]	211.0	91.2	29.0
Acibenzolar-S-methyl	Pesticide	8.07	[M+H]	211.0	136.2	41.0
Aflatoxin M1 #	Mycotoxin	5.98	[M+H]	329.1	229.0	41.7
Aflatoxin M1 #	Mycotoxin	5.98	[M+H]	329.1	273.1	24.5
Alanycarb	Pesticide	9.13	[M+H]	400.2	195.1	21.7
Alanycarb	Pesticide	9.13	[M+H]	400.2	383.1	7.1
Aldicarb	Pesticide	4.37	[M+H]	208.1	89.0	23.0
Aldicarb	Pesticide	4.37	[M+H]	208.1	116.0	11.0
Aldicarb sulfone	Pesticide	4.37	[M+H]	223.1	150.9	34.4
Aldicarb sulfone	Pesticide	4.37	[M+H]	223.1	166.0	15.8
Aldicarb sulfoxide	Pesticide	3.57	[M+H]	207.0	89.0	14.2
Aldicarb sulfoxide	Pesticide	3.57	[M+H]	207.0	132.0	6.3
Ametryn	Pesticide	7.05	[M+H]	228.1	96.0	35.0
Ametryn	Pesticide	7.05	[M+H]	228.1	186.1	25.0
Aminocarb	Pesticide	2.99	[M+H]	209.1	122.0	38.2
Aminocarb	Pesticide	2.99	[M+H]	209.1	136.9	23.7
Aminocarb	Pesticide	2.99	[M+H]	209.1	152.2	13.9
Amitraz	Pesticide	8.60	[M+H]	294.2	91.2	57.0
Amitraz	Pesticide	8.60	[M+H]	294.2	148.3	22.0
Azoxystrobin	Pesticide	7.68	[M+H]	404.1	329.0	30.7
Azoxystrobin	Pesticide	7.68	[M+H]	404.1	344.1	25.0
Azoxystrobin	Pesticide	7.68	[M+H]	404.1	372.0	14.2
Benalaxyl	Pesticide	8.61	[M+H]	326.2	148.1	29.0
Benalaxyl	Pesticide	8.61	[M+H]	326.2	294.1	15.0
Bendiocarb	Pesticide	6.57	[M+H]	224.0	108.9	17.7
Bendiocarb	Pesticide	6.57	[M+H]	224.0	167.1	10.2
Benfuracarb	Pesticide	4.01	[M+H]	411.1	160.0	35.2
Benfuracarb	Pesticide	4.01	[M+H]	411.1	192.1	12.3
Benzoximate	Pesticide	8.75	[M+H]	364.1	77.1	50.8
Benzoximate	Pesticide	8.75	[M+H]	364.1	105.0	24.4
Benzoximate	Pesticide	8.75	[M+H]	364.1	199.0	10.2
Bitertanol	Pesticide	8.74	[M+H]	338.2	70.0	10.1
Bitertanol	Pesticide	8.74	[M+H]	338.2	99.1	13.8
Bitertanol	Pesticide	8.74	[M+H]	338.2	269.2	8.3
Boscalid	Pesticide	7.89	[M+H]	343.0	270.9	35.0
Boscalid	Pesticide	7.89	[M+H]	343.0	272.0	30.2

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Boscalid	Pesticide	7.89	[M+H]	343.0	307.0	20.6
Bromuconazole I	Pesticide	8.13	[M+H]	377.8	159.0	29.5
Bromuconazole I	Pesticide	8.13	[M+H]	377.8	161.0	30.9
Bromuconazole I	Pesticide	8.13	[M+H]	377.8	172.9	30.0
Bromuconazole II	Pesticide	8.54	[M+H]	377.8	159.0	29.5
Bromuconazole II	Pesticide	8.54	[M+H]	377.8	161.0	30.9
Bromuconazole II	Pesticide	8.54	[M+H]	377.8	172.9	30.0
Bupirimate	Pesticide	7.99	[M+H]	317.1	166.1	24.3
Bupirimate	Pesticide	7.99	[M+H]	317.1	210.2	24.1
Bupirimate	Pesticide	7.99	[M+H]	317.1	272.1	19.6
Buprofezin	Pesticide	9.05	[M+H]	306.1	106.0	27.1
Buprofezin	Pesticide	9.05	[M+H]	306.1	116.0	16.1
Buprofezin	Pesticide	9.05	[M+H]	306.1	201.1	12.1
Butafenacil	Pesticide	8.10	[M+NH ₄]	492.1	331.0	24.1
Butafenacil	Pesticide	8.10	[M+NH ₄]	492.1	349.0	14.8
Butocarboxim	Pesticide	5.88	[M+H]	213.1	75.1	19.0
Butocarboxim	Pesticide	5.88	[M+H]	213.1	116.0	17.0
Butoxycarboxim	Pesticide	4.37	[M+H]	223.0	121.0	27.0
Butoxycarboxim	Pesticide	4.37	[M+H]	223.0	166.1	15.3
Carbaryl	Pesticide	6.87	[M+H]	202.0	117.1	24.0
Carbaryl	Pesticide	6.87	[M+H]	202.0	127.0	28.9
Carbaryl	Pesticide	6.87	[M+H]	202.0	145.1	10.2
Carbendazim	Pesticide	4.09	[M+H]	192.1	132.0	30.4
Carbendazim	Pesticide	4.09	[M+H]	192.1	160.1	18.2
Carbetamide	Pesticide	6.22	[M+H]	237.1	72.1	23.8
Carbetamide	Pesticide	6.22	[M+H]	237.1	120.0	16.2
Carbetamide	Pesticide	6.22	[M+H]	237.1	192.0	10.2
Carbofuran	Pesticide	6.60	[M+H]	222.0	77.1	42.6
Carbofuran	Pesticide	6.60	[M+H]	222.0	165.1	12.1
Carbofuran-3-hydroxy	Pesticide	5.23	[M+H]	238.1	163.1	15.7
Carbofuran-3-hydroxy	Pesticide	5.23	[M+H]	238.1	181.0	10.2
Carboxin	Pesticide	6.81	[M+H]	236.1	87.0	33.0
Carboxin	Pesticide	6.81	[M+H]	236.1	143.0	21.0
Cardinazole *	Veterinary medicines/drugs	5.47	[M+H]	245.2	75.0	34.3
Cardinazole *	Veterinary medicines/drugs	5.47	[M+H]	245.2	118.0	10.3
Carfentrazone-ethyl	Pesticide	8.44	[M+H]	412.0	346.0	23.3
Carfentrazone-ethyl	Pesticide	8.44	[M+H]	412.0	365.9	17.9
Carfentrazone-ethyl	Pesticide	8.44	[M+H]	412.0	384.0	14.4
Chloramphenicol *	Veterinary medicines/drugs	5.46	[M-H]	321.0	152.1	17.5
Chloramphenicol *	Veterinary medicines/drugs	5.46	[M-H]	321.0	256.8	8.0
Chlorantraniliprole	Pesticide	7.48	[M+H]	481.9	177.0	44.3
Chlorantraniliprole	Pesticide	7.48	[M+H]	481.9	283.9	12.1
Chlorantraniliprole	Pesticide	7.48	[M+H]	481.9	450.8	17.8
Chlorfluazuron	Pesticide	9.61	[M+H]	541.8	158.0	19.9
Chlorfluazuron	Pesticide	9.61	[M+H]	541.8	347.0	40.5

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Chlorfluazuron	Pesticide	9.61	[M+H]	541.8	348.9	41.4
Chlorfluazuron	Pesticide	9.61	[M+H]	541.8	384.9	21.3
Chlorotoluron	Pesticide	7.18	[M+H]	213.0	46.0	16.1
Chlorotoluron	Pesticide	7.18	[M+H]	213.0	72.1	18.5
Chloroxuron	Pesticide	8.15	[M+H]	291.0	46.0	19.4
Chloroxuron	Pesticide	8.15	[M+H]	291.0	72.1	20.5
Chloroxuron	Pesticide	8.15	[M+H]	291.0	218.0	26.1
Chlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	98.0	40.0
Chlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	154.1	31.0
Chlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	444.1	20.5
Chlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	462.1	17.3
Cinoxacin *	Veterinary medicines/drugs	6.06	[M+H]	263.1	189.0	26.8
Cinoxacin *	Veterinary medicines/drugs	6.06	[M+H]	263.1	217.0	21.0
Cinoxacin *	Veterinary medicines/drugs	6.06	[M+H]	263.1	245.0	13.9
Ciprofloxacin *	Veterinary medicines/drugs	5.00	[M+H]	332.1	231.1	35.6
Ciprofloxacin *	Veterinary medicines/drugs	5.00	[M+H]	332.1	245.1	24.2
Ciprofloxacin *	Veterinary medicines/drugs	5.00	[M+H]	332.1	288.1	17.6
Clethodim	Pesticide	8.99	[M+H]	360.1	164.1	18.0
Clethodim	Pesticide	8.99	[M+H]	360.1	166.1	24.0
Clethodim	Pesticide	8.99	[M+H]	360.1	268.1	12.0
Clofentezine	Pesticide	8.95	[M+H]	303.0	102.0	51.0
Clofentezine	Pesticide	8.95	[M+H]	303.0	138.0	19.0
Clothianidin	Pesticide	4.96	[M+H]	250.0	131.9	16.6
Clothianidin	Pesticide	4.96	[M+H]	250.0	169.0	12.7
Cyazofamid	Pesticide	8.26	[M+H]	325.0	107.9	13.7
Cyazofamid	Pesticide	8.26	[M+H]	325.0	215.9	17.5
Cyazofamid	Pesticide	8.26	[M+H]	325.0	217.0	18.1
Cycluron	Pesticide	7.52	[M+H]	199.1	46.1	16.4
Cycluron	Pesticide	7.52	[M+H]	199.1	69.1	21.3
Cycluron	Pesticide	7.52	[M+H]	199.1	72.1	22.1
Cymoxanil	Pesticide	8.76	[M+H]	199.0	112.8	40.3
Cymoxanil	Pesticide	8.76	[M+H]	199.0	140.9	29.4
Cymoxanil	Pesticide	8.76	[M+H]	199.0	184.1	17.4
Cyproconazole	Pesticide	8.02	[M+H]	292.0	70.0	31.0
Cyproconazole	Pesticide	8.02	[M+H]	292.0	125.0	29.0
Cyprodinil	Pesticide	8.28	[M+H]	226.0	77.0	61.0
Cyprodinil	Pesticide	8.28	[M+H]	226.0	93.0	47.0
Diclobutrazol	Pesticide	8.33	[M+H]	328.0	70.0	21.9
Diclobutrazol	Pesticide	8.33	[M+H]	328.0	123.0	54.1
Diclobutrazol	Pesticide	8.33	[M+H]	328.0	159.0	37.9
Diclotophos	Pesticide	4.92	[M+H]	238.0	108.9	32.4
Diclotophos	Pesticide	4.92	[M+H]	238.0	127.0	17.8
Diclotophos	Pesticide	4.92	[M+H]	238.0	192.5	10.2
Diethofencarb	Pesticide	7.67	[M+H]	268.0	124.0	32.0
Diethofencarb	Pesticide	7.67	[M+H]	268.0	226.1	10.2

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Difenoconazole	Pesticide	8.92	[M+H]	406.0	188.0	44.5
Difenoconazole	Pesticide	8.92	[M+H]	406.0	251.0	25.5
Difenoconazole	Pesticide	8.92	[M+H]	406.0	337.0	17.6
Difloxacin *	Veterinary medicines/drugs	5.28	[M+H]	400.1	299.1	29.0
Difloxacin *	Veterinary medicines/drugs	5.28	[M+H]	400.1	356.1	19.5
Difloxacin *	Veterinary medicines/drugs	5.28	[M+H]	400.1	382.1	21.8
Diflubenzuron	Pesticide	8.40	[M+H]	311.0	140.9	32.9
Diflubenzuron	Pesticide	8.40	[M+H]	311.0	158.0	14.2
Dimethoate	Pesticide	5.16	[M+H]	229.8	124.9	21.7
Dimethoate	Pesticide	5.16	[M+H]	229.8	171.0	15.3
Dimethoate	Pesticide	5.16	[M+H]	229.8	198.8	10.2
Dimethomorph	Pesticide	7.86	[M+H]	388.1	165.1	31.5
Dimethomorph	Pesticide	7.86	[M+H]	388.1	273.1	30.5
Dimethomorph	Pesticide	7.86	[M+H]	388.1	301.0	20.8
Dimetridazole *	Veterinary medicines/drugs	3.81	[M+H]	142.1	54.0	32.4
Dimetridazole *	Veterinary medicines/drugs	3.81	[M+H]	142.1	81.1	26.4
Dimetridazole *	Veterinary medicines/drugs	3.81	[M+H]	142.1	96.1	16.4
Dimoxystrobin	Pesticide	8.43	[M+H]	327.2	115.9	22.0
Dimoxystrobin	Pesticide	8.43	[M+H]	327.2	204.9	10.2
Dimoxystrobin	Pesticide	8.43	[M+H]	327.2	238.1	10.6
Diniconazole	Pesticide	8.85	[M+H]	326.0	70.0	25.9
Diniconazole	Pesticide	8.85	[M+H]	326.0	159.1	31.2
Diniconazole	Pesticide	8.85	[M+H]	326.0	172.9	27.0
Dinotefuran	Pesticide	3.44	[M+H]	203.0	113.1	10.2
Dinotefuran	Pesticide	3.44	[M+H]	203.0	129.1	11.6
Dinotefuran	Pesticide	3.44	[M+H]	203.0	157.2	10.2
Dioxacarb	Pesticide	8.50	[M+H]	224.1	123.0	21.0
Dioxacarb	Pesticide	8.50	[M+H]	224.1	167.0	11.0
Diuron	Pesticide	7.50	[M+H]	233.0	46.0	16.8
Diuron	Pesticide	7.50	[M+H]	233.0	72.1	18.7
Diuron	Pesticide	7.50	[M+H]	233.0	160.0	26.9
Doramectin *	Veterinary medicines/drugs	9.92	[M+NH ₄] ⁺	916.5	331.2	24.1
Doramectin *	Veterinary medicines/drugs	9.92	[M+NH ₄] ⁺	916.5	333.2	19.4
Doramectin *	Veterinary medicines/drugs	9.92	[M+NH ₄] ⁺	916.5	593.4	12.5
Doxycycline *	Veterinary medicines/drugs	6.83	[M+H]	445.2	321.1	31.0
Doxycycline *	Veterinary medicines/drugs	6.83	[M+H]	445.2	428.2	18.5
Emamectin B1a	Pesticide	9.27	[M+H]	886.5	158.0	40.0
Emamectin B1a	Pesticide	9.27	[M+H]	886.5	82.1	40.0
Enoxacin *	Veterinary medicines/drugs	4.83	[M+H]	321.1	234.1	20.4
Enoxacin *	Veterinary medicines/drugs	4.83	[M+H]	321.1	257.1	17.2
Enoxacin *	Veterinary medicines/drugs	4.83	[M+H]	321.1	303.1	17.6
Enrofloxacin *	Veterinary medicines/drugs	5.11	[M+H]	360.2	245.1	26.7
Enrofloxacin *	Veterinary medicines/drugs	5.11	[M+H]	360.2	316.1	19.0
Enrofloxacin *	Veterinary medicines/drugs	5.11	[M+H]	360.2	342.2	21.0
Epichlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	98.0	40.0

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Epichlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	444.1	20.5
Epichlortetracycline *	Veterinary medicines/drugs	6.00	[M+H]	479.1	462.1	17.3
Epioxytetracycline *	Veterinary medicines/drugs	5.01	[M+H]	461.2	426.1	24.3
Epioxytetracycline *	Veterinary medicines/drugs	5.01	[M+H]	461.2	444.1	17.7
Epitetracycline *	Veterinary medicines/drugs	5.00	[M+H]	445.2	410.1	18.6
Epitetracycline *	Veterinary medicines/drugs	5.00	[M+H]	445.2	427.2	12.5
Epoxiconazole	Pesticide	8.30	[M+H]	330.0	100.9	43.7
Epoxiconazole	Pesticide	8.30	[M+H]	330.0	121.0	21.1
Epoxiconazole	Pesticide	8.30	[M+H]	330.0	123.0	17.6
Eprinomectin B1a *	Veterinary medicines/drugs	9.68	[M+H]	914.5	154.1	32.7
Eprinomectin B1a *	Veterinary medicines/drugs	9.68	[M+H]	914.5	186.1	18.3
Eprinomectin B1a *	Veterinary medicines/drugs	9.68	[M+H]	914.5	298.2	21.5
Etaconazole	Pesticide	8.33	[M+H]	328.0	55.1	21.4
Etaconazole	Pesticide	8.33	[M+H]	328.0	159.0	27.2
Etaconazole	Pesticide	8.33	[M+H]	328.0	204.6	17.4
Ethiofencarb	Pesticide	7.80	[M+H]	226.0	77.0	55.0
Ethiofencarb	Pesticide	7.80	[M+H]	226.0	79.1	34.4
Ethiofencarb	Pesticide	7.80	[M+H]	226.0	107.1	14.6
Ethiofencarb	Pesticide	7.80	[M+H]	226.0	121.0	18.7
Ethiofencarb	Pesticide	7.80	[M+H]	226.0	169.3	8.2
Ethiprole	Pesticide	7.75	[M+H]	396.9	255.0	35.8
Ethiprole	Pesticide	7.75	[M+H]	396.9	350.9	21.2
Ethirimol	Pesticide	5.67	[M+H]	209.8	98.0	27.3
Ethirimol	Pesticide	5.67	[M+H]	209.8	140.1	22.4
Ethofumesate	Pesticide	7.71	[M+H]	287.0	121.0	18.5
Ethofumesate	Pesticide	7.71	[M+H]	287.0	163.0	12.6
Etoxazole	Pesticide	9.50	[M+H]	360.1	113.0	54.2
Etoxazole	Pesticide	9.50	[M+H]	360.1	141.0	30.8
Etoxazole	Pesticide	9.50	[M+H]	360.1	304.0	18.2
Famoxadone	Pesticide	8.61	[M+H]	392.0	238.0	16.0
Famoxadone	Pesticide	8.61	[M+H]	392.0	331.0	13.0
Fenamidone	Pesticide	7.78	[M+H]	312.1	236.1	14.7
Fenamidone	Pesticide	7.78	[M+H]	312.1	264.1	10.2
Fenarimol	Pesticide	8.19	[M+H]	331.0	258.9	25.9
Fenarimol	Pesticide	8.19	[M+H]	331.0	268.0	23.6
Fenazaquin	Pesticide	10.01	[M+H]	307.2	57.0	24.4
Fenazaquin	Pesticide	10.01	[M+H]	307.2	147.0	20.3
Fenazaquin	Pesticide	10.01	[M+H]	307.2	161.1	17.0
Fenbuconazole	Pesticide	8.33	[M+H]	337.1	70.1	21.0
Fenbuconazole	Pesticide	8.33	[M+H]	337.1	91.0	33.1
Fenbuconazole	Pesticide	8.33	[M+H]	337.1	125.0	30.9
Fenhexamid	Pesticide	8.12	[M+H]	302.0	55.0	35.3
Fenhexamid	Pesticide	8.12	[M+H]	302.0	97.0	23.4
Fenhexamid	Pesticide	8.12	[M+H]	302.0	143.0	30.7
Fenobucarb	Pesticide	7.70	[M+H]	208.1	95.0	14.7

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Fenobucarb	Pesticide	7.70	[M+H]	208.1	152.1	10.2
Fenoxycarb	Pesticide	8.43	[M+H]	302.0	88.0	19.4
Fenoxycarb	Pesticide	8.43	[M+H]	302.0	116.0	11.7
Fenpropimorph	Pesticide	7.64	[M+H]	304.0	117.0	65.0
Fenpropimorph	Pesticide	7.64	[M+H]	304.0	147.0	39.0
Fenpyroximate	Pesticide	9.64	[M+H]	422.2	214.1	29.9
Fenpyroximate	Pesticide	9.64	[M+H]	422.2	231.1	24.8
Fenpyroximate	Pesticide	9.64	[M+H]	422.2	366.2	15.8
Fipronil	Pesticide	8.34	[M-H]	435.0	250.0	35.0
Fipronil	Pesticide	8.34	[M-H]	435.0	330.0	20.0
Fipronil sulfone	Pesticide	8.50	[M-H]	451.0	415.0	25.0
Fipronil sulfone	Pesticide	8.50	[M-H]	451.0	282.0	27.0
Fipronil sulfide	Pesticide	8.30	[M-H]	419.0	383.0	20
Fipronil sulfide	Pesticide	8.30	[M-H]	419.0	314.0	30
Fipronil desulfinyl	Pesticide	8.27	[M-H]	387.0	282.0	35
Fipronil desulfinyl	Pesticide	8.27	[M-H]	387.0	331.0	35
Flonicamid	Pesticide	3.99	[M+H]	230.1	174.0	25.0
Flonicamid	Pesticide	3.99	[M+H]	230.1	203.1	23.0
Fluazinam	Pesticide	9.20	[M-H]	462.8	398.0	16.0
Fluazinam	Pesticide	9.20	[M-H]	462.8	415.9	19.3
Fludioxinil	Pesticide	6.05	[M+H]	249.1	131.1	39.7
Fludioxinil	Pesticide	6.05	[M+H]	249.1	161.1	19.2
Flufenacet	Pesticide	8.20	[M+H]	364.0	152.1	18.6
Flufenacet	Pesticide	8.20	[M+H]	364.0	194.0	10.0
Flufenoxuron	Pesticide	9.44	[M+H]	489.2	140.9	40.6
Flufenoxuron	Pesticide	9.44	[M+H]	489.2	158.1	17.8
Flumequine *	Veterinary medicines/drugs	7.09	[M+H]	262.1	125.9	49.7
Flumequine *	Veterinary medicines/drugs	7.09	[M+H]	262.1	202.0	32.9
Flumequine *	Veterinary medicines/drugs	7.09	[M+H]	262.1	244.1	19.0
Fluometuron	Pesticide	7.00	[M+H]	232.9	46.1	17.9
Fluometuron	Pesticide	7.00	[M+H]	232.9	72.0	18.9
Fluometuron	Pesticide	7.00	[M+H]	232.9	160.0	27.1
Fluoxastrobin	Pesticide	8.13	[M+H]	459.1	188.0	34.7
Fluoxastrobin	Pesticide	8.13	[M+H]	459.1	367.0	23.7
Fluoxastrobin	Pesticide	8.13	[M+H]	459.1	427.0	17.4
Fluquinconazole	Pesticide	8.13	[M+H]	375.9	108.0	50.0
Fluquinconazole	Pesticide	8.13	[M+H]	375.9	307.1	26.0
Fluquinconazole	Pesticide	8.13	[M+H]	375.9	349.0	19.0
Flusilazole	Pesticide	8.43	[M+H]	316.1	165.1	27.2
Flusilazole	Pesticide	8.43	[M+H]	316.1	219.1	30.7
Flusilazole	Pesticide	8.43	[M+H]	316.1	247.1	18.2
Flutolanil	Pesticide	7.92	[M+H]	324.1	242.1	35.0
Flutolanil	Pesticide	7.92	[M+H]	324.1	262.1	31.0
Flutriafol	Pesticide	7.19	[M+H]	302.0	70.0	18.8
Flutriafol	Pesticide	7.19	[M+H]	302.0	109.0	29.5

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Flutriafol	Pesticide	7.19	[M+H]	302.0	123.0	28.0
Forchlorfenuron	Pesticide	7.32	[M+H]	248.0	93.0	32.5
Forchlorfenuron	Pesticide	7.32	[M+H]	248.0	129.0	17.5
Forchlorfenuron	Pesticide	7.32	[M+H]	248.0	155.0	15.1
Formetanate	Pesticide	3.03	[M+H]	222.1	93.0	35.4
Formetanate	Pesticide	3.03	[M+H]	222.1	120.0	26.8
Formetanate	Pesticide	3.03	[M+H]	222.1	165.1	15.3
Fuberidazole	Pesticide	4.91	[M+H]	185.1	65.1	42.9
Fuberidazole	Pesticide	4.91	[M+H]	185.1	129.0	35.4
Fuberidazole	Pesticide	4.91	[M+H]	185.1	157.1	21.7
Furalaxyl	Pesticide	7.74	[M+H]	302.1	95.0	39.0
Furalaxyl	Pesticide	7.74	[M+H]	302.1	242.1	21.0
Furathiocarb	Pesticide	9.13	[M+H]	383.1	194.9	18.5
Furathiocarb	Pesticide	9.13	[M+H]	383.1	252.1	12.7
Halofenozide	Pesticide	7.78	[M+H]	331.1	105.0	18.0
Halofenozide	Pesticide	7.78	[M+H]	331.1	139.0	22.6
Halofenozide	Pesticide	7.78	[M+H]	331.1	275.0	6.3
Hexaconazole	Pesticide	8.67	[M+H]	314.0	70.0	21.0
Hexaconazole	Pesticide	8.67	[M+H]	314.0	159.0	31.7
Hexaconazole	Pesticide	8.67	[M+H]	314.0	184.9	22.7
Hexaflumuron	Pesticide	8.99	[M+H]	461.0	141.0	57.0
Hexaflumuron	Pesticide	8.99	[M+H]	461.0	158.0	23.0
Hexythiazox	Pesticide	9.36	[M+H]	353.1	168.0	25.0
Hexythiazox	Pesticide	9.36	[M+H]	353.1	228.0	15.3
Hexythiazox	Pesticide	9.36	[M+H]	353.1	271.0	13.4
Hydramethylnon	Pesticide	8.89	[M+H]	495.2	151.0	55.0
Hydramethylnon	Pesticide	8.89	[M+H]	495.2	323.1	30.8
Hydramethylnon	Pesticide	8.89	[M+H]	495.2	368.0	35.1
Hydroxyipronidazole *	Veterinary medicines/drugs	4.67	[M+H]	186.1	121.0	27.1
Hydroxyipronidazole *	Veterinary medicines/drugs	4.67	[M+H]	186.1	122.0	20.4
Hydroxyipronidazole *	Veterinary medicines/drugs	4.67	[M+H]	186.1	168.1	13.5
Hydroxymetronidazole *	Veterinary medicines/drugs	1.62	[M+H]	188.1	123.1	12.8
Hydroxymetronidazole *	Veterinary medicines/drugs	1.62	[M+H]	188.1	126.0	17.5
Hydroxymetronidazole *	Veterinary medicines/drugs	1.62	[M+H]	188.1	144.0	13.2
Imazalil	Pesticide	7.05	[M+H]	297.0	159.0	23.2
Imazalil	Pesticide	7.05	[M+H]	297.0	200.9	18.2
Imidacloprid	Pesticide	5.06	[M+H]	256.0	175.1	18.7
Imidacloprid	Pesticide	5.06	[M+H]	256.0	209.0	15.9
Indoxacarb	Pesticide	8.86	[M+H]	528.0	150.0	23.6
Indoxacarb	Pesticide	8.86	[M+H]	528.0	203.0	38.3
Indoxacarb	Pesticide	8.86	[M+H]	528.0	292.9	14.2
Ipconazole	Pesticide	8.95	[M+H]	334.2	70.0	37.0
Ipconazole	Pesticide	8.95	[M+H]	334.2	125.0	47.0
Ipronidazole *	Veterinary medicines/drugs	5.50	[M+H]	170.1	109.1	25.5
Ipronidazole *	Veterinary medicines/drugs	5.50	[M+H]	170.1	124.0	17.9

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Iprovalicarb	Pesticide	8.16	[M+H]	321.2	91.0	45.3
Iprovalicarb	Pesticide	8.16	[M+H]	321.2	116.1	20.0
Iprovalicarb	Pesticide	8.16	[M+H]	321.2	119.1	19.4
Isocarbophos	Pesticide	7.30	[M+H]	307.0	121.1	31.6
Isocarbophos	Pesticide	7.30	[M+H]	307.0	230.8	20.2
Isocarbophos	Pesticide	7.30	[M+H]	307.0	273.1	5.6
Isoprocarb	Pesticide	7.18	[M+H]	194.1	77.0	35.7
Isoprocarb	Pesticide	7.18	[M+H]	194.1	95.1	15.3
Isoprocarb	Pesticide	7.18	[M+H]	194.1	137.1	9.7
Isoproturon	Pesticide	7.35	[M+H]	207.1	46.1	17.5
Isoproturon	Pesticide	7.35	[M+H]	207.1	72.1	18.5
Isoproturon	Pesticide	7.35	[M+H]	207.1	165.1	14.4
Ivermectin B1a *	Veterinary medicines/drugs	10.13	[M+NH ₄]	892.5	307.2	23.1
Ivermectin B1a *	Veterinary medicines/drugs	10.13	[M+NH ₄]	892.5	569.3	13.7
Kresoxim-methyl	Pesticide	8.47	[M+H]	314.1	206.1	10.2
Kresoxim-methyl	Pesticide	8.47	[M+H]	314.1	222.1	13.1
Kresoxim-methyl	Pesticide	8.47	[M+H]	314.1	267.1	10.2
Linuron	Pesticide	7.81	[M+H]	249.1	160.0	25.0
Linuron	Pesticide	7.81	[M+H]	249.1	182.1	21.0
Lomefloxacin *	Veterinary medicines/drugs	5.14	[M+H]	352.1	265.1	23.2
Lomefloxacin *	Veterinary medicines/drugs	5.14	[M+H]	352.1	308.2	16.8
Lufenuron	Pesticide	8.86	[M+NH ₄]	528.1	203.0	32.6
Lufenuron	Pesticide	8.86	[M+NH ₄]	528.1	249.0	15.9
Lufenuron	Pesticide	8.86	[M+NH ₄]	528.1	293.0	12.1
Mandipropamid	Pesticide	7.89	[M+H]	412.1	125.0	36.0
Mandipropamid	Pesticide	7.89	[M+H]	412.1	328.1	14.9
Mandipropamid	Pesticide	7.89	[M+H]	412.1	356.1	10.2
Marbofloxacin *	Veterinary medicines/drugs	4.59	[M+H]	363.1	72.1	22.6
Marbofloxacin *	Veterinary medicines/drugs	4.59	[M+H]	363.1	320.1	15.2
Mefenacet	Pesticide	8.12	[M+H]	299.0	120.0	24.8
Mefenacet	Pesticide	8.12	[M+H]	299.0	148.1	14.3
Mepanipyrim	Pesticide	8.32	[M+H]	224.0	77.0	55.0
Mepanipyrim	Pesticide	8.32	[M+H]	224.0	106.0	35.0
Mepronil	Pesticide	7.95	[M+H]	270.1	91.0	39.8
Mepronil	Pesticide	7.95	[M+H]	270.1	118.9	23.7
Mepronil	Pesticide	7.95	[M+H]	270.1	228.1	15.0
Mesotrione	Pesticide	6.03	[M+H]	340.0	104.0	30.5
Mesotrione	Pesticide	6.03	[M+H]	340.0	228.0	16.5
Metalaxyl	Pesticide	7.33	[M+H]	280.1	192.2	25.0
Metalaxyl	Pesticide	7.33	[M+H]	280.1	220.2	19.0
Metconazole	Pesticide	8.71	[M+H]	320.1	70.1	24.0
Metconazole	Pesticide	8.71	[M+H]	320.1	125.0	38.2
Metconazole	Pesticide	8.71	[M+H]	320.1	177.0	22.7
Methabenzthiazuron	Pesticide	7.46	[M+H]	222.0	124.0	29.2
Methabenzthiazuron	Pesticide	7.46	[M+H]	222.0	150.0	33.1

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Methabenzthiazuron	Pesticide	7.46	[M+H]	222.0	165.1	16.5
Methamidophos	Pesticide	1.41	[M+H]	141.9	94.0	14.1
Methamidophos	Pesticide	1.41	[M+H]	141.9	109.9	15.4
Methamidophos	Pesticide	1.41	[M+H]	141.9	125.0	14.1
Methiocarb	Pesticide	7.80	[M+H]	226.0	77.0	55.0
Methiocarb	Pesticide	7.80	[M+H]	226.0	79.1	34.4
Methiocarb	Pesticide	7.80	[M+H]	226.0	107.1	14.6
Methiocarb	Pesticide	7.80	[M+H]	226.0	121.0	18.7
Methiocarb	Pesticide	7.80	[M+H]	226.0	169.3	8.2
Methomyl	Pesticide	4.16	[M+H]	163.1	73.0	27.9
Methomyl	Pesticide	4.16	[M+H]	163.1	87.9	10.2
Methomyl	Pesticide	4.16	[M+H]	163.1	106.1	10.2
Methoprotryne	Pesticide	7.16	[M+H]	272.1	170.0	28.5
Methoprotryne	Pesticide	7.16	[M+H]	272.1	198.0	23.0
Methoprotryne	Pesticide	7.16	[M+H]	272.1	240.2	19.1
Methoxyfenozide	Pesticide	7.99	[M+H]	369.2	149.1	17.1
Methoxyfenozide	Pesticide	7.99	[M+H]	369.2	313.1	10.2
Metobromuron	Pesticide	7.22	[M+H]	258.9	148.0	15.5
Metobromuron	Pesticide	7.22	[M+H]	258.9	169.9	19.0
Metribuzin	Pesticide	6.46	[M+H]	215.1	84.1	31.0
Metribuzin	Pesticide	6.46	[M+H]	215.1	187.1	25.0
Metronidazole *	Veterinary medicines/drugs	2.58	[M+H]	172.1	82.1	25.0
Metronidazole *	Veterinary medicines/drugs	2.58	[M+H]	172.1	128.1	15.0
Mevinphos-I	Pesticide	5.30	[M+H]	225.0	108.9	31.7
Mevinphos-I	Pesticide	5.30	[M+H]	225.0	127.0	17.0
Mevinphos-I	Pesticide	5.30	[M+H]	225.0	192.9	10.2
Mevinphos-II	Pesticide	5.81	[M+H]	225.0	108.9	31.7
Mevinphos-II	Pesticide	5.81	[M+H]	225.0	127.0	17.0
Mevinphos-II	Pesticide	5.81	[M+H]	225.0	192.9	10.2
Mexacarbate	Pesticide	4.37	[M+H]	223.1	136.1	37.5
Mexacarbate	Pesticide	4.37	[M+H]	223.1	151.1	24.0
Mexacarbate	Pesticide	4.37	[M+H]	223.1	166.1	15.1
Monceren (Pencycuron)	Pesticide	8.81	[M+H]	329.1	125.0	31.0
Monceren (Pencycuron)	Pesticide	8.81	[M+H]	329.1	218.1	23.0
Monocrotophos	Pesticide	4.57	[M+H]	224.0	98.1	12.6
Monocrotophos	Pesticide	4.57	[M+H]	224.0	127.0	16.4
Monocrotophos	Pesticide	4.57	[M+H]	224.0	192.9	10.2
Monolinuron	Pesticide	6.98	[M+H]	215.0	98.9	33.1
Monolinuron	Pesticide	6.98	[M+H]	215.0	126.0	17.9
Monolinuron	Pesticide	6.98	[M+H]	215.0	148.0	14.6
Moxidectin *	Veterinary medicines/drugs	10.03	[M+H]	640.4	496.2	10.2
Moxidectin *	Veterinary medicines/drugs	10.03	[M+H]	640.4	498.3	10.2
Moxidectin *	Veterinary medicines/drugs	10.03	[M+H]	640.4	528.3	10.2
Myclobutanil	Pesticide	8.05	[M+H]	289.0	70.0	41.0
Myclobutanil	Pesticide	8.05	[M+H]	289.0	125.0	39.0

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Nalidixic acid *	Veterinary medicines/drugs	6.88	[M+H]	233.1	187.0	25.2
Nalidixic acid *	Veterinary medicines/drugs	6.88	[M+H]	233.1	215.0	13.8
Neburon	Pesticide	8.46	[M+H]	275.0	57.0	21.3
Neburon	Pesticide	8.46	[M+H]	275.0	88.1	16.4
Nitenpyram	Pesticide	3.89	[M+H]	271.0	126.0	35.0
Nitenpyram	Pesticide	3.89	[M+H]	271.0	225.2	17.0
Norfloxacin *	Veterinary medicines/drugs	4.90	[M+H]	320.1	233.1	24.4
Norfloxacin *	Veterinary medicines/drugs	4.90	[M+H]	320.1	276.1	17.4
Norfloxacin *	Veterinary medicines/drugs	4.90	[M+H]	320.1	302.2	20.7
Nuarimol	Pesticide	7.74	[M+H]	315.1	243.0	24.6
Nuarimol	Pesticide	7.74	[M+H]	315.1	252.1	22.3
Ofloxacin *	Veterinary medicines/drugs	4.83	[M+H]	362.2	261.1	26.4
Ofloxacin *	Veterinary medicines/drugs	4.83	[M+H]	362.2	318.2	18.2
Ofloxacin *	Veterinary medicines/drugs	4.83	[M+H]	362.2	344.1	19.8
Omethoate	Pesticide	3.10	[M+H]	214.0	124.9	22.3
Omethoate	Pesticide	3.10	[M+H]	214.0	155.0	15.8
Omethoate	Pesticide	3.10	[M+H]	214.0	182.8	10.2
Orbifloxacin *	Veterinary medicines/drugs	5.14	[M+H]	396.2	267.0	36.2
Orbifloxacin *	Veterinary medicines/drugs	5.14	[M+H]	396.2	295.1	23.2
Orbifloxacin *	Veterinary medicines/drugs	5.14	[M+H]	396.2	352.1	16.9
Ornidazole *	Veterinary medicines/drugs	4.61	[M+H]	220.3	82.0	29.0
Ornidazole *	Veterinary medicines/drugs	4.61	[M+H]	220.3	128.0	16.4
Oxadixyl	Pesticide	6.19	[M+H]	279.1	132.1	31.3
Oxadixyl	Pesticide	6.19	[M+H]	279.1	133.1	21.6
Oxadixyl	Pesticide	6.19	[M+H]	279.1	219.1	10.2
Oxamyl	Pesticide	3.96	[M+H]	237.0	71.9	19.9
Oxamyl	Pesticide	3.96	[M+H]	237.0	90.1	10.6
Oxamyl	Pesticide	3.96	[M+H]	237.0	220.0	6.5
Oxolinic acid *	Veterinary medicines/drugs	6.30	[M+H]	262.1	160.0	38.1
Oxolinic acid *	Veterinary medicines/drugs	6.30	[M+H]	262.1	216.0	29.3
Oxolinic acid *	Veterinary medicines/drugs	6.30	[M+H]	262.1	244.0	18.7
Oxytetracycline *	Veterinary medicines/drugs	5.01	[M+H]	461.2	201.1	40.0
Oxytetracycline *	Veterinary medicines/drugs	5.01	[M+H]	461.2	337.1	30.0
Oxytetracycline *	Veterinary medicines/drugs	5.01	[M+H]	461.2	426.1	20.8
Paclobutrazol	Pesticide	7.91	[M+H]	294.0	70.1	20.9
Paclobutrazol	Pesticide	7.91	[M+H]	294.0	125.0	37.5
Paclobutrazol	Pesticide	7.91	[M+H]	294.0	165.0	22.9
Penconazole	Pesticide	8.60	[M+H]	284.1	70.1	18.1
Penconazole	Pesticide	8.60	[M+H]	284.1	159.0	30.1
Phenmedipham	Pesticide	7.43	[M+H]	301.1	136.0	20.4
Phenmedipham	Pesticide	7.43	[M+H]	301.1	168.0	10.2
Picoxystrobin	Pesticide	8.40	[M+H]	368.1	115.0	45.4
Picoxystrobin	Pesticide	8.40	[M+H]	368.1	145.1	21.2
Picoxystrobin	Pesticide	8.40	[M+H]	368.1	205.0	10.2
Pipemidic acid *	Veterinary medicines/drugs	4.41	[M+H]	304.2	215.0	34.2

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Pipemidic acid *	Veterinary medicines/drugs	4.41	[M+H]	304.2	217.1	22.3
Pipemidic acid *	Veterinary medicines/drugs	4.41	[M+H]	304.2	286.1	19.1
Piperonyl butoxide	Pesticide	9.23	[M+H]	356.3	119.0	33.4
Piperonyl butoxide	Pesticide	9.23	[M+H]	356.3	149.1	31.5
Piperonyl butoxide	Pesticide	9.23	[M+H]	356.3	177.1	10.2
Pirimicarb	Pesticide	5.61	[M+H]	239.1	72.0	21.5
Pirimicarb	Pesticide	5.61	[M+H]	239.1	108.9	30.8
Pirimicarb	Pesticide	5.61	[M+H]	239.1	182.1	16.1
Prochloraz	Pesticide	8.64	[M+H]	376.0	70.1	25.8
Prochloraz	Pesticide	8.64	[M+H]	376.0	266.0	16.8
Prochloraz	Pesticide	8.64	[M+H]	376.0	307.9	10.2
Promecarb	Pesticide	7.90	[M+H]	208.1	109.0	16.3
Promecarb	Pesticide	7.90	[M+H]	208.1	151.1	10.2
Prometon	Pesticide	6.67	[M+H]	226.1	100.0	29.5
Prometon	Pesticide	6.67	[M+H]	226.1	142.1	23.2
Prometon	Pesticide	6.67	[M+H]	226.1	184.0	18.7
Prometryn	Pesticide	7.60	[M+H]	242.2	158.0	23.7
Prometryn	Pesticide	7.60	[M+H]	242.2	185.9	18.0
Prometryn	Pesticide	7.60	[M+H]	242.2	200.0	18.7
Propamocarb	Pesticide	2.89	[M+H]	189.1	74.1	24.9
Propamocarb	Pesticide	2.89	[M+H]	189.1	102.0	17.3
Propamocarb	Pesticide	2.89	[M+H]	189.1	144.1	13.2
Propargite	Pesticide	9.43	[M+H]	368.2	175.1	23.0
Propargite	Pesticide	9.43	[M+H]	368.2	231.1	15.0
Propham	Pesticide	7.14	[M+H]	180.0	77.0	30.0
Propham	Pesticide	7.14	[M+H]	180.0	120.0	17.0
Propham	Pesticide	7.14	[M+H]	180.0	138.0	9.4
Propiconazole	Pesticide	8.68	[M+H]	342.1	122.9	55.0
Propiconazole	Pesticide	8.68	[M+H]	342.1	172.8	36.6
Propoxur	Pesticide	6.53	[M+H]	210.0	93.0	23.9
Propoxur	Pesticide	6.53	[M+H]	210.0	111.0	14.3
Propoxur	Pesticide	6.53	[M+H]	210.0	168.1	10.2
Pymetrozine	Pesticide	3.00	[M+H]	218.0	78.1	61.0
Pymetrozine	Pesticide	3.00	[M+H]	218.0	79.1	61.0
Pymetrozine	Pesticide	3.00	[M+H]	218.0	105.0	27.0
Pyracarbolid	Pesticide	6.67	[M+H]	218.1	97.0	37.0
Pyracarbolid	Pesticide	6.67	[M+H]	218.1	125.0	25.0
Pyraclostrobin	Pesticide	8.71	[M+H]	387.8	163.1	24.0
Pyraclostrobin	Pesticide	8.71	[M+H]	387.8	164.1	17.5
Pyraclostrobin	Pesticide	8.71	[M+H]	387.8	194.0	12.4
Pyridaben	Pesticide	9.78	[M+H]	365.0	147.0	33.0
Pyridaben	Pesticide	9.78	[M+H]	365.0	309.0	19.0
Pyrimethanil	Pesticide	7.49	[M+H]	200.1	82.0	27.0
Pyrimethanil	Pesticide	7.49	[M+H]	200.1	107.0	24.5
Pyrimethanil	Pesticide	7.49	[M+H]	200.1	168.1	30.3

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Pyriproxyfen	Pesticide	9.33	[M+H]	322.0	96.0	21.0
Pyriproxyfen	Pesticide	9.33	[M+H]	322.0	185.0	31.0
Quinoxifen	Pesticide	9.53	[M+H]	308.1	162.0	49.7
Quinoxifen	Pesticide	9.53	[M+H]	308.1	197.2	36.3
Quinoxifen	Pesticide	9.53	[M+H]	308.1	213.9	32.4
Ronidazole *	Veterinary medicines/drugs	2.92	[M+H]	201.1	55.0	22.3
Ronidazole *	Veterinary medicines/drugs	2.92	[M+H]	201.1	110.0	17.1
Ronidazole *	Veterinary medicines/drugs	2.92	[M+H]	201.1	140.0	10.2
Rotenone *	Pesticide	8.37	[M+H]	395.1	192.1	24.2
Rotenone *	Pesticide	8.37	[M+H]	395.1	195.0	34.8
Rotenone *	Pesticide	8.37	[M+H]	395.1	213.1	23.0
Sarafloxacin *	Veterinary medicines/drugs	5.35	[M+H]	386.1	342.1	18.8
Sarafloxacin *	Veterinary medicines/drugs	5.35	[M+H]	386.1	368.1	22.5
Secbumeton	Pesticide	6.70	[M+H]	226.2	100.0	37.0
Secbumeton	Pesticide	6.70	[M+H]	226.2	170.1	25.0
Siduron	Pesticide	7.77	[M+H]	233.3	94.0	31.0
Siduron	Pesticide	7.77	[M+H]	233.3	137.2	23.0
Simetryn	Pesticide	6.43	[M+H]	214.1	96.0	24.6
Simetryn	Pesticide	6.43	[M+H]	214.1	124.1	19.9
Simetryn	Pesticide	6.43	[M+H]	214.1	144.1	20.7
Spinetoram	Pesticide	8.96	[M+H]	748.5	98.1	65.0
Spinetoram	Pesticide	8.96	[M+H]	748.5	142.2	43.0
Spinosad D	Pesticide	8.96	[M+H]	746.5	99.1	39.0
Spinosad D	Pesticide	8.96	[M+H]	746.5	125.0	51.0
Spinosad D	Pesticide	8.96	[M+H]	746.5	142.1	30.3
Spinosad A	Pesticide	8.75	[M+H]	732.4	98.1	45.0
Spinosad A	Pesticide	8.75	[M+H]	732.4	100.9	46.2
Spinosad A	Pesticide	8.75	[M+H]	732.4	142.1	28.9
Spirodiclofen	Pesticide	9.57	[M+H]	411.1	71.0	16.6
Spirodiclofen	Pesticide	9.57	[M+H]	411.1	294.8	24.7
Spirodiclofen	Pesticide	9.57	[M+H]	411.1	312.9	11.7
Spiromesifen	Pesticide	9.43	[M+H]	371.1	187.2	28.9
Spiromesifen	Pesticide	9.43	[M+H]	371.1	255.0	23.3
Spiromesifen	Pesticide	9.43	[M+H]	371.1	273.1	9.4
Spirotetramat	Pesticide	8.16	[M+H]	374.1	216.1	33.7
Spirotetramat	Pesticide	8.16	[M+H]	374.1	302.1	16.8
Spirotetramat	Pesticide	8.16	[M+H]	374.1	330.2	15.4
Spiroxamine	Pesticide	7.84	[M+H]	298.2	72.1	38.4
Spiroxamine	Pesticide	7.84	[M+H]	298.2	100.0	30.4
Spiroxamine	Pesticide	7.84	[M+H]	298.2	144.2	20.1
Sulfachlorpyridazine *	Veterinary medicines/drugs	4.68	[M+H]	285.0	108.0	24.1
Sulfachlorpyridazine *	Veterinary medicines/drugs	4.68	[M+H]	285.0	156.0	15.0
Sulfadiazine *	Veterinary medicines/drugs	3.17	[M+H]	251.1	96.1	22.2
Sulfadiazine *	Veterinary medicines/drugs	3.17	[M+H]	251.1	108.0	23.3
Sulfadiazine *	Veterinary medicines/drugs	3.17	[M+H]	251.1	156.0	15.3

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Sulfadimethoxine *	Veterinary medicines/drugs	5.03	[M+H]	311.1	108.0	29.0
Sulfadimethoxine *	Veterinary medicines/drugs	5.03	[M+H]	311.1	156.0	21.3
Sulfadimethoxine *	Veterinary medicines/drugs	5.03	[M+H]	311.1	245.1	19.0
Sulfadoxine *	Veterinary medicines/drugs	5.03	[M+H]	311.1	108.0	25.6
Sulfadoxine *	Veterinary medicines/drugs	5.03	[M+H]	311.1	156.0	18.1
Sulfaethoxyipyridazine *	Veterinary medicines/drugs	5.34	[M+H]	295.2	92.1	30.3
Sulfaethoxyipyridazine *	Veterinary medicines/drugs	5.34	[M+H]	295.2	140.1	19.6
Sulfaethoxyipyridazine *	Veterinary medicines/drugs	5.34	[M+H]	295.2	156.0	18.7
Sulfamerazine *	Veterinary medicines/drugs	3.93	[M+H]	265.1	156.0	17.3
Sulfamerazine *	Veterinary medicines/drugs	3.93	[M+H]	265.1	172.0	16.4
Sulfamethazine *	Veterinary medicines/drugs	4.44	[M+H]	279.1	108.0	27.6
Sulfamethazine *	Veterinary medicines/drugs	4.44	[M+H]	279.1	124.0	25.1
Sulfamethazine *	Veterinary medicines/drugs	4.44	[M+H]	279.1	186.0	17.4
Sulfamethizole *	Veterinary medicines/drugs	4.34	[M+H]	271.0	92.1	26.2
Sulfamethizole *	Veterinary medicines/drugs	4.34	[M+H]	271.0	108.0	23.4
Sulfamethizole *	Veterinary medicines/drugs	4.34	[M+H]	271.0	156.0	14.4
Sulfamethoxazole *	Veterinary medicines/drugs	4.75	[M+H]	254.1	92.1	26.2
Sulfamethoxazole *	Veterinary medicines/drugs	4.75	[M+H]	254.1	108.0	23.4
Sulfamethoxazole *	Veterinary medicines/drugs	4.75	[M+H]	254.1	156.0	15.8
Sulfamethoxyipyridazine *	Veterinary medicines/drugs	4.44	[M+H]	281.1	92.1	28.7
Sulfamethoxyipyridazine *	Veterinary medicines/drugs	4.44	[M+H]	281.1	108.0	25.6
Sulfamoxole *	Veterinary medicines/drugs	4.99	[M+H]	268.1	108.0	24.1
Sulfamoxole *	Veterinary medicines/drugs	4.99	[M+H]	268.1	113.0	19.2
Sulfamoxole *	Veterinary medicines/drugs	4.99	[M+H]	268.1	156.0	16.1
Sulfaquinoxaline *	Veterinary medicines/drugs	5.92	[M+H]	301.1	92.1	29.0
Sulfaquinoxaline *	Veterinary medicines/drugs	5.92	[M+H]	301.1	108.0	25.5
Sulfaquinoxaline *	Veterinary medicines/drugs	5.92	[M+H]	301.1	156.0	16.6
Sulfathiazole *	Veterinary medicines/drugs	3.51	[M+H]	256.0	108.0	23.2
Sulfathiazole *	Veterinary medicines/drugs	3.51	[M+H]	256.0	156.0	14.9
Sulfentrazone *	Pesticide	6.69	[M+H]	387.0	272.9	29.6
Sulfentrazone *	Pesticide	6.69	[M+H]	387.0	279.8	27.7
Sulfentrazone *	Pesticide	6.69	[M+H]	387.0	307.0	21.3
Sulfisomidine *	Veterinary medicines/drugs	4.44	[M+H]	279.1	124.0	21.9
Sulfisomidine *	Veterinary medicines/drugs	4.44	[M+H]	279.1	156.0	20.3
Sulfisomidine *	Veterinary medicines/drugs	4.44	[M+H]	279.1	186.0	16.0
Sulfisoxazole *	Veterinary medicines/drugs	4.99	[M+H]	268.0	108.1	22.6
Sulfisoxazole *	Veterinary medicines/drugs	4.99	[M+H]	268.0	113.0	18.0
Sulfisoxazole *	Veterinary medicines/drugs	4.99	[M+H]	268.0	156.0	16.2
Tebuconazole	Pesticide	8.57	[M+H]	308.0	70.1	22.6
Tebuconazole	Pesticide	8.57	[M+H]	308.0	125.0	37.7
Tebuconazole	Pesticide	8.57	[M+H]	308.0	151.0	25.4
Tebufenozide	Pesticide	8.40	[M+H]	353.1	105.0	40.3
Tebufenozide	Pesticide	8.40	[M+H]	353.1	133.1	19.0
Tebufenozide	Pesticide	8.40	[M+H]	353.1	297.2	7.8
Tebufenpyrad	Pesticide	9.19	[M+H]	334.2	117.0	35.9

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Tebufenpyrad	Pesticide	9.19	[M+H]	334.2	145.0	27.0
Tebufenpyrad	Pesticide	9.19	[M+H]	334.2	147.1	25.2
Tebuthiuron	Pesticide	6.74	[M+H]	229.0	116.0	27.0
Tebuthiuron	Pesticide	6.74	[M+H]	229.0	172.1	17.9
Teflubenzuron	Pesticide	9.27	[M+H]	379.0	195.9	22.1
Teflubenzuron	Pesticide	9.27	[M+H]	379.0	338.9	10.2
Teflubenzuron	Pesticide	9.27	[M+H]	379.0	358.9	10.2
Temephos	Pesticide	9.20	[M+H]	467.0	405.0	21.0
Temephos	Pesticide	9.20	[M+H]	467.0	419.1	27.0
Terbumeton	Pesticide	6.70	[M+H]	226.2	142.1	23.1
Terbumeton	Pesticide	6.70	[M+H]	226.2	170.1	18.0
Terbumeton	Pesticide	6.70	[M+H]	226.2	184.1	18.7
Terbutryn	Pesticide	7.60	[M+H]	242.1	91.0	27.6
Terbutryn	Pesticide	7.60	[M+H]	242.1	158.1	23.7
Terbutryn	Pesticide	7.60	[M+H]	242.1	186.0	18.7
Ternidazole *	Veterinary medicines/drugs	3.85	[M+H]	186.2	82.0	27.2
Ternidazole *	Veterinary medicines/drugs	3.85	[M+H]	186.2	128.0	15.3
Tetraconazole	Pesticide	8.23	[M+H]	372.0	123.0	55.0
Tetraconazole	Pesticide	8.23	[M+H]	372.0	158.9	30.3
Tetracycline *	Veterinary medicines/drugs	5.04	[M+H]	445.2	154.1	30.0
Tetracycline *	Veterinary medicines/drugs	5.04	[M+H]	445.2	410.1	19.1
Thiabendazole	Pesticide	4.78	[M+H]	202.0	131.0	33.4
Thiabendazole	Pesticide	4.78	[M+H]	202.0	175.0	25.7
Thiacloprid	Pesticide	5.85	[M+H]	253.0	90.0	36.4
Thiacloprid	Pesticide	5.85	[M+H]	253.0	98.9	41.5
Thiacloprid	Pesticide	5.85	[M+H]	253.0	126.0	21.4
Thiamethoxam	Pesticide	4.41	[M+H]	292.0	131.9	22.3
Thiamethoxam	Pesticide	4.41	[M+H]	292.0	181.0	22.4
Thiamethoxam	Pesticide	4.41	[M+H]	292.0	211.1	12.1
Thidiazuron	Pesticide	6.53	[M+H]	221.0	94.0	14.6
Thidiazuron	Pesticide	6.53	[M+H]	221.0	102.0	16.5
Thidiazuron	Pesticide	6.53	[M+H]	221.0	127.9	16.8
Thiobencarb	Pesticide	8.84	[M+H]	258.0	89.0	49.0
Thiobencarb	Pesticide	8.84	[M+H]	258.0	99.0	47.7
Thiobencarb	Pesticide	8.84	[M+H]	258.0	125.0	19.6
Thiofanox	Pesticide	6.22	[M+H]	219.0	116.9	44.9
Thiofanox	Pesticide	6.22	[M+H]	219.0	132.1	25.5
Tinidazole *	Veterinary medicines/drugs	3.93	[M+H]	248.2	121.0	16.9
Tinidazole *	Veterinary medicines/drugs	3.93	[M+H]	248.2	128.1	21.6
Triadimefon	Pesticide	8.02	[M+H]	294.0	129.0	21.9
Triadimefon	Pesticide	8.02	[M+H]	294.0	141.0	22.4
Triadimefon	Pesticide	8.02	[M+H]	294.0	197.0	15.7
Triadimenol	Pesticide	7.91	[M+H]	296.1	70.0	33.0
Triadimenol	Pesticide	7.91	[M+H]	296.1	227.1	17.0
Trichlorfon	Pesticide	5.03	[M+H]	256.9	79.0	30.0

* Veterinary medicine/drug

Mycotoxin

Appendix 2 (continued). MRM transitions for pesticides, veterinary medicines/drugs, and aflatoxin M1

Name of compound	Category	RT (min)	ESI	Q1	Q3	CE (V)
Trichlorfon	Pesticide	5.03	[M+H]	256.9	108.9	17.5
Tricyclazole	Pesticide	6.25	[M+H]	190.0	109.0	35.7
Tricyclazole	Pesticide	6.25	[M+H]	190.0	136.0	28.7
Tricyclazole	Pesticide	6.25	[M+H]	190.0	163.0	22.8
Trifloxystrobin	Pesticide	8.92	[M+H]	409.0	116.0	22.8
Trifloxystrobin	Pesticide	8.92	[M+H]	409.0	145.0	44.0
Trifloxystrobin	Pesticide	8.92	[M+H]	409.0	186.0	17.9
Triflumizole	Pesticide	8.99	[M+H]	346.0	43.1	23.2
Triflumizole	Pesticide	8.99	[M+H]	346.0	73.1	16.7
Triflumizole	Pesticide	8.99	[M+H]	346.0	278.1	10.2
Triflumuron	Pesticide	8.71	[M+H]	359.1	139.0	45.0
Triflumuron	Pesticide	8.71	[M+H]	359.1	156.2	23.0
Triticonazole	Pesticide	8.19	[M+H]	318.1	70.0	35.0
Triticonazole	Pesticide	8.19	[M+H]	318.1	125.0	49.0
Vamidothion	Pesticide	5.27	[M+H]	288.0	118.0	22.7
Vamidothion	Pesticide	5.27	[M+H]	288.0	146.1	12.2
Zoxamide	Pesticide	8.61	[M+H]	336.0	159.0	39.3
Zoxamide	Pesticide	8.61	[M+H]	336.0	186.9	22.2
Zoxamide	Pesticide	8.61	[M+H]	336.0	203.9	16.9

* Veterinary medicine/drug

Mycotoxin

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