



## Trace level quantitation of pesticide residues in fresh fruits using LC-MS/MS

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### Keywords

TraceFinder, pesticide residues, grape, apple, QuEChERS, LC-MS/MS, TSQ Quantis

### Application benefits

- No cleanup, acetonitrile extract dilute-and-shoot method
- Sub-ppb level sensitivity (e.g. 0.001 mg/kg)
- Low cost, simple, sensitive and rugged method
- Compliance with the EU and FSSAI MRLs

### Goal

The objective was to provide an analytical solution for the trace level quantitation of 160 pesticides (parent, isomers and metabolites) in table grapes and in apple using liquid chromatography-tandem mass spectrometry. The optimized method was validated in accordance with the EU SANTE guidelines and further evaluated for compliance with the Food Safety and Standards Authority of India (FSSAI) as well as European Union (EU) MRLs.

### Introduction

In India, the commercial cultivation of grapes and apples requires frequent applications of pesticides throughout the growing season to control a variety of pests and diseases. Consequently, the occurrence of pesticide residues is a primary concern for the stakeholders of both crops. The minimization of

pesticide residues, especially in grapes, is challenging because besides direct application, pesticide residues may also occur in grapes from indirect sources such as soil, contaminated agro-inputs (e.g., manures, fertilizers, growth regulators, irrigation water, etc.), and drift from adjoining fields of other crops. In India in 2017, grape production was 2683 metric tons, whereas apple production was 2242 metric tons.<sup>1</sup> Until recently, Indian food testing laboratories analyzed pesticide residues in class-specific groups using a combination of GC- and HPLC-based methods. This approach required several days to complete the analysis. However, the present situation demands rapid methods and shorter turn-around times. Currently, 282 pesticides are registered in India under the Central Insecticide Board and Registration Committee (CIBRC) for their crop management.<sup>2</sup> There are 51 chemicals registered and recommended for grapes as per APEDA.<sup>3</sup>

The European Commission (EC) and FSSAI have set the maximum residue levels (MRLs) for pesticides and their metabolites in grape and apples.<sup>4,5</sup> Therefore, it is important to develop a fast, robust, sensitive, and cost-effective method able to produce results for LC-amenable pesticides that comply with the new MRLs recently set by the FSSAI.

For extraction of residues, the AOAC version of the QuEChERS (Quick, Easy, Cheap, Effective, Rugged and Safe) method was selected as it is widely used for the analysis of pesticide residues in fruit.<sup>6</sup> The instrument method plays an important role in delivering accurate and precise results to meet the regulatory requirements. Therefore, the Thermo Scientific™ TSQ Quantis™ triple quadrupole mass spectrometer system was used for data acquisition with instrument control, and the data processing, carried out using Thermo Scientific™ TraceFinder™ software.

This work aimed to develop an analytical solution validated in accordance with the EU SANTE/11813/ 2017 guidelines.<sup>7</sup> This method was applied to real samples to demonstrate the workflow, which meets the SANTE guideline requirements in terms of identification of incurred residues.

## Experimental

### Chemicals and apparatus

- Acetonitrile, Optima™ LC/MS Grade, Fisher Scientific™
- Methanol, Optima™ LC/MS Grade, Fisher Scientific™
- Water, Optima™ LC/MS Grade, Fisher Scientific™
- Formic acid (85%), Fisher Scientific™
- Acetic acid (100%), Fisher Scientific™
- Ammonium formate, LC/MS Grade, Fisher Scientific™
- Anhydrous magnesium sulfate, Fisher Scientific™
- Sodium acetate, Fisher Scientific™
- LC/MS pesticides mix reference standards, Restek™ P/N 31971
- Analytical balance (Aczet, CY2202, San Diego, CA) and precision balance (Aczet, CY205C, San Diego, CA)
- Vortex mixer (Thermo Scientific, P/N 88880017TS, also known as 88880017)
- Refrigerated centrifuge (Thermo Scientific™ Sorvall™ ST8 ventilated benchtop centrifuge)
- Variable volume micropipettes (Thermo Scientific)
- QuEChERS Salts (AOAC 2007.01) Mylar Pouch 6 g magnesium sulfate (anhydrous), 1.5 g sodium acetate 50 pk Thermo Scientific™ (P/N 60105-341)

## Sample preparation

The grape and apple samples collected from a local market were homogenized using a rotating blade chopper (Model: Maharaja Whiteline) to get a uniform slurry. Homogenized sub-samples were extracted using the AOAC Official Method 2007.01 QuEChERS procedure, which is outlined below<sup>6</sup>.

Sample extraction and cleanup:

- Weigh 15 g homogenized sample into a 50 mL extraction tube.
- For the recovery experiment, spike the samples before the addition of the extraction solvent.
- Add 15 mL of acetonitrile (containing 1% acetic acid).
- Shake vigorously and vortex for 1 minute on a vortex mixer at 2500 rpm.
- Add 6 g anhydrous MgSO<sub>4</sub> and 1.5 g sodium acetate to the tube and again mix vigorously for 1 minute on a vortex mixer at 2500 rpm.
- Centrifuge at 5000 rpm for 5 min.
- Dilute the supernatant with water (1:4 ratio, v:v).
- Transfer the extract into an LC vial for instrumental analysis.
- Inject 5 µL of extract into the LC-MS/MS.
- For the recovery experiment: screen the samples for the target list of analytes and check for any residues of analytes of interest. If there is no detection of target pesticides, use this sample as a blank, for spiking, and for the preparation of matrix-matched calibration standards.

## LC-MS/MS analysis

The Thermo Scientific™ Vanquish™ Flex UHPLC system was coupled with the Thermo Scientific™ TSQ Quantis™ quadrupole tandem mass spectrometer with a heated electrospray ionization (HESI) source. The optimized LC-MS/MS conditions are detailed in Table 1.

**Table 1. LC-MS/MS instrument conditions**

### Liquid chromatography method

Instrumentation:	Vanquish Flex UHPLC			
Column:	Thermo Scientific™ Hypersil GOLD™ (100 mm × 2.1 mm × 1.9 µm) (P/N 25002-102130)			
Sample compartment temp.:	10 °C			
Column oven temp.:	25 °C			
Injection volume:	5 µL			
Mobile phase:	A: 2 mM ammonium formate + 0.1% formic acid in water/ acetonitrile (90:10, v/v) B: 2 mM ammonium formate + 0.1% formic acid in water/ acetonitrile (10:90, v/v)			
Total run time:	18.0 min			
Gradient program:	<i>Time</i>	<i>Flow Rate</i>	<i>%B</i>	<i>Curve</i>
	0.000	0.400	1	5
	1.500	0.400	1	5
	5.000	0.400	50	5
	8.500	0.400	95	5
	13.500	0.400	95	5
	14.000	0.400	1	5
	18.000	0.400	1	5

### Mass spectrometry method

Instrumentation:	TSQ Quantis triple quadrupole tandem mass spectrometer			
Method type:	Time-based selected-reaction monitoring (t-SRM)			
Ion source type:	HESI			
Spray voltage:	Static Positive: 3500 V Negative: 2500 V			
Sheath gas:	50 Arb			
Aux gas:	10 Arb			
Sweep gas:	1 Arb			
Ion transfer tube temp.:	325 °C			
Vaporizer temp.:	350 °C			
Source position:	Vertical between M and Horizontal1			

## Data acquisition and processing

The data acquisition was performed by using the instrument conditions in Table 1. The data acquisition and processing were carried out using Thermo Scientific™ TraceFinder™ software version 4.1. The data was acquired in t-SRM mode, which includes two or more transitions per analyte. The target list of analytes given in Table 2 (Appendix) with their SRM transition, collision energies, and retention time (min). For data processing, the ion ratio ( $\pm 30\%$ ), retention time ( $\pm 0.1$  min), linearity ( $>0.99$  with residuals  $\pm 20$ ), recovery (70–120%) and precision ( $\pm 20\%$ ) were set as performance criteria by the EU SANTE guidelines.<sup>7</sup>

## Results and discussion

### LC-MS/MS analysis

The liquid chromatographic method was optimized, which offered excellent separation for the target analytes and absence of an isobaric interference from the matrix. The extracted ion chromatogram (XIC) is shown in Figure 1 for 160 compounds at 0.01 mg/L.

The data points/scans per peak depended on the dwell time required to monitor the transition. In this method, automatic optimized dwell time is  $<10$  ms per transition, which offered at minimum 12–15 points per peak. Here ametryn has more than 12 points per peak as shown in Figure 2. The optimized instrument conditions provided excellent selectivity, repeatability, and reproducibility.

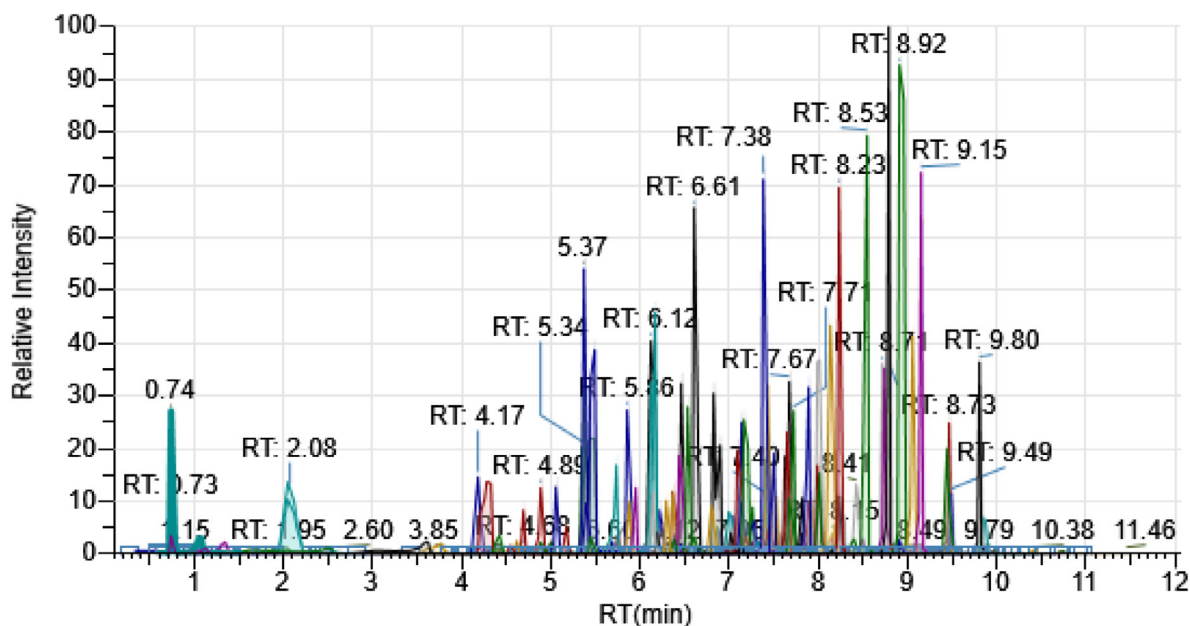
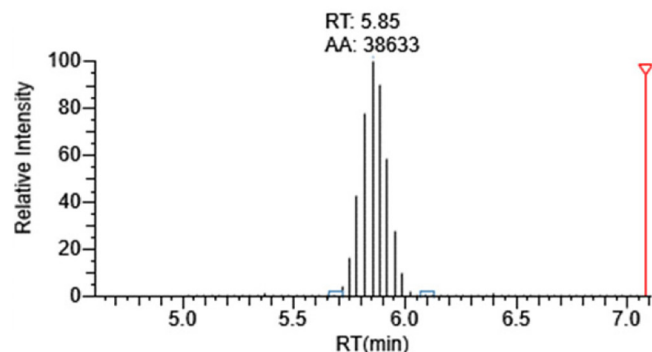


Figure 1. Total ion chromatograms with overlay extraction ions (160 compounds) in a single window

28th jan 2019\_002 Ametryn m/z: 186.100



28th jan 2019\_002 Ametryn m/z: 96.000

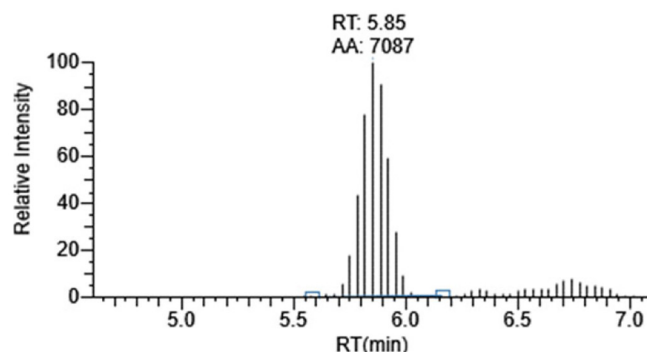


Figure 2. Impact of optimized dwell time on the data points per peak.

## Identification

The data was processed automatically using user-defined parameters. Color-coded flags indicate whether results pass or fail the user-defined acceptance criteria set in the processing method. The results that passed user-defined criteria (based on SANTE guidelines<sup>7</sup>) are shown in green (Figure 3), which minimizes the time required for review. A red flag indicates further investigation is required and dependent on the reason provided by the flag. As per SANTE guidelines, identification of dimethoate is shown with two transitions (230.0→199.0 and 230.0→125.0) at the same retention time (4.68 min) and ion ratio 50.27% (39.53–73.41%) in comparison with a neat standard (39.53–73.41%). The linearity for dimethoate provided correlation coefficient >0.999 with <20% residuals (Figure 3).

## Method performance

The linearity was plotted in the range of 0.0005 to 0.025 mg/L with a 1/x weighting factor and linear equation. The linear curve offered excellent correlation coefficients (>0.99) with < 20% residuals for all the target analytes in both solvents as well as in both matrices. The lowest calibration level (0.0005 mg/kg) showed

good sensitivity with  $\geq 10:1$  signal-to-noise ratio. The high sensitivity was enabled after dilution, without the need for cleanup. Since the extracts are diluted four-fold before analysis, the limit of quantitation (LOQ) with acceptable recoveries and precision was 0.005 mg/kg except carbofuran and 3-hydroxy carbofuran in both matrices. The recovery experiments were carried out at 0.005 (LOQ) and 0.01 ( $2 \times$  LOQ) mg/kg to demonstrate the method accuracy and precision. Average recoveries were observed in the range of 76–116% with <15 % RSD (Table 3), which were within acceptance criteria (recovery 70–120% and precision <20%) of SANTE guideline criteria. Also, the optimized method was tested for repeatability of results obtained for a long sequence of injections for grape (n=50) and apple (n=55) based on a typical 24-hour schedule of a commercial food testing laboratory. The time required to process the data through TraceFinder software was approximately 90 minutes considering manual revision. The repeatability was <15% for an area without internal standard correction and the retention time variation  $< \pm 0.05$  min in both matrices. The repeatability of response for selected pesticides in grape and apple is shown in Figure 4.

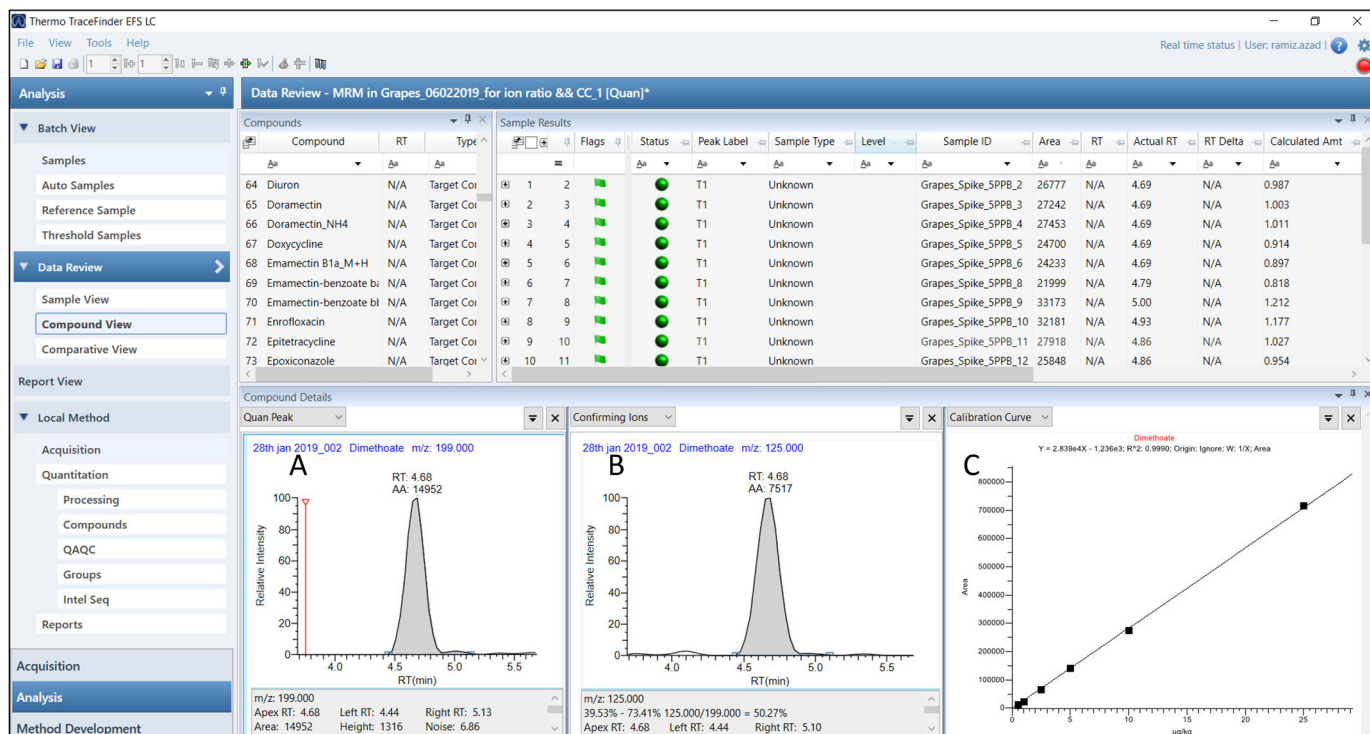


Figure 3. (A) Extracted ion chromatogram (XIC) for quantifier ion of dimethoate (B), identification based on selection confirmed with ion ratio, and (C) calibration curve

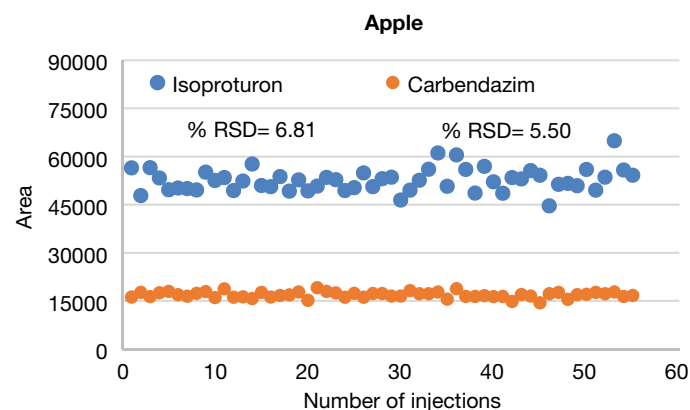
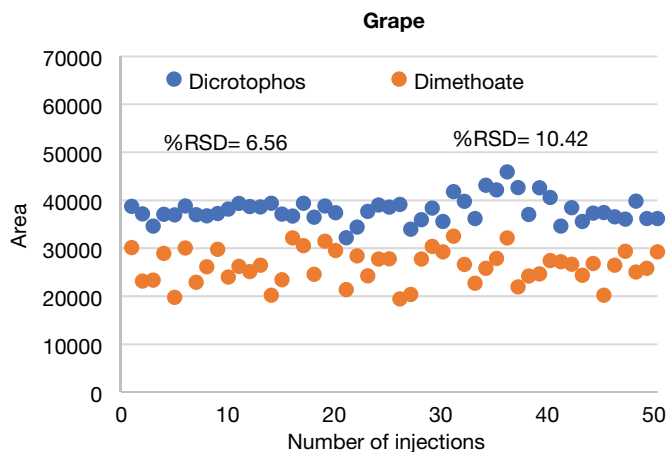


Figure 4. Area repeatability shown for dicrotophos and dimethoate in grape (n=50), and for isoproturon and carbendazim in apple (n=55)

### Application of the method to real samples

This method was applied to grape and apple samples (n=5 each) collected from the local market and analyzed for pesticides residue analysis. After the data review, there were no residues detected in apple samples. In the grape samples, a total of 10 different pesticides were identified and quantified. The concentration observed in grape samples were 0.015–2.2 mg/kg. However, spirotetramat and carbendazim were monitored as parent compounds. The detail list with their concentrations is given in Figure 5.

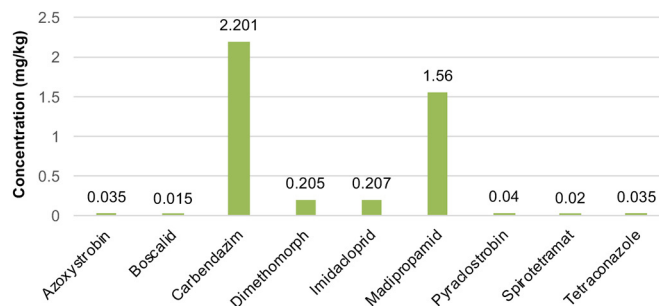


Figure 5. Incurred residue found in grape sample

### Conclusion

This application note describes a sensitive, robust, and low-cost method the quantification and identification of 160 pesticides and at low mg/kg levels grape and apple. Using this approach, at least 70 injections (standards, samples, blank) could be completed in a day (24-hour cycle) to increase the sample throughput of commercial food testing laboratories. The validation data fully meets the requirement of the EU SANTE guidelines. TraceFinder software used for data acquisition and data processing. The color-coded flagging of results outside of the acceptance criteria enables faster processing of the data and automatically identifies results in need of further investigation. The overall outcome is reduced time for reviewing data, with an overall increase in efficiency and productivity. The optimized method meets the EU and FSSAI MRLs for the LC-amenable pesticides in grape and apple.

### References

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- Insecticides / Pesticides Registered under section 9(3) of the Insecticides Act, 1968, for use in the Country. (As on 15/05/2019) [http://ppqs.gov.in/sites/default/files/list\\_of\\_pesticide\\_registered\\_us\\_93.pdf](http://ppqs.gov.in/sites/default/files/list_of_pesticide_registered_us_93.pdf)
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## Appendix

Table 2 (part 1). List of pesticides with MRM transitions used

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
1	3-Hydroxycarbofuran	4.41	Positive	238.1	163	19
		4.41	Positive	238.1	181	15
2	Acephate	4.70	Positive	184.1	49	35
		4.70	Positive	184.1	143	11
3	Acetamiprid	4.85	Positive	223	99	53
		4.85	Positive	223	126	29
4	Aldicarb sulfone**	1.90	Positive	240.1	86.2	28
		1.90	Positive	240.1	148.2	19
5	Ametryn	5.75	Positive	228.1	96	35
		5.75	Positive	228.1	186.1	25
6	Aminocarb	0.74	Positive	209.1	137.1	33
		0.74	Positive	209.1	152	19
7	Amitraz*	8.15	Positive	294.2	91.2	57
		8.15	Positive	294.2	148.3	22
8	Avermectin B1a	9.51	Positive	890.5	305	35
		9.51	Positive	890.5	567.5	17
9	Azoxystrobin	7.38	Positive	404.1	344.1	33
		7.38	Positive	404.1	372.1	19
10	Benalaxyl*	8.12	Positive	326.2	148.1	29
		8.12	Positive	326.2	294.1	15
11	Bendiocarb	6.81	Positive	224.1	109	33
		6.81	Positive	224.1	167.1	15
12	Benzoximate	8.71	Positive	364	105	31
		8.71	Positive	364	199	11
13	Bifenazate*	7.64	Positive	301.1	170.1	27
		7.64	Positive	301.1	198.1	13
14	Bitertanol	7.75	Positive	338.2	70	29
		7.75	Positive	338.2	269.2	13
15	Boscalid	7.48	Positive	343	140	25
		7.48	Positive	343	307	27
16	Bromucanazole-I	7.31	Positive	378	70	47
		7.31	Positive	378	159	37
17	Bromucanazole-II	7.62	Positive	378	70	47
		7.62	Positive	378	159	37
18	Bupirimate	7.40	Positive	317	108	35
		7.40	Positive	317	166.1	33
19	Buprofezin	8.73	Positive	306.2	116.2	23
		8.73	Positive	306.2	201.1	17
20	Butafenacil	8.00	Positive	492.1	331	27
		8.00	Positive	492.1	349	19
21	Butocarboxim	5.16	Positive	213.1	75.1	19
		5.16	Positive	213.1	116	17
22	Butoxycarboxim*	1.87	Positive	223.1	106	13
		1.87	Positive	223.1	166	11
23	Carbendazim*	1.64	Positive	192.2	132.1	41
		1.64	Positive	192.2	160.2	25
24	Carbetamide	5.45	Positive	237.1	118.1	17
		5.45	Positive	237.1	192	13

\*Parent compound

\*\* Only metabolite

**Table 2 (part 2). List of pesticides with MRM transitions used**

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
25	Carbofuran*	6.09	Positive	222.1	123	19
		6.09	Positive	222.1	165.1	15
26	Carboxin	6.37	Positive	236.1	87	35
		6.37	Positive	236.1	143	11
27	Chlorantraniliprole	6.87	Positive	484	285.9	53
		6.87	Positive	484	452.9	29
28	Chlorotoluron	6.22	Positive	213.1	46.2	28
		6.22	Positive	213.1	72.2	19
29	Chloroxuron	7.30	Positive	291.1	72.4	35
		7.30	Positive	291.1	218.1	25
30	Clethodim*	8.88	Positive	360.101	164	33
		8.88	Positive	360.101	268.1	19
31	Clothianidin	4.34	Positive	250	132	57
		4.34	Positive	250	169	22
32	Cyazofamid	8.16	Positive	325.2	108	35
		8.16	Positive	325.2	261.2	17
33	Cycluron	6.24	Positive	199.1	89	33
		6.24	Positive	199.1	69.1	19
34	Cyproconazole	7.16	Positive	292	70	29
		7.16	Positive	292	125	15
35	Cyprodinil	7.29	Positive	226	77	33
		7.29	Positive	226	93	15
36	Cyromazine	0.73	Positive	167.1	85.1	31
		0.73	Positive	167.1	125.1	11
37	Desmedipham	7.13	Positive	318.1	154	27
		7.13	Positive	318.1	182	13
38	Diclobutrazol	7.54	Positive	328.2	59.1	29
		7.54	Positive	328.2	70.2	13
39	Dicrotophos	3.59	Positive	238.1	112.1	25
		3.59	Positive	238.1	193	27
40	Diethofencarb	7.16	Positive	268.1	124	47
		7.16	Positive	268.1	226.1	37
41	Difenoconazole	8.24	Positive	406.1	251.1	47
		8.24	Positive	408.2	253.1	37
42	Dimethoate	4.68	Positive	230	125	35
		4.68	Positive	230	199	33
43	Dimethomorph-I	6.90	Positive	388.1	165.1	23
		6.90	Positive	388.1	301	17
44	Dimethomorph-II	7.03	Positive	388.1	165.1	27
		7.03	Positive	388.1	301	19
45	Dimoxystrobin	7.89	Positive	327.1	116	19
		7.89	Positive	327.1	205	17
46	Diniconazole	7.95	Positive	326.2	70.2	13
		7.95	Positive	326.2	159	11
47	Dinotefuran	1.37	Positive	203.1	129.2	41
		1.37	Positive	203.1	157.2	25
48	Dioxacarb	4.61	Positive	224.1	123	17
		4.61	Positive	224.1	167	13

\*Parent compound

\*\* Only metabolite



**Table 2 (part 3). List of pesticides with MRM transitions used**

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
49	Diuron	6.21	Positive	233.1	72	19
		6.21	Positive	235.1	72.1	15
50	Doramectin	9.96	Positive	916.6	331.4	35
		9.96	Positive	916.6	593.5	11
51	Emamectin-benzoate b1a	8.18	Positive	886.5	82.1	53
		8.18	Positive	886.5	158.1	29
52	Epoconazole	7.44	Positive	330	101.1	28
		7.44	Positive	330	121.1	19
53	Eprinomectin	9.15	Positive	914.6	154.2	35
		9.15	Positive	914.6	186.2	25
54	Etaconazole	7.44	Positive	328.1	159	33
		7.44	Positive	328.1	205	19
55	Ethirimol	4.40	Positive	210.2	98.1	57
		4.40	Positive	210.2	140.1	22
56	Etoxazole	9.46	Positive	360.1	57.2	35
		9.46	Positive	360.1	141	17
56	Fenamidone	7.40	Positive	312.1	92	33
		7.40	Positive	312.1	236.1	19
58	Fenarimol	7.31	Positive	331	81	29
		7.31	Positive	331	268	15
59	Fenazaquin	9.69	Positive	307.1	147	33
		9.69	Positive	307.1	161.1	15
60	Fenbuconazole	7.75	Positive	337	70	31
		7.75	Positive	337	124.9	11
61	Fenpropimorph	6.79	Positive	304	117	27
		6.79	Positive	304	147	13
62	Fenpyroximate	9.44	Positive	422	135.1	29
		9.44	Positive	422	366.1	13
63	Fenuron	4.19	Positive	165.1	46	25
		4.19	Positive	165.1	72.1	27
64	Fipronil*	8.18	Negative	435	250	47
		8.18	Negative	435	330	37
65	Fluazinam	9.11	Negative	462.7	397.80	47
		9.11	Negative	462.7	415.70	37
66	Flubendiamide	8.11	Positive	683.1	274.1	35
		8.11	Positive	683.1	408	33
67	Flufenacet*	7.86	Positive	364.1	152.1	23
		7.86	Positive	364.1	194.2	17
68	Fluometuron	6.30	Positive	233.1	46	27
		6.30	Positive	233.1	72.1	19
69	Fluoxastrobin	7.90	Positive	459.2	188	19
		7.90	Positive	459.2	427.2	17
70	Flusilazole	7.71	Positive	316.1	165.1	13
		7.71	Positive	316.1	247.1	11
71	Flutriafol	6.38	Positive	302.1	70.1	41
		6.38	Positive	302.1	123	25
72	Flutolanil	7.82	Positive	324.1	242.1	17
		7.82	Positive	324.1	262.1	13

\*Parent compound

\*\* Only metabolite

**Table 2 (part 4). List of pesticides with MRM transitions used**

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
73	Forchlorfenuron	6.37	Positive	248	93.1	19
		6.37	Positive	248	129.1	15
74	Formetanate-HCL	1.11	Positive	222.1	120	35
		1.11	Positive	222.1	165	11
75	Fuberidazole	2.5	Positive	185	65	53
		2.5	Positive	185	157	29
76	Furalaxyl	7.16	Positive	302.1	95	28
		7.16	Positive	302.1	242.1	19
77	Furathiocarb	9.06	Positive	383.1	195.1	35
		9.06	Positive	383.1	252.1	25
78	Hexaconazole	7.78	Positive	314.1	70	33
		7.78	Positive	314.1	159	19
79	Hexythiazox	9.32	Positive	353.1	168	57
		9.32	Positive	353.1	228	22
80	Imazalil	6.10	Positive	297.0	159	35
		6.10	Positive	297.0	201	17
81	Imidacloprid	4.55	Positive	256	175.1	33
		4.55	Positive	256	209.1	19
82	Indoxacarb	8.76	Positive	528	203	29
		8.76	Positive	528	218	15
83	Ipconazole-I	8.21	Positive	334.2	70	33
		8.21	Positive	334.2	125	15
84	Ipconazole-II	8.25	Positive	334.2	70	31
		8.25	Positive	334.2	125	11
85	Iprovalicarb	7.27	Positive	321.2	119	27
		7.27	Positive	321.2	203.1	13
86	Isoprocarb	6.63	Positive	194.1	95	29
		6.63	Positive	194.1	137	13
87	Isoproturon	6.46	Positive	207.2	46.1	25
		6.46	Positive	207.2	72.1	27
88	Ivermectin	10.74	Positive	892.6	307.3	47
		10.74	Positive	892.6	569.5	37
89	Linuron	7.22	Positive	249.1	160	47
		7.22	Positive	249.1	182.1	37
90	(Monceren) Pencycuron	7.95	Positive	329.1	125	35
		7.95	Positive	329.1	218.1	33
91	Mandipropamid	7.48	Positive	412.1	328.1	23
		7.48	Positive	412.1	356.1	17
92	Mefenacet	7.44	Positive	299	120.1	27
		7.44	Positive	299	148.1	19
93	Mepanipyrim	7.60	Positive	224	77	19
		7.60	Positive	224	106	17
94	Mepronil	7.67	Positive	270.1	119.1	13
		7.67	Positive	270.1	228	11
95	Metalaxyl*	6.44	Positive	280.1	192.2	41
		6.44	Positive	280.1	220.2	25
96	Metconazole	7.81	Positive	320.1	70	17
		7.81	Positive	320.1	125	13

\*Parent compound

\*\* Only metabolite

**Table 2 (part 5). List of pesticides with MRM transitions used**

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
97	Methabenzthiazuron	6.12	Positive	222.1	150.3	19
		6.12	Positive	222.1	165.2	15
98	Methamidophos	0.70	Positive	142	94	35
		0.70	Positive	142	125	11
99	Methiocarb*	7.15	Positive	226.1	121.1	53
		7.15	Positive	226.1	169.1	29
100	Methoprotryne	5.72	Positive	272.2	198	28
		5.72	Positive	272.2	240.2	19
101	Methoxyfenozide	7.65	Positive	369.1	149.1	35
		7.65	Positive	369.1	313.2	25
102	Metobromuron	6.65	Positive	259	148.2	33
		6.65	Positive	259	170.2	19
103	Metribuzin	5.75	Positive	215.1	84.1	57
		5.75	Positive	215.1	187.1	22
104	Mevinphos Isomer-I	4.41	Positive	225.101	127.1	35
		4.41	Positive	225.101	193.2	17
105	Mevinphos Isomer-II	4.99	Positive	225.102	127.1	33
		4.99	Positive	225.102	193.2	19
106	Mexacarbate	2.08	Positive	223.2	151	29
		2.08	Positive	223.2	166.1	15
107	Monocrotophos	2.49	Positive	224.1	98	33
		2.49	Positive	224.1	127.1	15
108	Monolinuron	6.47	Positive	215.1	99	31
		6.47	Positive	215.1	126.1	11
109	Moxidectin	10.40	Positive	640.4	498.5	27
		10.40	Positive	640.4	528.5	13
110	Myclobutanil	7.43	Positive	289	70	29
		7.43	Positive	289	125	13
111	Nitenpyram	2.57	Positive	271	126	25
		2.57	Positive	271	225.2	27
112	Omethoate	0.85	Positive	214	124.9	47
		0.85	Positive	214	182.8	37
113	Oxadixyl	5.73	Positive	279.1	132.1	47
		5.73	Positive	279.1	219.1	37
114	Paclbutrazol	7.02	Positive	294	70	35
		7.02	Positive	294	125	33
115	Penconazole	7.81	Positive	284.1	70	23
		7.81	Positive	284.1	159	17
116	Phenmedipham	7.13	Positive	301.2	107.9	27
		7.13	Positive	301.2	168	19
117	Picoxystrobin	8.23	Positive	368	145	19
		8.23	Positive	368	205	17
118	Piperonyl butoxide	8.60	Positive	356.2	119.1	13
		8.60	Positive	356.2	177.2	11
119	Pirimicarb	4.17	Positive	239.2	72.1	41
		4.17	Positive	239.2	182.1	25
120	Prochloraz	7.56	Positive	376	70	17
		7.56	Positive	376	308	13

\*Parent compound

\*\* Only metabolite

**Table 2 (part 6). List of pesticides with MRM transitions used**

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
121	Promecarb*	7.32	Positive	208.1	109	19
		7.32	Positive	208.1	151	15
122	Prometon	5.32	Positive	226.1	86	35
		5.32	Positive	226.1	142	11
123	Prometryne	6.41	Positive	242.2	158.1	53
		6.41	Positive	242.2	200.1	29
124	Propamocarb+	1.33	Positive	189.2	102	28
		1.33	Positive	189.2	144	19
125	Propiconazole	7.92	Positive	342.1	69	35
		7.92	Positive	342.1	159	25
126	Prothioconazole*	7.86	Positive	344.1	125.1	33
		7.86	Positive	344.1	188.9	19
127	Pyracarbolid	6.16	Positive	218.1	97	57
		6.16	Positive	218.1	125	22
128	Pyraclostrobin	8.41	Positive	388	163	35
		8.41	Positive	388	194	17
129	Pyridaben	9.80	Positive	365	147	33
		9.80	Positive	365	309	19
130	Pyrimethanil	6.24	Positive	200	82	29
		6.24	Positive	200	107	15
131	Pyriproxyfen	9.15	Positive	322	96	33
		9.15	Positive	322	185	15
132	Quinoxifen	8.91	Positive	308.1	162.1	31
		8.91	Positive	308.1	197.1	11
133	Rotenone	7.86	Positive	395.1	192.1	27
		7.86	Positive	395.1	213.1	13
134	Secbumeton	5.38	Positive	226.2	100	29
		5.38	Positive	226.2	170.1	13
135	Siduron	7.02	Positive	233.3	94	25
		7.02	Positive	233.3	137.2	27
136	Simetryn	5.16	Positive	214	124	47
		5.16	Positive	214	144	37
137	Spinetoram*	8.00	Positive	748.5	98.1	47
		8.00	Positive	748.5	142.2	37
138	Spinosad (Spinosyn A)	7.52	Positive	732.5	98.1	35
		7.52	Positive	732.5	142.2	33
139	Spinosad (Spinosyn D)	7.83	Positive	746.8	98.3	23
		7.83	Positive	746.8	142.4	17
140	Spiromesifen	9.84	Positive	371.2	255.2	27
		9.84	Positive	371.2	273.2	19
141	Spiroxamine	6.85	Positive	298.2	100.1	19
		6.85	Positive	298.2	144.2	17
142	Tebufenozide	7.99	Positive	353.2	133	13
		7.99	Positive	353.2	297.2	11
143	Tebufenpyrad	8.81	Positive	334	117	41
		8.81	Positive	334	145	25
144	Tebuthiuron	5.34	Positive	229.1	116.1	17
		5.34	Positive	229.1	172.4	13

\*Parent compound

\*\* Only metabolite

**Table 2 (part 7). List of pesticides with MRM transitions used**

Sr. No	Compound	RT (min)	Polarity	Precursor (m/z)	Product Ion (m/z)	Collision Energy (V)
145	Terbumeton	5.38	Positive	226.1	100	19
		5.38	Positive	226.1	170.1	15
146	Terbutryn	6.51	Positive	242.1	68.1	35
		6.51	Positive	242.1	186.1	11
147	Tetraconazole	7.59	Positive	372.1	70	53
		7.59	Positive	372.1	159	29
148	Thiabendazole	2.10	Positive	202.1	131.2	28
		2.10	Positive	202.1	175.1	19
149	Thiacloprid	5.38	Positive	253	99	35
		5.38	Positive	253	126	25
150	Thiamethoxam	3.73	Positive	292	181	33
		3.73	Positive	292	211	19
151	Thidiazuron	5.68	Positive	221.1	102.1	57
		5.68	Positive	221.1	127.9	22
152	Thiobencarb	8.49	Positive	258	125	35
		8.49	Positive	258	89	17
153	Thiophanate-methyl	5.94	Positive	343	151.1	33
		5.94	Positive	343	311	19
154	Triadimefon	7.47	Positive	294	197.1	29
		7.47	Positive	294	225	15
155	Triadimenol	7.02	Positive	296.1	70	33
		7.02	Positive	296.1	227.1	15
156	Tricyclazole	5.05	Positive	190	136	31
		5.05	Positive	190	163	11
157	Trifloxystrobin	8.79	Positive	409	186	27
		8.79	Positive	409	206	13
158	Triflumizole*	8.27	Positive	346.1	73	29
		8.27	Positive	346.1	278.1	13
159	Vamidothion	4.28	Positive	288	118	25
		4.28	Positive	288	146	27
160	Zoxamide	8.40	Positive	336.1	159	47
		8.40	Positive	336.1	187	37

\*Parent compound

\*\* Only metabolite

**Table 3 (part 1). Method validation data (recovery and % RSD)**

Sr. No.	Name of Compound	Apple				Ion Ratio at 0.005 mg/kg ( $\pm 30\%$ )	Grape				Ion Ratio at 0.005 mg/kg ( $\pm 30\%$ )
		0.005 (mg/kg)		0.01 (mg/kg)			0.005 (mg/kg)		0.01 (mg/kg)		
		% Rec.	% RSD	% Rec.	% RSD		% Rec.	% RSD	% Rec.	% RSD	
1	3-Hydroxycarbofuran	93	10.2	87	4.9	8.48	82	6.2	104	8.4	-7.48
2	Acephate	105	12.3	90	4.9	-2.22	114	3.5	110	0.3	-12.78
3	Acetamiprid	101	15.4	96	5.4	-3.10	114	17.9	101	15.8	-3.82
4	Aldicarb sulfone	104	12.1	95	10.4	-12.43	75	5.3	109	6.2	0.21
5	Ametryn	113	4.4	99	2.3	-2.17	86	3.9	105	4.4	7.75
6	Aminocarb	113	5.1	104	3.1	21.55	119	1.8	117	2.0	3.28
7	Amitraz	102	11.9	98	9.9	-22.99	87	7.2	98	9.7	4.93
8	Avermectin B1a	93	16.2	106	14.3	12.31	101	7.1	103	17.5	-1.14
9	Azoxystrobin	104	4.7	109	7.2	-7.92	91	11.2	95	3.8	4.03
10	Benalaxyl	119	13.3	117	2.8	-4.16	96	4.0	117	1.7	1.02
11	Bendiocarb	116	14.4	105	8.3	7.14	101	13.5	111	4.7	1.54
12	Benzoximate	95	4.5	80	6.2	-2.80	93	3.8	75	3.8	6.80
13	Bifenazate	89	14.8	104	15.5	13.49	95	6.0	100	5.1	1.57
14	Bitertanol	98	18.0	83	13.5	-0.65	99	6.9	95	4.0	-2.33
15	Boscalid	87	12.5	91	10.1	16.55	96	10.9	105	5.1	11.64
16	Bromucanazole I	103	4.6	104	16.2	8.38	114	7.3	118	7.9	-18.96
17	Bromucanazole II	82	17.8	91	14.7	-2.64	79	6.1	82	9.4	-6.60
18	Bupirimate	116	2.4	114	8.9	-3.62	113	6.3	119	4.3	-11.08
19	Buprofezin	83	11.8	72	3.8	3.43	118	1.1	106	16.5	4.59
20	Butafenacil	106	15.3	110	11.1	-9.97	106	13.1	104	7.0	5.88
21	Butocarboxim	94	18.5	83	9.3	0.59	74	2.9	79	17.9	0.29
22	Butoxycarboxim	104	1.6	91	1.7	-14.71	95	3.2	94	2.0	10.34
23	Carbendazim	110	6.9	120	1.9	-11.90	101	5.3	96	6.2	8.43
24	Carbetamide	106	13.3	88	3.9	-12.29	99	14.2	89	17.6	-13.57
25	Carbofuran	100	9.1	91	4.2	-2.15	96	7.3	81	7.5	-11.39
26	Carboxin	107	3.5	100	4.6	6.34	87	6.2	96	3.1	0.25
27	Chlorantraniliprole	113	9.9	93	3.6	17.59	98	10.3	118	6.6	2.85
28	Chlorotoluron	120	3.7	103	4.5	-11.42	102	5.5	119	4.9	16.25
29	Chloroxuron	119	14.8	115	4.3	-8.01	98	15.7	119	2.3	-5.72
30	Clethodim	112	5.2	83	9.3	-9.65	98	8.4	77	5.9	-7.69
31	Clothianidin	88	15.7	103	13.4	-1.59	116	10.3	91	7.0	-0.90
32	Cyazofamid	89	18.3	77	12.7	2.06	107	8.6	107	16.6	2.16
33	Cycluron	117	2.7	99	2.5	15.10	96	6.1	108	4.4	-12.62
34	Cyproconazole	118	15.6	106	7.9	-14.35	102	13.8	113	4.7	13.56
35	Cyprodinil	95	11.4	82	4.7	-0.62	98	10.2	89	4.3	-9.41
36	Cyromazine	93	5.6	117	9.0	0.82	87	4.4	99	3.9	-17.95
37	Desmedipham	110	4.9	99	3.8	-10.41	107	3.9	118	2.3	9.75
38	Diclobutrazol	102	6.7	89	10.7	27.62	105	12.1	90	4.5	4.86
39	Dicrotophos	112	3.8	97	3.7	-0.96	115	2.0	109	3.0	1.19
30	Diethofencarb	104	2.4	97	8.3	8.44	119	14.0	115	14.5	7.02
41	Difenoconazole	100	6.8	88	4.2	26.84	107	9.1	99	11.4	-12.18
42	Dimethoate	97	4.4	86	7.9	-9.08	98	6.2	95	1.9	2.63
43	Dimethomorph I	112	7.6	92	4.0	-1.54	88	2.1	106	3.3	1.40
44	Dimethomorph II	110	19.7	90	9.6	-1.83	90	2.5	99	6.5	-11.91
45	Dimoxystrobin	98	2.9	87	10.4	17.67	83	6.1	105	2.3	-9.62
46	Diniconazole	90	13.3	89	16.0	-19.41	118	0.5	77	9.9	-19.62
47	Dinotefuran	79	3.0	90	9.0	-0.74	109	5.3	115	2.0	0.92
48	Dioxacarb	88	15.7	72	9.0	-0.51	91	13.3	71	5.6	0.42

**Table 3 (part 2). Method validation data (recovery and % RSD)**

Sr. No.	Name of Compound	Apple				Ion Ratio at 0.005 mg/kg (±30%)	Grape				Ion Ratio at 0.005 mg/kg (±30%)
		0.005 (mg/kg)		0.01 (mg/kg)			0.005 (mg/kg)		0.01 (mg/kg)		
		% Rec.	% RSD	% Rec.	% RSD		% Rec.	% RSD	% Rec.	% RSD	
49	Diuron	99	14.4	89	3.2	1.93	90	9.2	105	5.2	-2.23
50	Doramectin	101	17.3	102	14.5	-0.51	118	14.9	80	15.7	-7.23
51	Emamectin-benzoate b1a	105	7.5	109	10.7	-15.15	104	13.8	82	16.4	-2.18
52	Epoxiconazole	97	5.4	80	12.0	-20.16	109	8.3	82	15.3	5.35
53	Eprinomectin	98	12.2	104	10.5	-21.99	75	19.8	105	14.8	-7.01
54	Etaconazole	104	5.5	94	3.5	11.69	110	8.7	113	3.5	-7.82
55	Ethirimol	85	6.2	91	7.6	-6.16	78	16.9	71	6.8	2.52
56	Etoxazole	104	7.9	97	10.8	11.29	76	2.7	98	3.6	17.42
57	Fenamidone	83	9.4	81	6.3	-4.53	83	10.1	71	7.1	-10.32
58	Fenarimol	100	15.2	101	16.3	4.07	119	2.6	104	15.0	9.80
59	Fenazaquin	101	7.0	84	7.7	-11.97	105	3.8	94	5.1	1.77
60	Fenbuconazole	100	14.9	85	7.4	-18.16	83	9.0	75	14.1	-3.35
61	Fenpropimorph	98	8.7	103	4.3	-12.33	97	5.9	112	7.3	2.69
62	Fenpyroximate	114	8.8	97	10.5	14.49	97	5.0	120	0.9	-19.35
63	Fenuron	111	10.9	93	6.6	23.31	94	12.6	107	6.3	10.82
64	Fipronil	96	11.1	111	4.0	0.66	118	9.9	115	6.5	20.01
65	Fluazinam†	76	16.9	86	11.3	-3.60	99	17.2	74	3.1	-2.80
66	Flubendiamide	112	10.4	93	9.7	-12.24	88	11.0	93	8.2	13.03
67	Flufenacet	107	18.1	95	12.4	3.68	76	15.6	82	17.2	18.10
68	Fluometuron	114	6.6	106	7.7	-9.53	89	10.0	119	7.6	15.81
69	Fluoxastrobin	94	5.7	102	6.8	-17.42	78	10.7	112	8.5	-14.25
70	Flusilazole	80	8.7	70	3.6	2.46	86	4.9	70	4.8	0.44
71	Flutolanil	91	17.6	96	1.9	19.76	104	13.8	72	12.6	-2.72
72	Flutriafol	89	11.4	77	8.0	11.73	90	13.4	71	5.4	-3.37
73	Forchlorfenuron	92	4.2	82	4.8	-15.87	82	6.1	100	6.0	3.75
74	Formetanate HCl	91	7.2	105	9.6	7.75	86	1.4	92	1.7	4.39
75	Fuberidazole	101	6.4	85	3.9	-8.86	75	6.7	71	7.0	-16.79
76	Furalaxyl	118	4.2	112	6.0	3.86	74	8.4	106	6.8	-3.31
77	Furathiocarb	86	4.4	82	3.7	-2.11	73	2.1	81	3.9	0.52
78	Hexaconazole	96	10.4	86	15.2	-7.89	97	15.8	105	18.4	-12.63
79	Hexythiazox	101	8.10	96	8.8	1.55	118	6.5	102	20.0	2.14
80	Imazalil	84	14.5	98	8.3	7.60	94	7.0	86	6.0	13.18
81	Imidacloprid	114	4.6	102	5.8	6.29	98	9.9	101	10.2	-0.71
82	Indoxacarb	95	15.4	88	13.3	-14.78	93	14.1	83	13.3	9.07
83	Ipconazole I	79	10.3	72	9.9	-14.81	93	19.1	74	15.7	11.17
84	Ipconazole II	88	10.1	80	17.2	-4.50	82	17.7	83	11.2	-5.81
85	Iprovalicarb	113	7.4	104	6.1	8.59	90	6.5	118	6.8	4.11
86	Isoprocarb	104	19.4	115	7.1	-12.31	102	15.1	96	16.0	-6.03
87	Isoproturon	83	8.7	79	3.5	24.58	92	4.6	71	6.0	1.54
88	Ivermectin	118	17.8	109	6.7	2.67	114	5.6	108	15.4	-0.39
89	Linuron	102	7.7	93	1.3	8.85	105	15.1	88	19.4	20.00
90	Mandipropamid	76	5.1	74	4.8	-22.21	90	6.1	108	4.8	1.37
91	Mefenacet	92	5.8	83	3.5	4.02	77	5.1	92	4.0	0.55
92	Mepanipyrim	103	7.5	80	5.4	23.10	102	4.3	83	6.2	4.74
93	(Monceren) Pencycuron	87	8.2	71	17.8	21.76	77	4.9	76	3.2	13.04
94	Mepronil	119	11.5	106	16.6	8.22	97	5.9	117	1.3	10.66
95	Metalaxyl	115	3.5	103	4.2	-4.38	89	4.8	95	5.8	7.89
96	Metconazole	96	7.9	98	1.5	-2.91	93	17.0	118	7.6	-11.55

**Table 3 (part 3). Method validation data (recovery and % RSD)**

Sr. No.	Name of Compound	Apple				Ion Ratio at 0.005 mg/kg (±30%)	Grape				Ion Ratio at 0.005 mg/kg (±30%)
		0.005 (mg/kg)		0.01 (mg/kg)			0.005 (mg/kg)		0.01 (mg/kg)		
		% Rec.	% RSD	% Rec.	% RSD		% Rec.	% RSD	% Rec.	% RSD	
97	Methabenzthiazuron	115	6.0	100	5.7	19.94	93	4.3	114	10.1	6.05
98	Methamidophos	108	7.0	105	1.1	-5.86	79	6.9	86	2.7	12.50
99	Methiocarb	105	10.7	80	8.2	2.42	87	7.8	81	9.1	5.23
100	Methoprotryne	108	6.9	96	5.2	-17.03	87	8.3	95	3.9	0.91
101	Methoxyfenozide	107	5.0	86	7.8	-7.16	76	2.3	94	2.4	14.61
102	Metobromuron	118	3.3	103	5.1	6.93	79	13.1	93	11.3	1.61
103	Metribuzin	114	19.0	86	14.5	7.70	102	8.3	117	6.1	5.69
104	Mevinphos I	105	8.1	95	4.7	19.19	120	9.1	109	9.7	-3.11
105	Mevinphos II	95	14.8	99	5.4	18.88	84	12.9	87	11.4	23.85
106	Mexacarbate	107	2.6	93	1.2	-9.36	96	3.3	96	1.1	1.92
107	Monocrotophos	107	2.5	97	5.6	6.17	114	2.2	117	3.0	1.46
108	Monolinuron	92	15.5	99	8.8	-9.20	101	7.5	81	4.5	-9.80
109	Moxidectin	98	19.0	86	19.5	4.06	82	14.8	96	8.6	1.06
110	Myclobutanil	110	11.5	105	4.0	-13.60	99	17.1	119	9.7	3.65
111	Nitenpyram	100	9.6	93	6.6	5.79	96	1.8	88	7.5	5.67
112	Omethoate	119	1.8	113	4.1	-12.55	111	2.4	115	2.1	20.64
113	Oxadixyl	109	4.8	93	3.1	12.67	102	7.5	85	3.5	8.66
114	Paclobutrazol	99	5.2	85	7.2	18.86	89	4.6	91	5.7	-8.54
115	Penconazole	107	6.4	88	10.4	-5.41	95	7.8	88	8.4	8.05
116	Phenmedipham	99	10.8	101	3.8	19.75	98	7.5	118	1.8	-2.57
117	Picoxystrobin	91	3.3	77	2.6	-6.55	93	4.8	73	1.8	4.27
118	Piperonyl butoxide	120	2.0	108	2.9	8.86	88	2.4	120	0.7	9.37
119	Pirimicarb	107	2.6	90	1.9	3.33	95	2.8	98	7.6	2.16
120	Prochloraz	115	7.8	102	6.7	15.78	101	6.6	101	5.7	-12.67
121	Promecarb	109	16.0	82	17.4	-10.84	112	7.0	116	3.7	-12.67
122	Prometon	115	9.5	87	1.9	-6.87	102	5.6	96	9.0	0.25
123	Prometryne	94	3.8	83	2.7	-5.82	90	2.8	81	1.6	0.66
124	Propamocarb	105	5.1	118	6.25	-4.46	92	1.7	97	1.8	19.52
125	Propiconazole	94	3.8	83	2.7	-20.92	90	10.0	75	8.1	3.11
126	Prothioconazole	98	5.2	110	3.6	4.05	108	5.3	120	0.9	3.75
127	Pyracarbolid	109	9.1	83	2.7	13.22	109	2.3	96	10.4	13.04
128	Pyraclostrobin	95	8.7	101	9.5	-7.64	568	5.1	797	29.5	2.74
129	Pyridaben	80	10	73	7.9	-5.02	85	4.5	71	4.0	2.07
130	Pirimethanil	81	9.1	79	6.25	3.55	95	18.5	87	5.3	15.50
131	Pyriproxyfen	74	2.6	70	2.3	-14.68	74	3.4	72	1.3	-3.64
132	Quinoxifen	99	4.8	94	4.3	12.11	104	9.7	112	2.5	-16.72
133	Rotenone	101	13.43	98	15.65	6.43	111	19.2	100	19.8	19.20
134	Secbumeton	108	9.6	90	2.0	-2.73	95	2.2	109	7.7	10.31
135	Siduron	116	3.9	104	7.2	11.05	101	10.5	119	1.8	-0.09
136	Simetryn	103	12.6	96	1.9	-7.68	94	10.5	96	7.7	-13.73
137	Spinetoram	94	8.6	88	6.6	-0.62	103	11.0	91	7.3	7.05
138	Spinosad (Spinosyn A)	117	5.1	108	6.0	-7.20	90	12.7	102	9.1	4.43
139	Spinosad (Spinosyn D)	117	11.5	94	7.2	4.40	109	11.1	100	10.7	9.02
140	Spiromesifen	107	8.9	99	9.1	-9.71	81	4.6	114	4.2	20.49
141	Spiroxamine	107	3.6	93	3.3	5.26	92	4.1	99	2.5	1.45
142	Tebufenozide	99	6.25	101	11.23	11.31	112	4.2	110	5.8	5.13
143	Tebufenpyrad	77	11.2	71	9.1	-1.26	99	6.3	87	4.2	15.34
144	Tebuthiuron	99	14.7	83	2.1	-8.50	78	1.2	89	19.7	9.05



Table 3 (part 4). Method validation data (recovery and % RSD)

Sr. No.	Name of Compound	Apple				Ion Ratio at 0.005 mg/kg ( $\pm 30\%$ )	Grape				Ion Ratio at 0.005 mg/kg ( $\pm 30\%$ )
		0.005 (mg/kg)		0.01 (mg/kg)			0.005 (mg/kg)		0.01 (mg/kg)		
		% Rec.	% RSD	% Rec.	% RSD		% Rec.	% RSD	% Rec.	% RSD	
145	Terbutmeton	108	6.8	91	2.0	9.95	99	5.2	100	7.7	-7.76
146	Terbutryn	110	4.0	98	2.1	-2.71	91	3.2	98	3.1	18.14
147	Tetraconazole	99	8.5	97	7.2	23.39	92	15.3	95	9.5	-10.62
148	Thiabendazole	98	5.9	89	3.5	8.11	89	4.7	83	2.4	6.10
149	Thiacloprid	98	15.8	77	7.2	-1.85	71	7.7	109	13.2	-4.38
150	Thiamethoxam	112	6.9	96	4.0	29.72	96	4.6	93	3.8	-0.21
151	Thidiazuron	114	9.5	95	5.7	-26.96	91	2.6	109	5.3	7.65
152	Thiobencarb	77	8.5	85	9.2	23.77	88	18.2	93	15.2	13.98
153	Thiophanate-methyl	110	10.1	105	5.1	6.04	119	5.1	88	10.3	29.18
154	Triadimefon	84	14.0	95	18.2	5.97	96	14.1	115	13.4	-5.13
155	Triadimenol	79	9.1	81	13.6	21.61	80	11.9	90	5.8	14.97
156	Tricyclazole	93	13.0	93	4.8	5.64	104	6.3	93	14.6	4.29
157	Trifloxystrobin	72	5.3	72	4.9	-8.44	90	1.9	117	4.4	6.49
158	Triflumizole	93	9.6	99	11.6	9.56	113	5.4	115	3.4	29.27
159	Vamidothion	104	7.3	85	7.2	8.96	94	6.2	99	9.1	-13.76
160	Zoxamide	109	5.6	104	18.8	15.35	94	5.6	102	16.5	-15.76

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