APPLICATION NOTE 65607

Simultaneous screening and quantitation of pesticides residue in milk at trace level using high resolution Orbitrap GC-MS

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Goal

The objective of this work was to develop and evaluate an analytical method for the simultaneous screening and quantitation of 162 pesticide residues in milk using gas chromatography (GC) and high resolution accurate mass spectrometry (HRAM). The optimized method was developed following the European Union SANTE guidelines and assessed against the fulfillment of the Food Safety and Standards Authority of India (FSSAI) as well as the European Commission (EC) MRLs requirement for milk.

Introduction

Pesticide residue analysis is an essential aspect of ensuring a safe global food supply chain. There are many pesticides authorized for use on crops, and these pesticides have the potential to accumulate in the environment and enter the food chain via various routes. Due to this environmental contamination, these pesticides could be deposited in animal tissues as well as in milk[1].

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With the available technologies, such as GC-MS/MS, it is possible to check and quantify the presence of pesticides in milk with unit mass resolution as per the SANTE/11813/2017 confirmation and quantification criteria[2]. When using triple quadrupole MS, the selectivity required to separate target pesticides from the chemical background is achieved using selected reaction monitoring (SRM). SRM is used in targeted experiments in which the mass spectrometer is pre-programmed, utilizing a list of predefined target compounds such as pesticides. During acquisition, the targeting of specific lists of compounds limits the scope of analysis and can result in non-detection (false negative) for untargeted compounds. This limitation has motivated laboratories to develop methods using high-resolution mass spectrometry that can operate in full scan with a higher mass resolving power than triple quadrupoles, but also provide similar analytical performance. In addition to the instrument, sample preparation is also equally important. For sample preparation, there are few methods reported for multi-pesticides residue analysis with respect to their scope. However, to cover the target list of diversified chemistries, the most popular QuEChERS is preferred[3].

This work aimed to optimize the method for pesticide residues screening and quantification in milk by using EN QuEChERS sample preparation in combination with the Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS system in full scan mode. The data acquisition and processing was carried out using Thermo Scientific™ TraceFinder™ software. The optimized method was validated as per the SANTE/11813/2017 validation guidelines[2].

Experimental

Instrument conditions

The Thermo Scientific™ TRACE™ 1310 gas chromatograph was coupled with the Exactive GC Orbitrap GC-MS system with electron impact (EI) ionization to provide high-resolution, accurate-mass analysis. The specific, optimized GC-Orbitrap conditions are given in Table 1.

Table 1. GC-Orbitrap instrument conditions

a) Gas chromatography method	
Instrumentation	TRACE 1310 GC with Thermo Scientific™ TriPlus™ RSH autosampler
Column	Thermo Scientific™ TraceGOLD™ TG-5SIL-MS (30 m x 0.25 mm i.d. x 0.25 µm) P/N 26096-1420
Injector	Programmed temperature vaporizing injector (PTV)
Liner	Siltek™ six baffle PTV liner (P/N 453T2120)
Injector mode	Cold splitless
Splitless time	2.0 min
Split flow	50.0 mL/min
Purge flow	5.0 mL/min
Stop purge for	0.50 min
Injection volume	1 µL
Column flow	1.20 mL/min
Carrier gas and purity	Helium (99.999%)
Vacuum compensation	On
PTV program	85 ˚C, 0.10 min hold, 2.5 ˚C/min to 300 ˚C, 3.0 min hold, 14.5 ˚C/min to 320 ˚C, 5.0 min hold, 75.0 mL/min flow
Cleaning phase	On
Post-cycle temperature	Cool down
Total run time	35.6 min
GC oven program	90 ˚C, 5 min hold, 25 ˚C/min to 180 ˚C, 5 ˚C/min to 280 ˚C, 10 ˚C/min to 300 ˚C, 5 min hold
b) Orbitrap mass spectrometry method	
Instrumentation	Exactive GC Orbitrap System with ExtractaBrite ion source and VPI technology
Acquisition mode	Full scan
MS transfer line temp.	310 ˚C
Ion source temp.	320 ˚C
Electron energy	70 eV
Resolving power	60,000 (FWHM at *m/z* 200)
Mass range	50–500 Da
Ionization	Electron ionization (EI)

Sample preparation

Reagents and chemicals

- Acetonitrile, Fisher Scientific™ Optima™ grade [514 L-16923 U]
- Anhydrous Magnesium Sulfate, Thermo Scientific [P/N 80020-415-500]
- EN 15662 QuEChERS Extraction kit (4 g anhydrous $MgSO_4$, 1 g sodium chloride, 1 g Na_3Citrate, and 500 mg Na_2Citrate), Thermo Scientific™ [60105-216]
- Bulk C_{18} Octadecyl Endcapped, Thermo Scientific™ [P/N 80020-413-100]
- Bulk PSA (Primary Secondary Amine), Thermo Scientific™ [80020-416-100]

Sample extraction and clean-up

The EN 15662 buffered QuEChERS method was used for extraction[3].

- Homogenized sample (10 g) was weighed into a 50 mL extraction tube.
- Recovery spike samples (n=6 for each level) were prepared by spiking blank samples with the pesticides mix at 0.005, 0.010, and 0.025 mg/kg. Recovery samples were spiked before the addition of water and extraction solvent.
- HPLC grade water (10 mL) was added.
- Acetonitrile (10 mL) was added to the tube.
- The tube was shaken vigorously for 1 minute on a vortex mixer at 2500 rpm.
- The EN 15662 QuEChERS Extraction kit was added to the tube, and the tube was again mixed vigorously for 1 minute on a vortex mixer at 2500 rpm.
- The tube was centrifuged at 5000 rpm for 5 min.
- The supernatant (1 mL) was transferred into the 2 mL microcentrifuge tube containing 150 mg $MgSO_4$, 25 mg PSA, and 50 mg C_{18}.
- Samples were vortexed for 1 min and centrifuged at 5000 rpm for 5 min.
- The supernatant was collected and transferred into a GC vial for instrumental analysis.
- The matrix blank (unspiked) extract was prepared by following the above protocol for matrix-matched calibration standards.
- Matrix-matched (MM) calibration standards: the matrix-matched calibration standards were prepared by post-extraction spiking as shown in Table 2b.
- The final extract and MM standards were injected into the Exactive GC-Orbitrap system.

Table 2a. Solvent calibration standards preparation

Working std. (µg/mL)	Vol. taken from working std. (µL)	Solvent (µL)	Final conc. (mg/kg)	Total volume (µL)
2	50	950	0.100	1000
1	50	950	0.050	1000
0.5	50	950	0.025	1000
0.2	50	950	0.010	1000
0.1	50	950	0.005	1000
0.05	50	950	0.0025	1000
0.02	50	950	0.001	1000

Table 2b. Matrix-matched calibration standards preparation

Working std. (µg/mL)	Vol. taken from working std. (µL)	Extracted matrix (µL)	Final conc. (mg/kg)	Total volume (µL)
2	50	950	0.100	1000
1	50	950	0.050	1000
0.5	50	950	0.025	1000
0.2	50	950	0.010	1000
0.1	50	950	0.005	1000
0.05	50	950	0.0025	1000
0.02	50	950	0.001	1000

Data acquisition and processing

The data acquisition and processing were carried out by using Thermo Scientific™ TraceFinder™ software, version 4.1. The data were acquired in full scan mode with a 1 µL injection. For data processing, identification and quantitation of analytes, the mass error (±5.0 PPM) for base peak and confirmatory ions, retention time (±0.10 min), linearity (>0.99 with residuals ±20%), recovery (70–120%) and precision (±20%) were set as user-defined filters as per SANTE guidelines.

Results and discussion

Milk contains water (80–90%), fat (1–9%), protein (4–5%), and carbohydrates (4–5%). Determination of pesticide residues in milk is challenging due to its complex chemical background and high amount of fat. Therefore, the EN QuEChERS method was optimized by use of a higher amount of C_{18} along with primary secondary amine (25 mg) cleanup. The C_{18} (50 mg/mL) offered an excellent response for all target analytes and minimized background noise levels. The higher amount of C_{18} has an adverse effect on sensitivity for 20% compounds. The cleanup, i.e., 25 mg PSA + 50 mg C_{18} + 150 mg $MgSO_4$, was selected for further recovery and precision experiments. Detail results for compounds chosen are presented in Figure 1.

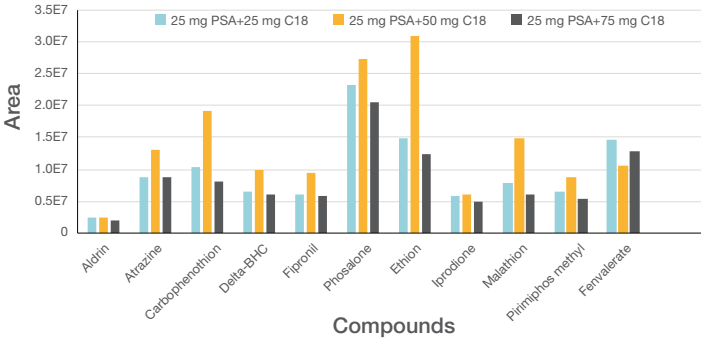

Figure 1. Optimization of C_{18} for the cleanup and detection of pesticides in milk

GC-Orbitrap analysis

Generally, a non-polar solvent is preferred for GC analysis. In this experiment, acetonitrile is used for extraction, followed by an injection into the GC-Orbitrap. It is a low molecular weight, high polarity solvent with a relatively high expansion volume and carries a high amount of matrix co-extractives, which may disturb the chromatography. By considering these challenges, the injection volume was reduced to 1 µL in the programmable temperature vaporization (PTV) injection program given in Table 1a, which offered symmetrical peaks for the target list of analytes. Using acetonitrile also gives an advantage as one can use the same extract for GC-MS and LC-MS, giving larger compound coverage. The gas chromatographic oven program was taken from the Thermo Scientific Pesticide Residue Analyzer Reference, Rev. 2, which offered excellent separation for the target analytes and absence of an isobaric interference from matrix[4]. An extracted ion chromatogram (XIC) for the target list of analytes is shown in Figure 2.

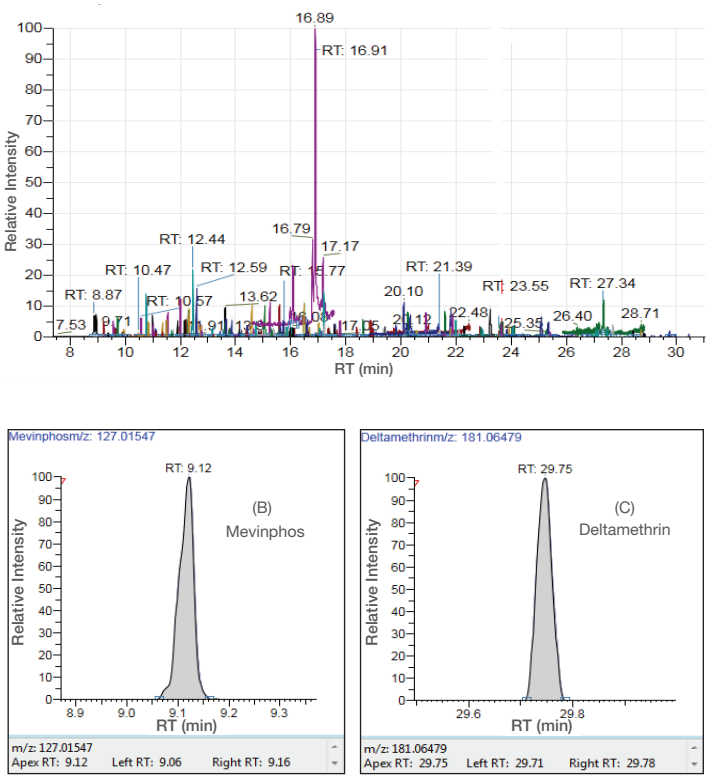

Figure 2. (A) Extracted ion chromatograms (XIC) for 162 compounds in milk spiked at 0.005 mg/kg level, first eluted compound mevinphos (B) and last eluted compound deltamethrin (C)

Method performance

Screening method

The screening detection limit (SDL) is defined as the lowest concentration for which it has been evident that the target analytes could detect at least >95% of the spiked samples and the false negative rate should be <5%. Also, at SDL, the analyte could be identified based on the base peak, but there is no guarantee about confirmation. SDLs were estimated in the range of 0.001–0.002 mg/kg for the target list of analytes in milk by injecting replicate samples (n=20). To confirm the identity of analytes, the following criteria were utilized based on the SANTE guidelines[2].

(i) Two ions per analyte included parent (base peak)/ characteristic confirming ions with mass accuracy ≤5 ppm and peak S/N >3:1.

(ii) Parent ion (base peak) and confirmatory ions must be fully overlapped in the extracted ion chromatogram.

(iii) Retention time (±0.1 min) have been compared with standards in the same sequence.

(iv) Optional: To increase the confidence in identification, an additional ion ratio was monitored (±30%) in comparison with the calibration standards from the same sequence.

In Figure 3, an identification of the fipronil spiked milk sample was demonstrated in full scan spectra for *m/z* 366.94294 (base peak) at 15.69 min retention time with 0.81 ppm mass error observed. This was further confirmed with confirmatory ions (product ions) *m/z* 212.94801 (1.59 ppm mass error) and *m/z* 214.94498 (1.33 ppm mass error). Additionally, an isotopic pattern was monitored for the base peak.

Figure 3. Extracted ion chromatogram along with spectra, isotopic pattern, and fragments for fipronil in the sample spiked at 0.005 mg/kg concentration

To examine the capability of GC-Orbitrap in terms of screening and sensitivity, the post-extraction spiked samples at different concentrations were evaluated. In Figure 4, those compounds met the identification and confirmation criteria as per the SANTE guidelines[2]. Out of 162 compounds, 123 (0.001 mg/kg), 137 (0.0025 mg/kg), 140 (0.005 mg/kg), 146 (0.01 mg/kg), 158 (0.025 mg/kg), and 162 (0.05 mg/kg) met the identification and confirmation criteria. Observed mass error within ±5 ppm has been demonstrated to assess the identification and confirmation criteria for the target analytes.

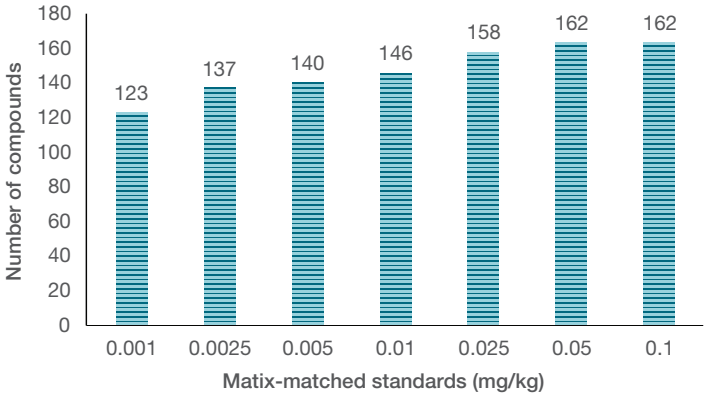

Figure 4. Minimum screened detected concentration for the 162 compounds

Quantitation

For confident quantitation, there is a requirement of symmetrical peak shape. An accurate quantitation is reliant upon several factors, one of which is an acquisition speed should be fast enough to provide at least 10 scans across the chromatographic peak even at high resolution setting (R=60,000). The optimized method provided sufficient scans (>12) per peak for the target list of analytes. This was demonstrated in Figure 5 for fipronil, which has >40 scans per peak with a 6 s peak width, with <2 ppm mass accuracy. Due to the sufficient number of scans per peak, better repeatability was obtained for target analytes.

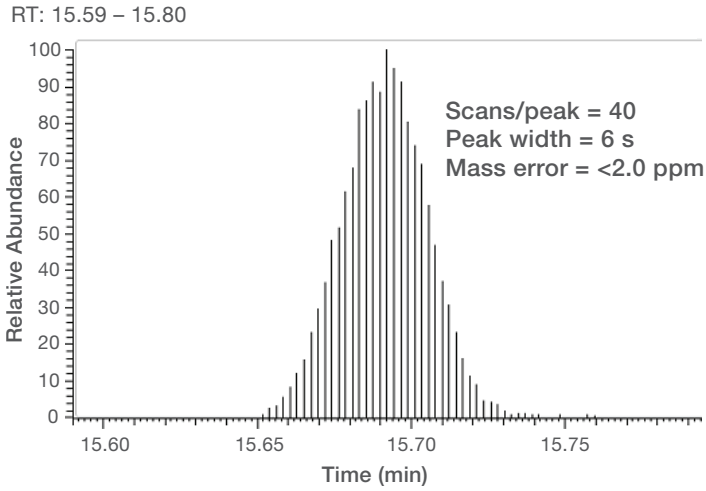

Figure 5. Extracted ion chromatogram for fipronil in spiked milk at 0.010 mg/kg showing scans/peak

Based on the user-defined criteria, the raw data was processed automatically with flagging to show when parameters were out of tolerance (Figure 6). These colored-coded flags indicate whether the results pass or fail as per the acceptance criteria given in the processing method. The green flag indicates that the analyte has a parent (base peak) with confirmatory ions at the same retention time (<0.1 min) with <±5 ppm mass accuracy error. With the green flagging, the user can quickly see which compounds meet the identification criteria and which do not. Where there is a red flag, the user is directed to the data that needs to be reviewed further. The most abundant and highest mass ion, i.e., parent/base peak ion (*m/z* 366.94294) at 0.005 mg/kg, was considered as quantitation ion. The matrix enhancement was observed for almost all target analytes. The matrix enhancement observed for α-HCH and fipronil are shown in Figure 7. Matrix enhancement has been found in matrix-matched standards as compared to solvent standards linearity (Table 3, Appendix). The linearity was assessed using matrix-matched standards across a concentration of 0.001–0.100 mg/kg. The coefficient of determination (R^2) was >0.99 for all target analytes with <20% residuals observed in the above range of matrix-matched standards.

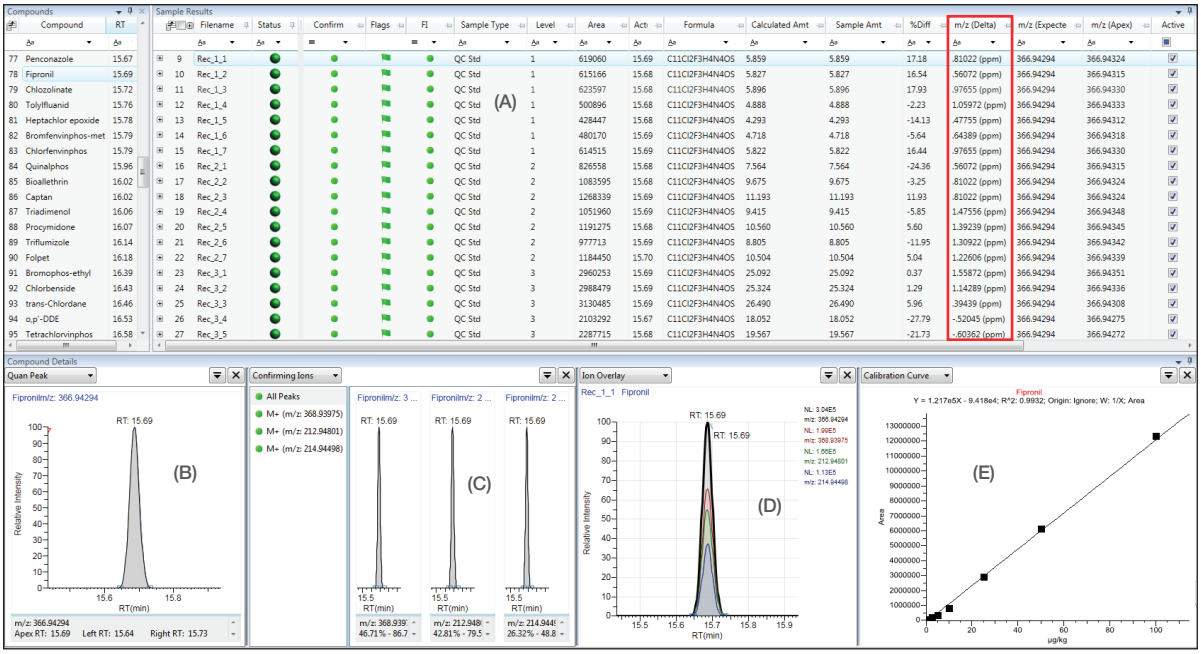

Figure 6. TraceFinder window showing the sample set (A), quantification ion of fipronil (B), confirming ions (C), overlay of confirming ion (D), and calibration curve for fipronil in milk matrix

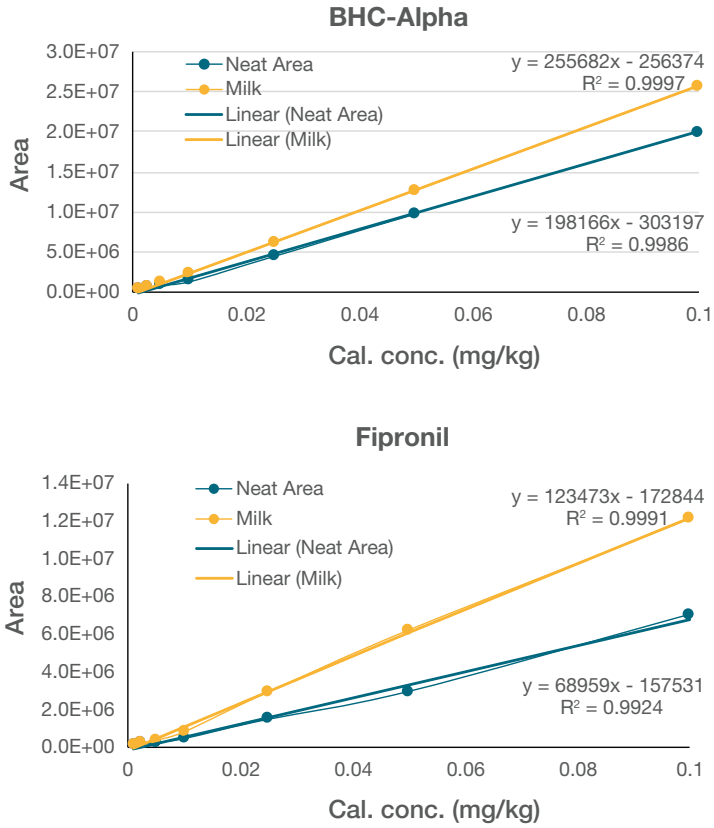

Figure 7. Matrix effect for BHC-Alpha and fipronil in milk

The limit of quantitation (LOQ) values observed in milk matrix were in the range of 0.005–0.01 mg/kg with acceptable recoveries (70–120%) and precision (<20%). The recovery experiment was carried out at 0.005, 0.01, and 0.025 mg/kg to demonstrate method accuracy and precision (n=6). The average recovery was observed in the range of 72–117% with <15% RSD (Table 3, Appendix), which were within acceptance criteria (recovery 70–120% and precision <20%) of SANTE guidelines[2].

The optimized method was tested by analyzing the whole sequence, which was assessed for the mass accuracy at different concentration levels with six replicates. The mass accuracy observed for all analyzed molecules was <5 ppm without using the lock mass. Enabling the lock mass during the acquisition of the data is beneficial for the mass correction, which gives the corrected mass with better mass accuracy. Corrected mass will always give better mass accuracy as compared to uncorrected mass. As the mass accuracy criteria given in the SANTE guidelines allow for a mass error of ±5 ppm, the mass accuracy was demonstrated without any mass correction by using the lock mass. The retention time repeatability for all the components between each injection also passing the criteria, i.e., <0.1 min. Ion ratios of the molecules were observed within the acceptance criteria of ±30% (relative) of average of calibration standards from same sequence. Consistency of the ion ratio for fipronil confirmatory ions (368.93975, 212.94801, 214.94498) throughout the whole sequence has been demonstrated in Figure 8.

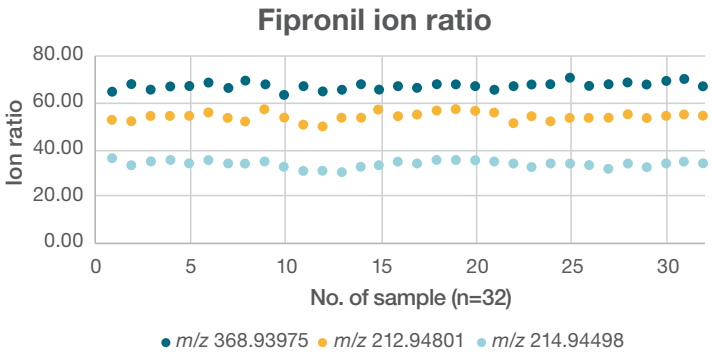

Figure 8. Ion ratio consistency for the fipronil confirming ions (*m/z* 368.93975, *m/z* 212.94801 and *m/z* 214.94498)

Conclusion

- The Thermo Scientific Exactive GC Orbitrap high-resolution mass spectrometer, in combination with TraceFinder software, is a high-performance analytical system offering a robust and sensitive performance for screening and quantitation of pesticide residues in milk.
- The data acquisition in full scan offered a retrospective of data analysis possibilities without losing data quality and also reduced the time required to optimize the method in comparison with the triple quadrupole system.
- The mass accuracy observed for all the target analytes is within ±5 ppm without any mass correction, even at trace levels (0.005 mg/kg).
- The ion ratio for the confirmatory ions has been observed within the acceptance criteria of ±30% (relative) of the average of calibration standards from the same sequence.
- The recovery as well as the precision have been observed within the acceptance criteria of 70–120% and ±20%, respectively.
- Use of the QuEChERS method for extraction followed by Exactive GC Orbitrap GC-MS system analysis could increase the overall high throughput.
- This method meets the SANTE guideline requirements in terms of identification and confirmation, followed by quantitation.
- This method complies with the EU as well as FSSAI MRLs requirements by achieving an excellent lower limit of quantitation (LOQ).

References

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Appendix

Table 3. List of pesticides with accurate masses used and validation data (linearity, recovery, and precision at three levels) as per the FSSAI[5] and EU[6] MRLs

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
1	3,4-Dichloroaniline	9.21	0.9956	35	160.97935	162.9764, 126.0105, 98.99960	0.005	91.4	14.9	2.89	88.8	12.7	3.13	89.9	11.6	2.20
2	4,4'-Dichlorobenzophenone	15.07	0.9980	44	138.99451	215.02582, 249.99467, 110.9996	0.005	98.0	13.7	3.22	89.5	10.9	3.58	85.6	10.0	2.46
3	Acrinathrin	24.06	0.9934	370	181.06479	180.08078, 208.07569	0.005	101.8	14.4	2.33	86.3	14.5	3.00	96.6	9.8	1.86
4	Alachlor	13.63	0.9980	51	160.11208	188.10699, 202.12264	0.005	101.8	11.8	2.61	94.0	8.7	3.24	86.4	14.0	1.96
5	Aldrin/Aldrin-r	14.79	0.9975	33	262.85681	260.85936, 290.92963	0.005	82.8	10.0	0.66	77.2	4.4	0.86	72.2	9.4	0.08
6	Alpha-BHC	11.50	0.9982	41	180.93730	218.91103, 108.96063, 145.96845	0.005	99.2	7.7	2.48	91.0	4.3	2.94	87.2	6.5	2.03

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
7	Atrazine	11.90	0.9984	38	200.06975	215.09322, 202.0668	0.005	96.3	13.4	1.93	92.1	11.6	2.41	86.3	14.8	1.36
8	Azinphos-ethyl	22.95	0.9969	77	132.04439	104.04947	0.010	n.d.	n.d.	n.d.	87.3	9.2	3.53	80.8	8.6	2.86
9	Azinphos-methyl	24.08	0.9980	43	132.04439	104.04948, 160.05054	0.005	106.4	10.5	3.17	99.7	11.6	3.90	102.7	3.1	2.69
10	Benfluralin	11.06	0.9928	68	264.02266	276.05905, 318.106	0.005	103.7	6.8	2.09	98.1	7.3	2.42	96.1	9.5	1.82
11	Benzonitrile, pentachloro-	12.16	0.9978	53	274.84384	276.84089, 272.84679, 239.87499	0.005	90.6	9.8	2.16	83.5	6.2	2.54	80.8	9.2	1.66
12	Beta-BHC	11.97	0.9974	40	180.93730	218.91103, 108.96063, 145.96845	0.005	91.3	14.4	2.61	89.7	8.7	2.89	92.2	10.5	2.15
13	Bifenthrin	21.81	0.9984	44	181.10118	166.0777, 182.10453, 167.08106	0.010	n.d.	n.d.	n.d.	101.4	12.0	2.74	91.2	7.4	1.78
14	Bromfenvinphos-methyl	15.87	0.9903	153	294.96883	169.96846, 338.91831	0.005	101.3	12.7	0.96	85.2	12.2	1.03	74.1	10.1	0.22
15	Bromophos	15.26	0.9960	55	330.87777	328.87982, 78.99452, 332.87491	0.005	95.6	13.9	-0.27	81.9	7.8	0.27	70.0	19.6	-0.28
16	Bromophos-ethyl	16.45	0.9967	53	300.84869	358.90906, 241.87159, 330.87776	0.005	100.7	14.3	-0.09	88.2	12.6	0.22	80.0	16.8	-0.51
17	Bromopropylate	21.81	0.9990	36	182.94400	184.94196, 340.89942, 338.90147	0.010	n.d.	n.d.	n.d.	101.8	11.9	2.77	89.6	11.1	1.76
18	Bupirimate	17.81	0.9965	55	208.14443	193.14477, 166.09748, 273.10158	0.005	106.7	12.7	2.05	99.2	12.2	2.32	95.3	11.0	1.38
19	Carbophenothion	19.74	0.9948	63	156.98733	170.96978, 199.00108, 295.98559	0.005	107.6	10.9	2.87	92.0	14.0	3.19	88.9	12.4	2.13
20	Carfentrazone-ethyl	19.69	0.9976	67	312.05905	310.01893, 330.02516, 340.09035	0.010	n.d.	n.d.	n.d.	112.6	10.1	1.09	101.0	8.6	0.05
21	Chlorbenside	16.49	0.9970	43	125.01525	127.0123, 267.98747	0.005	97.5	13.9	3.11	86.4	11.7	3.44	82.4	9.4	2.49
22	Chlorfenapyr	18.10	0.9956	45	247.04776	249.00256, 137.00268, 361.94277	0.005	104.4	13.8	2.15	96.0	11.0	2.79	93.2	10.8	1.35
23	Chlorfenson/Ovex	17.22	0.9966	38	174.96150	110.9996, 176.95855, 301.95657	0.005	105.5	13.2	2.49	93.4	10.8	2.80	90.2	9.7	2.07
24	Chlorfenvinphos	15.85	0.9949	91	266.93770	268.93457, 323.00012, 324.99717	0.005	108.1	12.5	1.57	91.5	9.2	1.91	81.0	17.0	0.93
25	Chlorobenzilate	18.62	0.9985	57	138.99452	251.0025, 252.99955, 140.99157	0.010	n.d.	n.d.	n.d.	104.9	10.2	3.61	91.9	14.9	2.59
26	Chloroneb	9.73	0.9987	28	190.96611	192.96316, 205.98958, 207.98663	0.005	94.7	14.6	3.27	86.1	10.1	3.87	89.5	7.6	2.82
27	Chlorpropham	10.99	0.9978	49	127.01832	171.00815, 129.01537, 213.0551	0.005	92.2	11.8	3.42	90.8	8.6	3.73	89.5	11.1	2.71
28	Chlorpyrifos(-ethyl)	14.65	0.9977	49	196.91964	257.89428, 313.95688	0.005	100.3	7.5	2.21	87.0	11.2	2.56	78.9	18.4	1.87

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
29	Chlorthiophos	19.00	0.9893	55	268.92590	270.92278, 296.9572, 207.95109	0.005	98.1	13.2	1.73	87.0	12.2	1.84	85.6	14.0	1.20
30	Chlozolinate	15.78	0.9969	81	185.98718	186.95862, 258.97975, 188.95567	0.005	105.4	5.1	2.55	93.2	9.4	2.78	86.9	13.9	1.90
31	*cis*-1,2,3,6-Tetrahydrophthalimide	9.66	0.9988	52	151.06277	123.06786, 122.06004	0.005	85.5	16.0	3.00	86.2	12.5	3.47	83.6	17.6	2.30
32	*cis*-Chlordane	16.92	0.9945	56	372.82542	374.82247, 236.84076, 376.81952	0.005	92.4	10.4	1.49	81.8	8.6	1.55	80.2	10.0	0.66
33	*cis*-Nonachlor	18.89	0.9943	35	408.78350	406.78645, 236.84076, 404.7894	0.005	98.7	10.9	1.58	84.9	8.9	2.37	80.2	8.9	1.59
34	Clomazone/ Dimethazone	12.01	0.9977	48	125.01525	204.1019, 89.03857	0.005	95.1	12.0	3.35	94.8	8.0	3.61	92.5	11.0	2.46
35	Coumaphos	25.24	0.9980	98	225.98498	96.95094, 210.00782, 109.00508	0.005	107.0	8.1	2.05	93.9	14.4	2.20	89.2	5.1	0.85
36	Cycloate	10.84	0.9979	44	154.12264	155.12599	0.005	96.9	6.3	2.91	91.2	4.8	3.13	85.8	7.2	2.22
37	Cyprodinil	15.59	0.9962	48	224.11822	225.12604, 208.08692, 210.10257	0.005	95.2	13.5	2.06	83.9	11.8	2.26	78.0	13.4	1.27
38	Delta-BHC	12.74	0.9984	84	180.93730	218.91103, 108.96063, 145.96845	0.005	92.1	13.1	2.51	83.5	3.8	3.04	76.5	12.3	1.91
39	Deltamethrin	29.75	0.9909	214	181.06479	171.98821, 173.98617, 252.9045	0.01	n.d.	n.d.	n.d.	76.2	7.8	2.13640	80.3	10.5	1.94378
40	Diazinone	12.31	0.9999	58	179.11789	137.07094, 199.06309, 276.0692	0.005	110.1	5.3	2.43	99.3	8.3	2.81	85.0	17.2	1.82
41	Dichloran	11.74	0.9979	38	175.96644	123.99485, 207.96148, 159.97153	0.005	95.7	11.4	2.57	89.3	9.5	2.98	88.3	8.4	2.07
42	Dieldrin	17.74	0.9967	27	262.85641	264.85346, 260.85936	0.005	99.2	13.5	1.84	87.6	10.5	2.34	81.9	11.1	1.36
43	Diphenamid	15.25	0.9972	43	167.08552	165.06987, 72.04439, 152.06205	0.005	112.5	6.8	2.60	96.5	11.3	2.82	91.0	12.0	1.82
44	Diphenylamine	10.76	0.9988	41	169.08860	168.08078, 167.07295	0.005	91.1	9.0	2.06	89.0	7.6	2.12	86.3	9.6	0.90
45	Disulfoton	12.58	0.9990	49	96.95076	88.03412, 141.96704, 153.01336	0.005	113.6	6.1	2.56	100.0	9.6	2.99	86.3	18.0	2.09
46	Edifenphos	19.81	0.9903	261	109.01064	172.98206, 186.04977, 310.02455	0.005	103.9	10.8	3.02	87.9	5.0	3.37	75.1	15.7	2.39
47	Endosulfan ether	13.20	0.9974	37	240.89539	238.89834, 169.96846, 276.87206	0.005	92.7	9.4	1.76	91.9	6.5	2.15	90.1	7.6	1.29
48	Endosulfan-α	16.92	0.9942	19	236.84076	192.93731, 242.91104	0.005	84.4	12.3	1.97	79.0	10.2	1.90	80.1	12.0	1.08
49	Endosulfan-β	18.70	0.9953	37	159.98411	236.84076, 169.96846, 192.93731	0.005	102.7	12.8	2.41	91.3	10.5	2.81	88.3	11.2	2.15
50	Endosulfan sulfate	19.93	0.9940	60	271.80962	228.89539, 236.84076, 269.81257	0.005	105.7	10.8	2.43	89.7	12.0	2.27	86.6	7.4	1.49

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
51	Endrin	18.37	0.9975	29	260.85937	242.95295, 280.92668	0.005	95.0	13.1	2.41	82.8	10.3	2.36	76.1	14.0	1.51
52	Endrin ketone	21.45	0.9958	28	249.84858	242.95295	0.005	102.0	18.2	2.86	96.1	17.2	2.45	90.9	13.0	1.42
53	Ethalfluralin	10.87	0.9994	66	276.05905	316.09035, 248.02775	0.010	n.d.	n.d.	n.d.	103.8	4.7	2.14	91.5	7.9	1.38
54	Ethion	18.91	0.9974	75	230.97315	124.98206, 202.94185, 153.01336	0.010	n.d.	n.d.	n.d.	105.4	11.4	2.53	92.8	13.8	1.43
55	Etofenprox	27.34	0.9994	71	161.11174	135.08044, 107.04914, 164.1151	0.005	94.3	10.8	2.38	87.0	13.9	3.23	87.8	3.3	1.98
56	Etridiazole	9.33	0.9982	47	182.91812	210.94942, 212.94646, 139.9123	0.010	n.d.	n.d.	n.d.	95.5	9.2	2.82	83.5	6.4	1.93
57	Famishes	17.09	0.9978	89	154.04468	303.10525, 217.00827, 260.05047	0.010	n.d.	n.d.	n.d.	101.7	12.8	2.94	93.2	13.8	2.35
58	Fenarimol	23.84	0.9984	12	138.99452	219.03197, 252.99955	0.005	105.3	6.4	2.82	98.3	5.4	3.34	96.9	4.8	2.60
59	Fenchlorphos/Ronnel	13.87	0.9980	56	284.93033	124.98206, 78.99434, 269.90685	0.005	95.9	13.5	1.59	85.1	7.7	1.89	83.9	10.3	0.90
60	Fenitrothion	14.21	0.9966	93	260.01409	127.01547, 277.01683	0.005	103.9	13.4	1.73	91.3	9.7	2.53	85.9	15.5	1.54
61	Fenpropathrin	22.11	0.9977	38	181.06479	265.07334, 209.08352	0.005	114.4	7.6	2.51	101.7	15.1	2.74	97.9	7.8	1.72
62	Fenthion	14.75	0.9975	51	278.01947	169.01402, 245.03958, 151.0576	0.005	101.1	14.9	1.69	89.8	12.2	2.20	80.7	18.4	1.16
63	Fenvalerate	28.41	0.9981	121	125.01525	225.07843, 167.0622	0.005	88.4	12.0	3.09	85.2	5.1	3.49	87.6	6.2	2.63
64	Fipronil	15.69	0.9952	97	366.94294	368.93975, 212.94801, 214.94498	0.005	103.9	16.2	0.81	101.9	12.0	1.13	93.6	14.5	-0.01
65	Fluazifop butyl	18.39	0.9978	70	282.07364	254.04234, 268.05799, 227.05525	0.010	n.d.	n.d.	n.d.	106.0	11.2	2.18	94.3	11.6	1.22
66	Fluchloralin	12.35	0.9956	129	264.02267	306.06962, 326.01499, 310.02008	0.010	n.d.	n.d.	n.d.	102.8	7.1	2.15	89.2	12.6	1.67
67	Flucythrinate	27.47	0.9994	73	157.04595	181.06479	0.005	107.2	5.1	2.71	99.8	12.6	3.13	100.9	5.8	2.35
68	Fluquinconazole	25.27	0.9981	61	340.03959	298.01779	0.005	111.5	6.3	0.21	98.4	13.9	0.91	91.1	8.5	-0.23
69	Fluridone	27.68	0.9990	93	328.09438	329.09958	0.005	95.9	9.5	0.35	89.6	11.9	0.95	87.2	8.9	-0.01
70	Flusilazole	17.77	0.9968	91	233.05926	206.05443, 314.09196	0.005	110.1	6.5	1.86	108.9	7.9	2.44	102.2	11.2	1.50
71	Flutolanil	17.19	0.9963	54	173.02087	145.02596, 281.06581, 323.11276	0.005	113.5	11.3	2.61	101.8	11.7	2.95	98.9	12.1	1.86
72	Flutriafol	17.02	0.9964	59	123.02407	164.06185, 219.0616, 220.06495	0.005	107.1	9.5	2.91	96.9	11.3	3.22	89.6	17.7	2.30
73	Fonofos	12.32	0.9998	52	108.98715	137.01845, 80.95585, 246.02964	0.005	111.7	5.1	2.90	99.8	8.5	3.18	88.3	14.3	2.16
74	Gamma-BHC	12.17	0.9982	46	180.93730	218.91103, 108.96063, 145.96845	0.005	100.1	8.1	2.72	91.3	5.5	2.90	88.0	8.2	1.88

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
75	Heptachlor	13.86	0.9972	48	100.00742	236.84076, 269.81257, 336.84874	0.005	92.4	12.3	2.33	82.4	7.4	2.69	78.5	12.3	1.81
76	Heptachlor epoxide	15.85	0.9974	40	352.84366	354.84071, 262.85641, 236.84076	0.005	98.2	10.3	0.74	89.3	8.7	1.00	80.8	12.1	0.02
77	Hexazinone	20.25	0.9965	47	171.08765	71.06037, 128.08183	0.005	114.4	4.4	2.49	99.9	10.6	2.60	93.7	8.2	2.06
78	Iodofenphos	17.21	0.9950	88	376.86595	378.863, 249.96148, 258.85727	0.005	97.1	13.1	1.11	83.5	8.0	1.83	75.8	16.2	0.57
79	Iprodione	21.47	0.9994	127	314.00937	186.95862, 188.95567, 316.00642	0.010	n.d.	n.d.	n.d.	102.7	13.3	1.16	93.4	11.0	-0.18
80	Isazofos	12.58	0.9996	42	118.98809	162.04268, 161.03504, 177.01202	0.005	108.9	7.4	3.15	99.9	10.8	3.49	89.2	13.2	2.61
81	Isodrin	15.58	0.9975	41	192.93731	194.93436, 262.85641, 264.85346	0.005	89.4	9.8	2.42	81.2	7.4	2.68	75.1	9.8	1.76
82	Isopropalin	15.38	0.9916	77	238.08223	280.12918, 264.13426, 222.08731	0.005	104.7	9.9	1.98	89.6	9.8	2.42	82.1	13.4	1.47
83	Lambda-Cyhalothrin	23.66	0.9993	75	181.06479	141.05103, 197.03394	0.010	n.d.	n.d.	n.d.	102.2	9.6	2.53	100.5	2.3	1.85
84	Leptophos	22.90	0.9969	100	171.00280	376.89851, 374.90055, 155.02564	0.005	98.3	8.5	1.91	85.2	11.6	3.09	83.2	8.9	1.89
85	Linuron	14.38	0.9950	103	61.05221	159.97153, 248.01138	0.005	92.1	16.4	2.75	85.4	10.6	2.99	81.7	4.9	2.37
86	Malathion	14.43	0.9966	117	124.98206	99.00767, 173.08083	0.005	101.2	14.0	3.38	88.4	8.8	3.61	78.1	17.7	2.56
87	Metalaxyl	13.78	0.9958	46	160.11240	206.11755, 234.11284	0.005	104.4	14.3	0.69	95.6	12.2	1.27	93.9	14.6	0.33
88	Metazachlor	15.61	0.9962	44	132.08078	133.0886, 209.06019, 211.05724	0.005	101.2	15.2	3.42	93.9	11.5	3.71	88.7	13.7	2.76
89	Methacrifos	9.64	0.9995	47	180.00045	207.99537, 124.98206, 209.00319	0.010	n.d.	n.d.	n.d.	104.9	6.4	2.99	90.4	11.7	1.85
90	Methoxychlor	21.99	0.9955	53	227.10666	228.11001	0.010	n.d.	n.d.	n.d.	105.7	11.7	2.46	92.6	8.4	1.06
91	Metolachlor	14.60	0.9978	49	162.12772	238.09931, 146.09642, 211.07584	0.005	105.6	12.7	2.66	95.9	10.8	2.88	88.5	13.6	1.91
92	Mevinphos	9.11	0.9986	207	109.00491	193.02604, 127.01547, 164.0233	0.010	n.d.	n.d.	n.d.	98.8	14.5	3.18	75.8	18.1	2.11
93	MGK 264 Isomer A	15.30	0.9977	45	164.07060	111.03148, 98.02365	0.005	99.6	12.6	2.79	91.7	11.6	2.92	85.7	12.9	2.01
94	MGK 264 Isomer B	15.65	0.9971	42	164.07060	210.14886, 209.14103, 257.17742	0.005	101.5	14.1	2.78	91.9	11.5	3.04	85.9	13.1	2.06
95	Myclobutanil	17.69	0.9952	52	179.02447	150.0105, 245.05885, 206.0731	0.005	112.0	6.2	2.51	96.0	12.3	2.93	90.5	12.8	2.06
96	Nitrofen	18.32	0.9970	83	202.01799	282.97975, 284.9768, 252.98176	0.010	n.d.	n.d.	n.d.	103.8	9.1	2.40	96.8	6.3	1.39

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
97	Norflurazon	19.79	0.9972	65	173.03210	145.02596, 303.03807, 302.03025	0.005	113.4	7.5	2.47	100.8	12.3	3.01	96.9	6.5	2.03
98	o,p'-DDE	16.60	0.9957	35	245.99976	247.99681, 176.06205, 317.93451	0.005	90.1	18.3	2.26	82.0	8.7	2.40	75.2	10.5	1.55
99	o,p'-DDT	18.98	0.9961	59	235.00758	237.00463, 245.99976	0.010	n.d.	n.d.	n.d.	89.2	7.7	2.38	73.7	9.9	1.62
100	o,p'-Methoxychlor	20.34	0.9975	60	121.06479	227.10666	0.010	n.d.	n.d.	n.d.	107.8	11.0	3.52	92.9	7.5	2.56
101	o,p'-DDD	17.78	0.9997	33	235.00758	165.06999, 199.03099	0.010	n.d.	n.d.	n.d.	103.4	9.0	2.48	87.3	10.6	1.48
102	Oxadiazone	17.61	0.9960	33	174.95862	258.03211, 302.02194	0.005	106.1	14.2	2.64	93.9	12.1	3.07	90.9	11.6	1.96
103	Oxyfluorfen	17.78	0.9962	97	252.03927	300.00337, 317.00611, 280.0216	0.005	113.2	15.0	2.06	105.1	11.4	2.53	106.4	8.3	1.43
104	p,p'-DDE	17.59	0.9959	33	245.99976	247.99681, 317.93451, 315.93746	0.005	92.0	13.0	1.87	82.0	11.5	2.52	76.2	11.1	1.46
105	p,p'-DDD	18.90	0.9943	44	235.00758	165.06987, 199.0309	0.005	107.8	10.3	2.03	91.9	10.8	2.54	87.3	11.0	1.49
106	p,p'-DDT	20.12	0.9948	87	235.00758	165.06987, 199.0309	0.010	n.d.	n.d.	n.d.	93.2	9.9	2.67	76.4	9.3	1.11
107	Paclobutrazol	16.68	0.9956	72	125.01525	236.05851, 167.02581, 138.02307	0.005	115.6	8.2	3.47	99.1	12.0	3.67	89.0	19.2	2.77
108	Parathion	14.85	0.9952	79	109.00491	155.00355, 139.02639, 291.03248	0.005	104.2	15.4	2.84	92.1	11.6	3.21	90.7	13.4	2.21
109	Parathion-methyl	13.58	0.9975	58	127.01547	263.00118, 245.99844	0.005	92.3	16.4	3.32	87.5	7.1	3.73	82.6	16.4	2.42
110	Pebulate	9.38	0.9972	41	128.10699	161.08689	0.005	91.1	13.0	3.27	90.4	4.7	3.59	88.4	6.6	2.71
111	Penconazole	15.74	0.9962	46	158.97628	248.0949, 160.97333, 250.09195	0.005	105.5	9.6	2.90	91.3	12.1	3.20	85.4	15.3	2.15
112	Pendimethalin	15.57	0.9913	78	252.09788	162.07876, 191.06893, 208.07167	0.005	102.4	11.4	2.23	88.3	10.9	2.47	81.6	12.9	1.39
113	Pentachloroaniline	13.17	0.9983	41	262.86244	191.9169, 202.87973, 229.89063	0.005	85.3	9.4	2.12	79.2	7.7	2.40	72.3	10.3	1.59
114	Pentachloroanisole	11.69	0.9977	35	264.83567	279.85915, 238.83781, 234.84372	0.005	85.4	5.6	1.98	79.2	3.6	2.57	75.9	6.1	1.73
115	Pentachlorobenzene	9.90	0.9993	23	249.84858	251.84563, 247.85154, 177.9137	0.005	75.9	10.4	1.72	76.8	4.8	2.21	75.1	3.2	1.49
116	Pentachlorothioanisole	14.40	0.9998	50	295.83631	245.84398, 262.85641, 297.83336	0.005	85.9	9.1	0.79	74.5	8.0	0.92	66.6	10.6	-0.33
117	Permethrin	25.34	0.9961	52	183.08044	161.00758, 168.05696	0.005	103.9	8.2	2.49	93.2	14.3	2.87	94.0	3.4	1.79
118	Phorate	11.36	0.9998	50	75.02629	96.95076, 230.97315, 260.01227	0.010	n.d.	n.d.	n.d.	101.9	10.6	2.93	89.9	15.8	2.19
119	Phosalone	22.86	0.9968	67	182.00033	121.04129, 183.99822	0.005	106.9	12.5	2.34	97.9	13.1	2.95	95.6	6.0	1.86
120	Phosmet	21.59	0.9980	97	160.03930	161.04300	0.010	n.d.	n.d.	n.d.	99.5	13.1	3.30	84.7	9.6	2.08

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
121	Piperonyl butoxide	20.90	0.9953	76	176.08318	149.0597, 177.091, 161.0597	0.005	112.8	6.4	2.41	99.0	13.3	2.93	94.5	9.1	1.93
122	Pirimiphos methyl	14.14	0.9981	59	290.07227	180.11314, 276.05662, 262.04097	0.005	100.0	13.6	1.20	91.3	12.3	1.70	81.9	18.3	0.89
123	Pirimiphos-ethyl	15.23	0.9965	46	168.05899	180.11313, 318.10357, 333.12705	0.005	102.4	15.2	2.74	90.8	13.8	3.05	86.5	13.7	1.99
124	Pretilachlor	17.38	0.9967	51	162.12772	202.12264, 238.09931	0.005	110.6	13.8	2.73	96.6	10.9	2.87	90.0	13.0	2.21
125	Procymidone	16.14	0.9967	43	283.01613	96.05696, 255.02122	0.005	104.6	13.5	1.56	93.0	10.6	2.02	87.8	10.5	1.10
126	Profenofos	17.45	0.9947	212	207.91063	205.91286, 138.99789, 266.88767	0.005	103.5	11.6	1.98	85.1	7.2	1.95	72.9	15.2	1.15
127	Profluralin	12.08	0.9942	66	318.06962	264.02267, 330.106, 186.03993	0.005	104.0	7.8	0.70	91.4	7.0	0.94	84.2	10.9	-0.03
128	Propachlor	10.57	0.9970	46	120.08077	176.10699, 93.0573, 169.02889	0.005	101.7	10.2	3.16	90.5	7.1	3.46	85.8	10.9	2.56
129	Propyzamide	12.29	0.9977	47	172.95555	174.9526, 254.0134, 256.01044	0.005	89.6	18.2	2.53	88.9	15.3	2.78	87.0	15.9	2.11
130	Pyraclofos	24.42	0.9926	198	194.02414	138.01050	0.005	96.0	15.6	1.52	81.9	7.4	2.79	77.0	8.8	1.40
131	Pyrazophos	23.93	0.9997	53	221.07949	193.04819, 232.10805, 265.08794	0.010	n.d.	n.d.	n.d.	100.4	11.4	1.76	96.8	4.1	0.67
132	Pyridaben	25.32	0.9994	73	309.08228	147.11682	0.005	103.8	17.4	-0.04	96.6	11.1	2.03	90.9	6.6	0.21
133	Pyridaphenthion	21.41	0.9985	93	199.08658	96.95076, 188.05802, 340.06411	0.010	n.d.	n.d.	n.d.	106.9	6.8	3.45	95.9	11.9	2.38
134	Pyrimethanil	12.45	0.9976	43	198.10257	199.11039, 183.07909	0.005	82.2	7.7	1.93	82.8	13.5	2.06	75.5	13.1	0.90
135	Pyriproxyfen	23.24	0.9967	12	136.07569	96.04439	0.005	109.9	8.9	2.95	98.0	13.9	3.72	99.0	3.2	2.48
136	Quinalphos	16.03	0.9972	57	146.04746	157.07602, 118.05255, 173.07094	0.005	104.1	15.1	3.22	93.0	13.3	3.52	87.0	17.3	2.61
137	Quintozene	12.08	0.9972	39	234.84372	213.87191, 248.84076, 294.83366	0.005	92.3	8.2	1.99	88.0	5.8		86.3	6.8	1.49
138	Resmethrin	21.00	0.9985	88	128.06205	143.08552, 171.08044	0.010	n.d.	n.d.	n.d.	99.9	11.4	3.26	90.9	9.4	2.42
139	Sulfotep	11.11	0.9974	53	173.95687	209.89698, 237.92828, 322.02218	0.010	n.d.	n.d.	n.d.	101.5	9.8	3.02	88.6	19.9	2.37
140	Sulprofos	19.42	0.9940	61	156.00619	140.02903, 112.92791, 322.02792	0.005	109.2	12.0	2.62	94.3	12.2	3.19	89.4	13.5	2.25
141	Tebuconazole	20.56	0.9961	59	125.01525	250.07417, 127.0123, 161.0309	0.005	109.0	6.6	3.10	95.6	13.1	3.55	88.4	14.7	2.55
142	Tebufenpyrad	22.29	0.9974	25	171.03197	318.13677, 276.08982, 145.0527	0.005	110.5	7.1	2.55	101.1	11.9	2.74	96.3	9.0	1.92
143	Tecnazene	10.47	0.9975	36	200.88269	260.87264, 177.91383, 214.87987	0.005	96.9	7.1	2.13	89.2	4.0	2.38	86.4	5.4	1.66

Sr. No.	Name of compound	RT (min)	R^2	% ME (*)	Target mass (quant ion) (*m/z*)	Confirming ions (*m/z*)	LOQ (mg/kg)	0.005 mg/kg (n=6)			0.010 mg/kg (n=6)			0.050 mg/kg (n=6)		
								% Rec.	% RSD	Mass error (ppm)	% Rec.	% RSD	Mass error (ppm)	% Rec	% RSD	Mass error (ppm)
144	Tefluthrin	12.60	0.9998	38	177.03218	141.05103, 197.03393, 127.03538	0.005	105.3	4.1	2.41	97.7	8.1	2.71	86.0	12.1	1.58
145	Terbacil	12.58	0.9969	77	161.01123	160.00341	0.005	102.5	11.4	2.67	90.2	10.4	3.10	83.0	17.0	2.28
146	Terbufos	12.21	0.9992	52	230.97315	96.95076, 202.94185, 174.91055	0.005	110.8	5.5	1.95	97.4	9.9	2.32	84.1	19.2	1.38
147	Terbuthylazine	12.19	0.9977	47	214.08540	173.04627, 138.07742, 216.08245	0.005	94.3	12.6	1.79	89.5	11.1	2.11	85.0	15.2	1.10
148	Tetramethrin	21.88	0.9991	62	164.07060	165.07417	0.010	n.d.	n.d.	n.d.	106.4	11.6	3.15	96.3	7.6	1.87
149	Tolclofos-methyl	13.62	0.9979	44	264.98496	266.982, 249.96166	0.005	96.9	12.9	2.12	88.3	10.0	2.58	81.0	17.0	1.53
150	*trans*-Chlordane	16.53	0.9973	42	372.82542	374.82247, 376.81952, 236.84076	0.005	94.0	10.7	0.65	84.7	8.8	1.40	76.7	12.1	0.47
151	*trans*-Chlorfenvinphos	17.04	0.9940	105	266.93770	268.93475, 169.96846, 323.00013	0.005	109.5	11.8	1.32	93.5	9.8	1.78	86.1	17.3	0.87
152	Transfluthrin	13.66	0.9982	30	161.01653	143.01031, 335.04564	0.005	88.1	13.6	2.69	89.6	11.0	2.74	87.0	12.6	1.78
153	*trans*-Nonachlor	17.01	0.9982	47	408.78350	236.84076, 271.80962, 262.85641	0.005	89.5	15.5	1.57	80.4	7.9	2.87	75.5	13.9	1.42
154	*trans*-permethrin	25.09	0.9978	64	183.08044	161.00758, 127.0309	0.005	106.3	7.6	2.26	88.7	12.7	2.63	86.3	2.6	1.76
155	Triadimefon	14.94	0.9957	52	208.02722	128.00234, 181.01612, 210.02426	0.005	104.5	14.8	1.75	91.7	11.9	2.25	87.1	17.0	1.30
156	Triadimenol	16.14	0.9954	72	112.05054	168.11314, 128.00234, 150.10257	0.005	110.2	9.2	2.34	95.4	12.1	2.75	86.7	19.3	1.76
157	Triallate	12.77	0.9975	55	268.03242	142.92166, 270.02947, 144.91871	0.005	93.0	10.4	2.06	87.4	7.7	2.17	81.6	12.8	1.77
158	Triazophos	19.37	0.9971	96	162.06619	172.08692, 177.03552, 257.00185	0.010	n.d.	n.d.	n.d.	106.8	11.0	2.63	91.4	14.2	2.09
159	Tricyclazole	17.37	0.9981	67	189.03552	161.0168, 135.01372, 118.05255	0.005	104.1	6.0	2.16	91.1	8.5	2.53	81.3	12.7	1.77
160	Triflumizole	16.20	0.9946	56	205.99789	178.98699, 278.0554, 218.04796	0.005	106.7	8.5	1.70	89.1	10.8	2.35	81.2	15.9	1.24
161	Trifluralin	11.01	0.9976	69	306.06961	248.02775, 290.0747	0.005	103.0	9.0	0.81	94.5	7.0	1.08	90.3	9.5	0.22
162	Vinclozolin	13.53	0.9964	39	178.04180	178.0418, 212.00283, 284.99539	0.005	94.4	11.9	2.51	94.3	9.8	2.95	93.5	11.7	1.73

*ME= matrix effect

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