Application Note

Food and Beverage Testing

Determination of 366 Pesticides in Cocoa Liquor

Using Agilent Captiva EMR-GPD passthrough cleanup and GC/MS/MS and LC/MS/MS detection

Authors

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Abstract

This application note describes the development and optimization of a method for the analysis of multiresidue pesticides in cocoa liquor. This method involves sample extraction with the Agilent Bond Elut QuEChERS AOAC extraction kit, followed by passthrough cleanup with the Agilent Captiva Enhanced Matrix Removal – General Pigment Dry (EMR-GPD) cartridge. The samples were then injected into a gas chromatography/triple quadrupole mass spectrometer (GC/MS/MS) and into a liquid chromatography/triple quadrupole mass spectrometer (LC/MS/MS) for analysis. The developed method provided efficient matrix removal, reliable target quantitation results, and was successfully utilized for the analysis of a large number of pesticides in the challenging cocoa liquor matrix. Robust method performance was observed for both GC-amenable (76) and LC-amenable (308) pesticides, with excellent accuracy and precision demonstrated by 70–120% recovery for over 92% of analytes and RSDs below 20% for all pesticides in cocoa liquor.

Introduction

Cocoa liquor is a key and central intermediate used in the manufacture of a wide range of cocoa-derived products, including chocolate, cocoa butter, and cocoa powder. Its production begins with the processing of cocoa beans (as shown in Figure 1) and it contains both cocoa butter and cocoa solids, making it the most representative and analytically challenging matrix for studying cocoa flavor, quality, safety, and authenticity.[1]

As cocoa beans are vulnerable to fungal infections and insect infestation, pesticides are often applied during cultivation and post-harvest processing. Consequently, regulatory agencies worldwide, such as the EU and US FDA, require stringent monitoring of pesticide residues in cacao-derived products to ensure consumer safety and compliance with maximum residue limits (MRLs).[2]

However, pesticide analysis in cocoa liquor presents significant analytical challenges. The high lipid content, natural pigments, and abundant matrix coextractives can cause severe matrix effects, detector contamination, and reduced method robustness. These issues demand highly sensitive, selective, and rugged instrumentation capable of operating reliably even in the presence of complex sample backgrounds.

To meet these analytical needs, the Agilent 8890/7010D GC/MS/MS and the Agilent 1290 Infinity III/6475 LC/MS/MS systems provide powerful complementary platforms for comprehensive pesticide monitoring. The 7010D GC/MS/MS, equipped with the high-efficiency electron ionization source and the industry-leading femtogram-level sensitivity, enables confident quantification of pesticide residues with outstanding selectivity through dynamic multiple reaction monitoring (dMRM). For thermally labile or highly polar pesticides that are unsuitable for GC analysis, the 6475 LC/MS/MS system offers superior sensitivity, robust spray stability, and advanced dMRM acquisition tailored for trace-level quantification, even in challenging matrices.

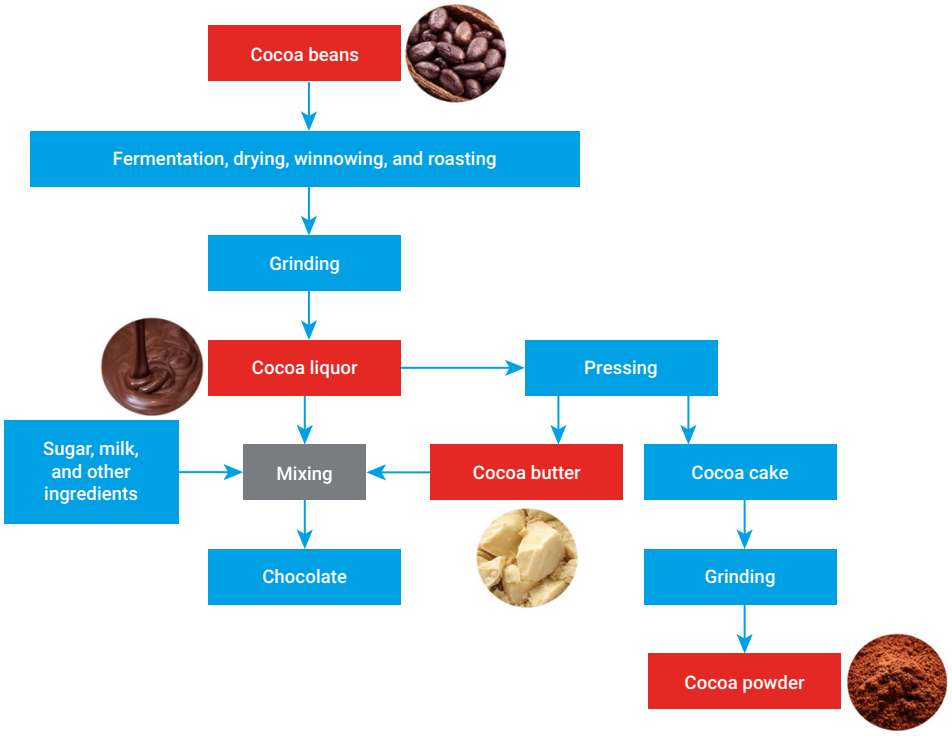

Figure 1. Manufacture process of the cocoa bean from farm to manufacturing.

This application note demonstrates a combined GC- and LC-based workflow that is optimized for cocoa liquor, including sample preparation, matrix cleanup strategies, and dMRM method development. As shown in Figure 2, 76 analytes were analyzed by GC/MS/MS and 308 analytes were analyzed by LC/MS/MS. The GC/MS/MS analysis included 18 analytes that can also be determined using LC/MS/MS; thus, this workflow covers a total of 366 unique pesticides. Together, the 7010D GC/MS/MS and 6475 LC/MS/MS deliver a comprehensive solution covering a broad range of pesticide chemistries while maintaining excellent accuracy, precision, and long-term instrument robustness.

The results highlight how the Agilent integrated workflow enables laboratories to efficiently achieve regulatory compliance and high confidence in pesticide residue testing of cocoa liquor and related complex food matrices.

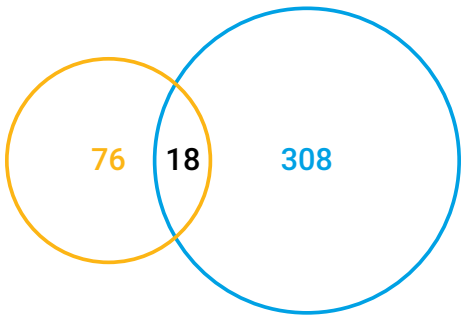

Figure 2. Number of pesticides analyzed by GC/MS/MS (orange) and LC/MS/MS (blue), including unique and common analytes.

Experimental

Reagents and samples

- Formic acid was obtained from Honeywell Fluka (Michigan, USA)
- Acetic acid was purchased from Sigma Aldrich (Missouri, USA)
- Pesticides standard (part numbers G3440-85041 and 5190-0551) and magnesium sulfate (part number 5982-0102) were obtained from Agilent
- Cocoa liquor was obtained from a customer

Sample preparation

A 1.5 g portion of cocoa liquor was weighed into a 50 mL tube and extracted using the QuEChERS AOAC method (part number 5982-5755). The extract was subsequently cleaned using a Captiva EMR-GPD 6 mL cartridge (part number 5610-2091). The EMR-GPD sorbent bed comprises Agilent proprietary materials, including Carbon S for pigment removal, primary secondary amine (PSA) for fatty acid removal, and EC-C18 for additional hydrophobic matrix reduction, providing highly selective and efficient matrix cleanup. Appropriate post-extraction treatments were applied to prepare the eluates for GC/MS/MS and LC/MS/MS analysis. The detailed sample preparation workflow is presented in Figure 3.

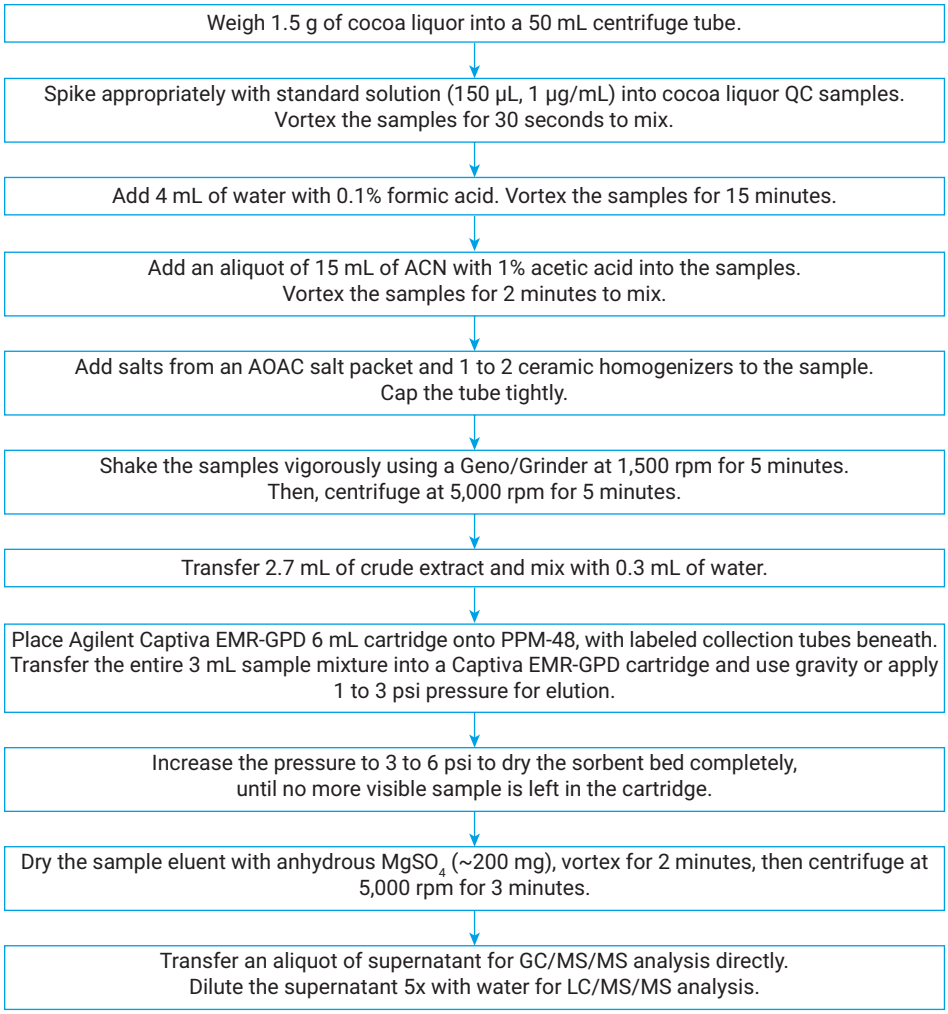

Figure 3. Sample preparation procedure for cocoa liquor.

Matrix-optimized MRM transitions

Matrix effects remain a significant challenge in pesticide analysis performed using MRM acquisition. The selectivity and performance of specific MRM transitions can vary across different sample matrices, potentially affecting analytical accuracy and reproducibility. Access to multiple MRM transitions per compound enables analysts to select the most suitable transitions for each matrix, thereby improving quantitation robustness, streamlining method development, and enhancing overall laboratory productivity.

The Agilent G9250AA Rev. A.04.02 Pesticides and Environmental Pollutants (P&EP) MRM Database is the most comprehensive GC/MS/MS MRM database available, featuring over 1,100 compounds and up to 10 MRM transitions per compound.[3] This extensive resource enables the selection of matrix-optimized MRM transitions for reliable and robust target compound analysis in cocoa liquor by GC/MS/MS. The optimized MRM transitions for the 76 pesticides analyzed by GC/MS/MS are listed in Appendix 1.

The optimized dMRM transitions for 308 pesticides analyzed by LC/MS/MS were obtained from application notes by Zou.[4]

Matrix-matched calibration

A matrix blank was prepared using an unfortified, blank sample of cocoa liquor. Calibration performance was evaluated using a series of matrix-matched calibration standards (postspiked standards), ranging from 2.5 to 100 ng/mL for pesticides analyzed by GC/MS/MS and 0.5 to 50 ng/mL for pesticides analyzed by LC/MS/MS.

Instrument parameters

The GC/MS/MS analysis parameters are shown in Table 1. The target compound MRM parameters are listed in Appendix 1. Figure 4 shows a typical GC/MS/MS MRM chromatogram of targeted pesticides spiked in cocoa liquor at a concentration of 10 ng/mL. Figure 5 shows a typical LC/MS/MS MRM chromatogram of targeted pesticides spiked in cocoa liquor at 10 ng/mL.

Other equipment utilized for sample preparation are as follows: VWR DVX-2500 Multi-Tube Vortexer (Massachusetts, USA), 2010 Geno/Grinder (California, USA), Eppendorf Centrifuge 5804R (Leipzig, Germany), Agilent positive pressure manifold 48 processors (PPM-48), Eppendorf Centrifuge 5430R (Leipzig, Germany). Sample preparation materials include Agilent Bond Elut QuEChERS

Table 1. Agilent GC/MS/MS parameters for pesticide analysis.

Gas Chromatography	
Model	Agilent 8890 GC
GC Column	Agilent HP-5Q, 30 m × 0.25 mm, 0.25 µm (p/n 19091S-433Q)
Column Pneumatics	Constant flow
Carrier Gas	Helium
Injection Volume	1.0 µL
Injector Mode	Split (split ratio 5:1)
Purge Flow to Split Vent	50 mL/min at 1.5 min
Inlet Temperature	60 °C for 0.2 min, then to 280 °C at 900 °C/min
Injector Liner	Agilent Ultra Inert fritted splitless liner (p/n 5190-5112)
Flow Rate	1.2 mL/min
Oven Temperature Program	60 °C for 1 min 40 °C/min to 170 °C 10 °C/min to 310 °C, hold 3.0 min
Equilibration Time	3 min
Mass Spectrometer	
Model	Agilent 7010D triple quadrupole GC/MS
Acquisition Mode	dMRM
Gain	10
He Quench Gas	2.25 mL/min
N_2 Collision Gas	1.5 mL/min
Transfer Line Temperature	280 °C
Ion Source Temperature	280 °C
Quad Temperature	150 °C

Table 2. Agilent LC/MS/MS parameters for pesticide analysis.

Liquid Chromatography	
Model	Agilent 1290 Infinity III UHPLC
LC Column	Agilent ZORBAX RRHD Eclipse Plus C18, 2.1 × 150 mm, 1.8 µm (p/n 959759-902)
Mobile Phase A	5 mM ammonium formate + 0.1% formic acid in water
Mobile Phase B	5 mm ammonium formate + 0.1% formic acid in methanol
Injection Volume	2.0 µL
Flow Rate	0.4 mL/min
Gradient	Time (min) %B 0 5 3 30 17 100 20 100
Post Time	3 min
Mass Spectrometer	
Model	Agilent 6475 triple quadrupole LC/MS
Acquisition Mode	dMRM
Drying Gas	200 °C at 9 L/min
Sheath Gas	400 °C at 12 L/min
Nebulizer	35 psi
Capillary Voltage	2,500 V (+), 3,000 V (–)
Nozzle Voltage	0 V (+/-)

EMR–Lipid polish pouch, 3.5 g anhydrous $MgSO_4$ (part number 5982-0102), and ceramic homogenizers, 50 mL tubes, 100/pk (part number 5982-9313).

Results and discussion

Both the GC/MS/MS and LC/MS/MS data were acquired in dMRM acquisition method with MassHunter acquisition software version 13.0 and processed by the Agilent MassHunter Qualitative and Quantitative Analysis software version 12.1.

Linearity

Matrix-matched calibration standards were prepared over a range of 2.5 to 100 ng/mL for GC/MS/MS pesticides and 0.5 to 50 ng/mL for LC/MS/MS pesticides. Results in Figure 6 show that all the targets met the calibration curve linearity requirement of $R^2 \geq 0.99$ for the 76 pesticides analyzed by

Table 3. R^2 Comparison of the pesticides analyzed by both GC/MS/MS and LC/MS/MS.

Name	GC/MS/MS	LC/MS/MS
Azinphos-methyl	0.998	0.997
Cadusafos	1.000	0.996
Chlorfenvinphos	0.996	0.997
Chlorpyrifos	0.999	0.997
Diazinon	0.999	0.998
Dimethoate	0.999	0.998
Diphenamid	0.999	0.997
Ethoprophos	1.000	0.995
Fensulfothion	0.996	0.997
Heptenophos	0.999	0.993
Isazofos	0.999	0.994
Metolachlor	1.000	0.998
Penconazole	0.998	0.994
Pirimiphos-methyl	1.000	0.998
Profenofos	0.996	0.997
Quinalphos	0.996	0.992
Quizalofop-ethyl	0.998	0.994
Triazophos	0.997	0.993

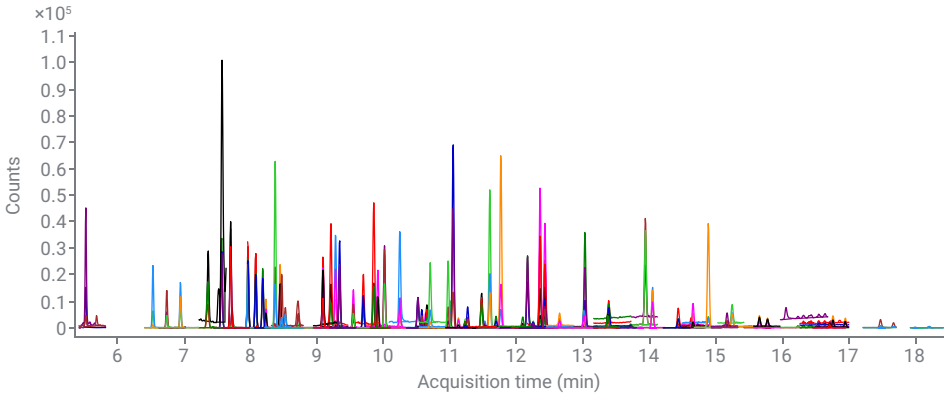

Figure 4. MRM chromatogram of 76 pesticides spiked at 10 ng/mL in cocoa liquor by GC/MS/MS analysis.

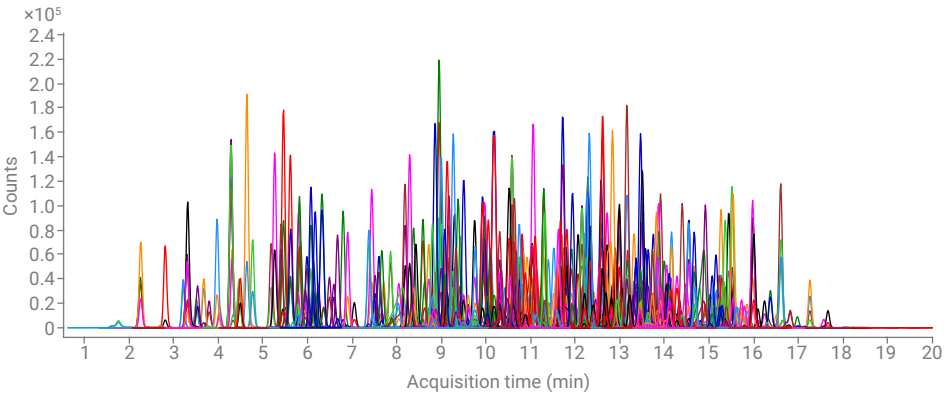

Figure 5. MRM chromatogram of 308 pesticides spiked at 10 ng/mL in cocoa liquor by LC/MS/MS analysis.

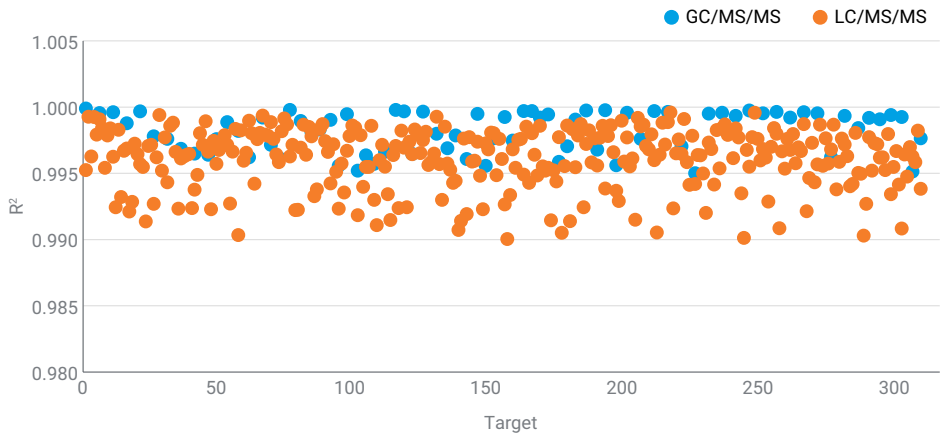

Figure 6. R^2 distribution of linearity curves for all the pesticides analyzed by both GC/MS/MS and LC/MS/MS.

GC/MS/MS and 308 pesticides by LC/MS/MS. Table 3 summarized the R^2 value comparison for the 18 pesticides that were analyzed by both GC/MS/MS and LC/MS/MS.

Recovery and reproducibility

Target recovery and reproducibility are strongly representative of quantitation accuracy and data quality and thus serve as important indicators of overall method performance. Recovery was calculated based on analyte response ratios between prespiked QC (10 µg/kg spike for GC/MS/MS and 2 µg/kg spike for LC/MS/MS) and corresponding matrix-matched calibration level. Figure 7 shows the pesticide recovery in cocoa liquor after QuEChERS sample preparation. Statistical analysis showed that more than 92% of the target compounds achieved recoveries between 70 and 120%.

Reproducibility was assessed by six replicate injections of prespiked samples analyzed by GC/MS/MS and LC/MS/MS, respectively. As shown in Figure 8, the RSD values for all pesticides were below 20%, demonstrating the excellent reproducibility of both analytical systems. Table 4 summarizes the recovery and RSD% for the 18 pesticides covered by both techniques. Both GC/MS/MS and LC/MS/MS show comparable results.

Combination of methods

The combined use of LC/MS/MS and GC/MS/MS enables comprehensive coverage of a broad range of pesticide residues and their metabolites in food matrices. Owing to the structural diversity of this large class of compounds, it is not feasible to analyze all pesticides using a single analytical technique based solely on either GC

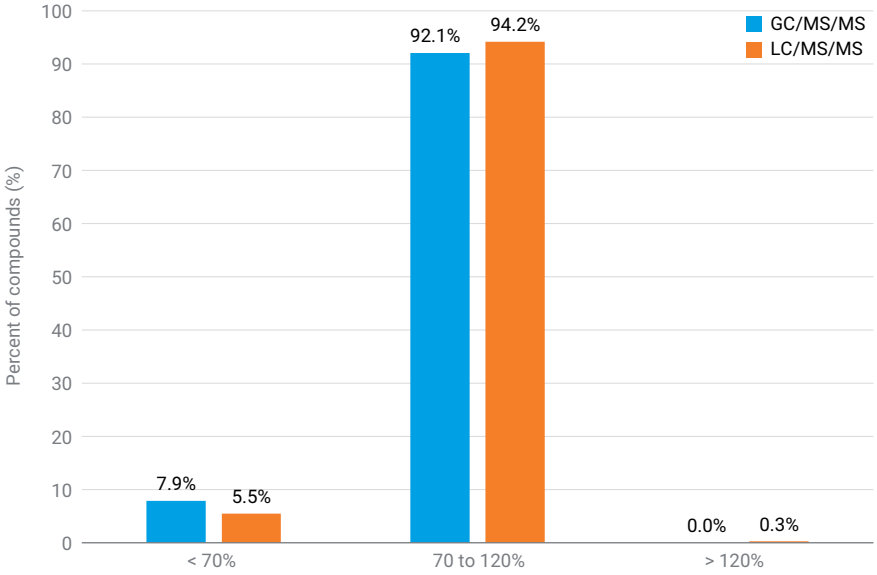

Figure 7. Pesticide recovery rate in QuEChERS cocoa liquor.

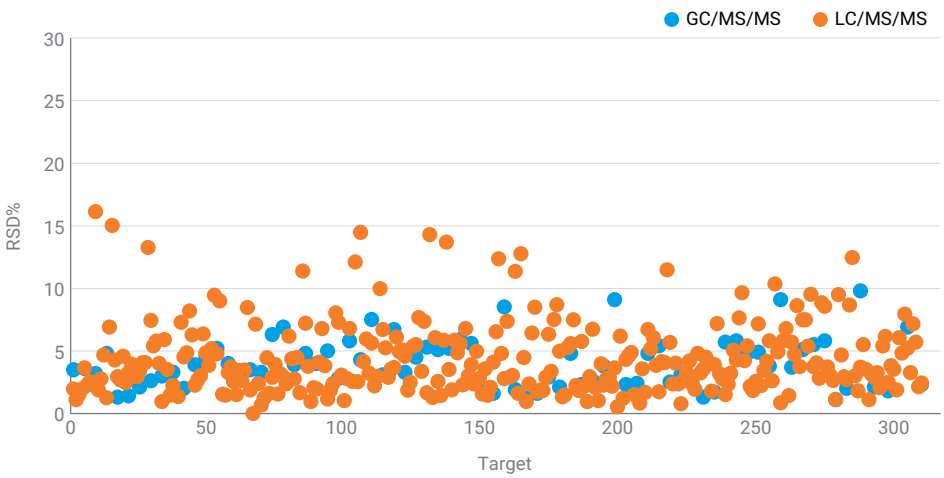

Figure 8. RSD% of prespiked pesticides in cocoa liquor.

or LC. Therefore, leveraging both complementary techniques is essential to achieve wide analytical coverage of pesticide residues that may pose risks to human health.

Certain classes of pesticides are more amenable to GC/MS/MS analysis, particularly halogenated and nonpolar compounds. Examples include hexachlorobenzene (HCB), hexachlorocyclohexane (HCH), DDE, DDT, DDD, dieldrin, endrin, endosulfan, heptachlor, and heptachlor epoxide. These compounds are generally not suitable for LC-based analysis and are therefore preferentially analyzed by GC/MS/MS. In contrast, highly polar and thermally labile compounds such as clothianidin, dinotefuran, imidacloprid, imazosulfuron, oxasulfuron, siduron, metoxuron, isoproturon, foramsulfuron, forchlorfenuron, halosulfuron-methyl, flazasulfuron, ethoxysulfuron, diflubenzuron, cinosulfuron, chlorsulfuron, azimsulfuron, and amidosulfuron are not amenable to GC analysis and are more effectively determined using LC/MS/MS.

Some pesticides are amenable to analysis by both analytical techniques. In this study, a total of 18 pesticides were analyzed using both LC/MS/MS and GC/MS/MS. These pesticides include azinphos-methyl, cadusafos, chlorfenvinphos, chlorpyrifos, diazinon, dimethoate, diphenamid,

Table 4. Recovery and RSD% comparison of the pesticides analyzed by both techniques.

Name	Recovery (%)		RSD (%)	
	GC/MS/MS	LC/MS/MS	GC/MS/MS	LC/MS/MS
Azinphos-methyl	85.9	98.9	4.8	15.0
Cadusafos	86.5	96.5	2.0	1.5
Chlorfenvinphos	92.1	100.1	5.2	6.3
Chlorpyrifos	78.0	94.1	3.5	6.3
Diazinon	84.3	93.0	3.1	2.9
Dimethoate	94.3	101.8	3.3	1.7
Diphenamid	87.3	99.1	4.5	2.0
Ethoprophos	87.2	101.0	1.9	2.5
Fensulfothion	91.5	102.2	8.5	5.4
Heptenophos	92.6	98.9	2.6	2.8
Isazofos	85.6	104.8	2.3	4.5
Metolachlor	86.6	95.9	3.1	2.9
Penconazole	85.2	93.4	5.7	2.4
Pirimiphos-methyl	84.9	89.8	3.8	5.0
Profenofos	84.5	90.9	9.1	4.2
Quinalphos	88.2	91.9	5.5	7.5
Quizalofop-ethyl	60.7	63.9	5.8	3.7
Triazophos	91.2	100.6	6.9	3.8

ethoprophos, fensulfothion, heptenophos, isazofos, metolachlor, penconazole, pirimiphos-methyl, profenofos, quinalphos, quizalofop-ethyl, and triazophos.

Figures 9 and 10 provide representative examples illustrating the complementary performance of GC/MS/MS and LC/MS/MS. Figure 9 shows the chromatograms of triazophos in a spiked matrix extract at 5 ng/mL, where LC/MS/MS exhibits superior detection sensitivity compared to GC/MS/MS. In contrast, Figure 10 presents the chromatograms of chlorpyrifos at the same concentration, for which GC/MS/MS delivers higher sensitivity. Together, these results underscore the value of employing both analytical platforms to achieve optimal sensitivity and reliable quantification across diverse pesticide classes.

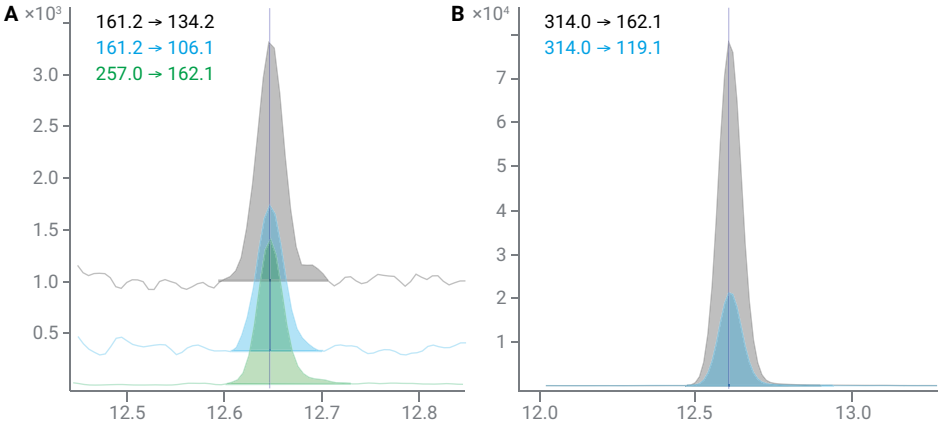

Figure 9. Analysis of triazophos by GC/MS/MS (A) and LC/MS/MS (B).

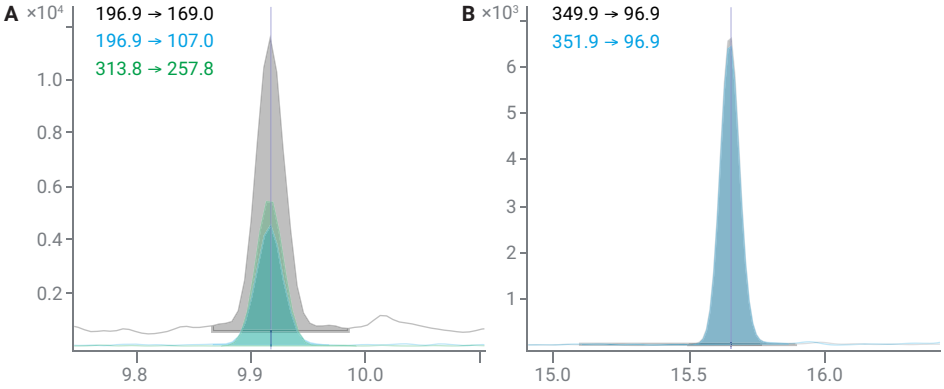

Figure 10. Analysis of chlorpyrifos by GC/MS/MS (A) and LC/MS/MS (B).

Conclusion

This study successfully demonstrated a robust and sensitive method for the quantitative analysis of 366 pesticides in cocoa liquor using the Agilent 8890/7010D GC/MS/MS and the 1290 Infinity III/6475 LC/MS/MS system.

To achieve the most efficient use of instrument cycle time, both GC/MS/MS and LC/MS/MS data were acquired in dMRM mode. The dMRM methods were created and developed based on the Agilent MRM databases.

The optimized workflow included sample

Appendix 1

GC/MS/MS MRM parameters of target pesticides

Name	RT (min)	Quantifier		Qualifier 1		Qualifier 2	
		Transition	CE (ev)	Transition	CE (ev)	Transition	CE (ev)
Mevinphos, E-	5.528	127.0 → 94.9	15	127.0 → 109.0	10	163.9 → 93.0	15
Heptenophos	6.534	124.0 → 89.0	10	124.0 → 63.0	35	249.9 → 124.0	5
Thionazin	6.745	143.0 → 79.0	10	143.0 → 52.1	20	175.0 → 79.0	10
Ethoprophos	6.946	157.9 → 97.0	15	157.9 → 114.0	5	157.9 → 81.0	15
Cadusafos	7.357	158.8 → 97.0	15	126.9 → 98.9	5	157.9 → 96.9	15
BHC-alpha	7.570	180.9 → 145.0	15	216.9 → 181.0	5	218.9 → 183.0	5
Hexachlorobenzene	7.703	283.8 → 213.9	30	283.8 → 248.8	15	248.9 → 214.0	15
Dimethoate	7.724	87.0 → 46.0	20	125.0 → 47.0	15	228.7 → 87.0	5
BHC-beta	7.963	181.0 → 145.0	15	216.9 → 181.1	5	218.9 → 183.1	5
BHC-gamma	8.081	181.0 → 145.0	15	216.9 → 181.0	5	218.9 → 183.1	5
Fonofos	8.183	246.1 → 109.0	15	246.1 → 137.0	5	109.0 → 62.9	15
Diazinon	8.232	137.1 → 84.0	10	199.1 → 135.1	10	199.1 → 93.0	15
Tefluthrin	8.372	177.1 → 127.1	15	177.1 → 87.0	30	197.0 → 141.1	10
BHC-delta	8.445	181.1 → 145.1	15	217.0 → 181.1	5	219.0 → 183.1	5
Isazofos	8.468	161.0 → 119.1	5	256.9 → 118.9	15	256.9 → 162.0	5
Chlorothalonil	8.526	265.9 → 133.0	45	265.9 → 230.9	20	265.9 → 168.0	30
Formothion	8.721	124.9 → 47.0	15	170.0 → 93.0	5	197.9 → 92.9	10
Parathion-methyl	9.088	125.0 → 47.0	10	125.0 → 79.0	5	262.9 → 109.0	10
Chlorpyrifos-methyl	9.089	124.9 → 47.0	15	285.9 → 93.0	25	287.9 → 92.9	20
Alachlor	9.211	188.1 → 160.1	10	188.1 → 132.1	20	237.1 → 160.1	10
Heptachlor	9.277	271.7 → 236.9	15	273.7 → 236.9	15	273.7 → 238.9	15
Ronnel	9.342	285.0 → 269.9	15	285.0 → 93.0	25	286.9 → 272.0	15
Fenitrothion	9.548	125.1 → 47.0	15	277.0 → 109.0	15	277.0 → 260.1	5
Pirimiphos-methyl	9.549	290.0 → 125.0	20	276.0 → 125.0	15	304.9 → 180.0	5
Malathion	9.699	126.9 → 99.0	5	157.8 → 125.0	5	172.9 → 99.0	15
Metolachlor	9.854	238.0 → 162.2	10	238.0 → 133.2	30	240.0 → 162.2	10
Aldrin	9.886	262.9 → 192.9	35	262.9 → 190.9	35	254.9 → 220.0	20
Chlorpyrifos	9.917	196.9 → 169.0	15	196.9 → 107.0	40	313.8 → 257.8	15
DCPA (Dacthal, chlorthal-dimethyl)	10.015	298.9 → 221.0	25	300.9 → 223.0	25	331.8 → 300.9	10
Diphenamid	10.243	167.1 → 165.1	20	239.0 → 72.0	10	239.0 → 167.1	0
Bromophos	10.250	330.9 → 315.9	20	330.9 → 93.0	30	125.0 → 47.0	15
Penconazole	10.515	248.0 → 157.1	25	248.0 → 192.1	15	159.0 → 123.0	20
Heptachlor exo-epoxide	10.574	352.8 → 262.9	15	352.8 → 316.8	5	354.8 → 264.9	15
Chlorfenvinphos	10.632	266.9 → 159.0	20	266.9 → 203.0	10	294.9 → 266.9	5
Heptachlor endo-epoxide	10.652	135.0 → 99.0	15	183.0 → 119.0	30	216.9 → 147.0	40
Quinalphos	10.702	146.0 → 118.0	10	157.0 → 102.0	30	192.9 → 129.0	10
Methidathion	10.970	144.9 → 85.0	5	144.9 → 58.1	15	124.9 → 47.0	15
Chlordane-trans	10.997	271.7 → 236.9	15	372.8 → 265.8	15	374.8 → 265.8	15
DDE-o,p'	11.048	246.0 → 176.2	30	248.0 → 176.2	30	317.8 → 248.0	15
Tetrachlorvinphos, E-isomer	11.125	330.8 → 108.9	15	328.8 → 108.9	15	332.8 → 108.8	15
Endosulfan I (alpha isomer)	11.229	194.9 → 160.0	5	194.9 → 125.0	20	276.7 → 241.9	15
Chlordane-cis	11.264	372.8 → 265.9	25	372.8 → 336.9	10	372.8 → 300.9	10

Name	RT (min)	Quantifier		Qualifier 1		Qualifier 2	
		Transition	CE (ev)	Transition	CE (ev)	Transition	CE (ev)
Prothiofos	11.476	162.0 → 63.1	30	266.9 → 239.0	5	308.9 → 238.9	15
Profenofos	11.520	207.9 → 63.0	30	207.9 → 98.9	25	338.8 → 268.7	15
DDE-p,p'	11.597	246.1 → 176.2	30	315.8 → 246.0	15	317.8 → 246.0	15
Dieldrin	11.691	262.9 → 193.0	35	237.0 → 142.9	25	277.0 → 241.0	5
DDD-o,p'	11.761	235.0 → 165.1	25	235.0 → 200.1	10	199.1 → 164.1	20
Endrin	12.093	262.8 → 193.0	35	244.8 → 210.0	10	244.8 → 173.0	30
Chlorobenzilate	12.164	139.1 → 75.1	30	251.1 → 111.1	35	251.1 → 139.1	15
Fensulfothion	12.249	291.8 → 156.0	15	291.8 → 108.8	15	292.8 → 96.8	20
Endosulfan II (beta isomer)	12.253	206.9 → 172.0	15	194.9 → 124.9	25	194.9 → 158.9	10
DDD-p,p'	12.352	237.0 → 165.1	25	237.0 → 200.1	15	199.1 → 164.1	20
Ethion	12.421	230.9 → 129.0	20	230.9 → 175.0	10	152.9 → 96.9	10
DDT-o,p'	12.426	235.0 → 165.2	20	235.0 → 199.1	15	237.0 → 165.2	20
Triazophos	12.646	161.2 → 134.2	5	161.2 → 106.1	10	257.0 → 162.1	5
Endosulfan sulfate	13.012	271.9 → 237.0	20	273.8 → 236.9	15	273.8 → 238.9	15
DDT-p,p'	13.026	235.0 → 165.2	20	235.0 → 199.2	15	237.0 → 165.2	20
Triphenyl phosphate	13.369	214.9 → 168.1	15	325.0 → 169.1	20	326.0 → 325.0	5
Piperonyl butoxide	13.383	176.1 → 103.1	25	176.1 → 131.1	15	176.1 → 117.1	20
Iprodione	13.714	313.8 → 244.9	10	313.8 → 55.9	20	187.0 → 124.0	25
Bifenthrin	13.935	181.2 → 165.2	25	181.2 → 166.2	10	166.2 → 165.2	20
Methoxychlor, p,p'-	14.045	227.0 → 141.1	40	227.0 → 212.1	15	227.0 → 169.1	25
Tetradifon	14.432	158.9 → 111.0	20	353.8 → 226.8	10	355.8 → 228.8	10
Azinphos-methyl	14.627	160.0 → 77.0	20	160.0 → 132.1	5	160.0 → 51.1	40
Leptophos	14.653	171.0 → 77.1	15	171.0 → 51.0	40	376.8 → 361.8	20
Mirex	14.880	271.8 → 236.8	20	236.9 → 142.9	30	236.9 → 118.9	30
Pyrazophos	15.166	221.0 → 193.1	10	221.0 → 149.0	15	232.0 → 204.1	10
Azinphos-ethyl	15.242	132.0 → 77.1	15	160.0 → 132.1	0	160.0 → 77.1	20
Permethrin, (1R)-cis-	15.650	183.1 → 168.1	10	183.1 → 153.1	15	163.0 → 127.0	5
Permethrin, (1R)-trans-	15.775	182.9 → 168.1	10	163.0 → 127.0	5	183.1 → 153.1	15
Cyfluthrin	16.227	162.9 → 127.0	5	162.9 → 90.9	15	206.0 → 150.0	40
Cypermethrin	16.544	163.0 → 127.0	5	181.0 → 152.1	25	163.0 → 91.0	10
Quizalofop-ethyl	16.708	163.0 → 100.0	20	163.0 → 136.0	10	371.8 → 298.9	10
Flucythrinate	16.754	156.9 → 107.1	15	198.9 → 157.0	10	198.9 → 107.0	25
Fenvalerate	17.468	167.0 → 125.1	5	208.9 → 141.1	15	224.9 → 119.0	15
Deltamethrin	18.203	252.9 → 174.0	5	250.7 → 93.0	20	250.7 → 172.0	5

Appendix 2

LC/MS/MS MRM parameters of target pesticides

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Cyromazine	2.252	167.1 → 85.0	21	167.1 → 68.0	43
Methamidophos	2.269	141.9 → 94.1	15	141.9 → 125.0	10
Acephate	2.814	183.9 → 143.0	7	183.9 → 125.0	19
Omethoat	3.213	214.0 → 125.0	25	214.0 → 109.0	30
Aminocarb	3.297	209.1 → 137.2	24	209.1 → 152.0	12
Pymetrozin	3.304	218.0 → 105.1	20	218.0 → 78.1	45
Butocarboxim sulfoxide	3.310	207.1 → 131.9	4	207.1 → 75.0	14
Dinotefuran	3.538	203.1 → 129.0	8	203.1 → 114.0	8
Aldicarb sulfon	3.672	223.1 → 86.2	15	223.1 → 148.1	7
Butoxycarboxim	3.675	240.0 → 106.0	12	240.0 → 44.1	54
Oxamyl	3.971	237.0 → 72.1	15	237.0 → 90.1	10
Nitenpyram	4.032	271.1 → 56.1	35	271.1 → 225.2	8
Oxydemeton-methyl	4.286	247.1 → 169.1	12	247.1 → 109.0	32
Demeton-s-methyl sulfoxide	4.291	247.0 → 169.0	12	247.0 → 109.0	30
Methomyl	4.320	162.9 → 88.1	15	162.9 → 106.1	5
Flonicamid	4.331	230.0 → 203.0	20	230.0 → 174.0	20
Demeton-s-methylsulfone	4.468	263.1 → 169.0	15	263.1 → 109.2	29
Monocrotophos	4.775	224.0 → 127.0	15	224.0 → 193.1	10
Dicrotophos	5.184	238.1 → 112.1	9	238.1 → 127.1	17
Ethiofencarb sulfone	5.260	275.1 → 107.0	29	275.1 → 201.0	7
Imidacloprid	5.454	256.0 → 175.1	20	256.0 → 209.1	15
Ethiofencarb sulfoxide	5.465	242.0 → 107.0	17	242.0 → 185.1	5
Clothianidin	5.512	250.2 → 169.1	11	250.2 → 132.1	17
Pirimicarb-desmethyl	5.621	225.1 → 71.9	21	225.1 → 168.0	13
Sulfadiazole (Ethidimuron)	5.622	265.1 → 207.9	12	265.1 → 57.0	32
Flumetsulam	5.795	326.0 → 129.2	25	326.0 → 262.1	20
Fenuron	5.807	165.1 → 72.0	16	165.1 → 76.9	32
Fuberidazol	5.820	185.1 → 157.1	25	185.1 → 156.1	35
Methiocarb sulfoxide	5.848	242.1 → 185.1	12	242.1 → 121.9	34
Metamitron	5.935	203.1 → 175.1	15	203.1 → 104.1	25
Trichlorfon	5.953	256.9 → 109.1	20	256.9 → 221.0	10
Dimethoate	5.982	230.0 → 125.0	20	230.0 → 199.0	10
Dioxacarb	6.059	224.0 → 123.0	15	224.0 → 167.0	5
Vamidothion	6.080	288.1 → 146.0	8	288.1 → 58.0	50
Acetamiprid	6.132	223.0 → 126.1	24	223.0 → 90.1	43
Chloridazon (Pyrazon)	6.247	222.0 → 77.1	40	222.0 → 104.1	25
Mexacarbate	6.330	223.1 → 151.0	24	223.1 → 166.1	12
Cymiazol	6.362	219.0 → 144.0	40	219.0 → 171.0	30
Cymoxanil	6.591	199.0 → 128.1	10	199.0 → 111.1	20
Oxycarboxin	6.673	268.1 → 175.0	15	268.1 → 147.0	27
Isocarbamide	6.795	186.1 → 87.0	16	186.1 → 130.0	10
Thiacloprid	6.902	253.0 → 126.0	25	253.0 → 90.1	45
Mevinphos	7.052	225.0 → 127.0	5	225.0 → 193.1	10

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Florasulam	7.455	360.0 → 129.0	38	360.0 → 192.0	16
Aldicarb	7.489	116.0 → 89.1	9	116.0 → 70.1	4
Fensulfothion oxon	7.608	292.9 → 237.0	20	292.9 → 265.0	12
DMSA	7.632	201.0 → 92.1	19	201.0 → 137.0	7
Metoxuron	7.662	229.0 → 72.0	21	229.0 → 156.0	27
Ethirimol	7.709	210.1 → 140.1	24	210.1 → 98.1	28
Allidochlor	7.743	174.1 → 98.1	12	174.1 → 41.2	30
Cythioate	7.784	298.0 → 217.0	17	298.0 → 125.0	27
Fensulfothion oxon sulfone	7.862	309.0 → 253.0	16	309.0 → 175.0	28
Paraoxon-methyl	7.891	248.0 → 109.1	30	248.0 → 202.1	15
Metolcarb	8.041	166.1 → 109.1	5	166.1 → 65.0	40
2-(1-Naphthyl)acetamide	8.188	186.1 → 141.0	17	186.1 → 115.0	45
Carbetamide	8.190	237.1 → 192.1	6	237.1 → 118.1	12
Phosphamidon (mix of isomers)	8.210	300.1 → 174.1	13	300.1 → 127.0	16
Pirimicarb	8.287	239.1 → 72.1	25	239.1 → 182.2	15
Quinoclamin	8.327	208.0 → 76.9	49	208.0 → 88.9	49
Atraton	8.381	212.2 → 170.1	16	212.2 → 100.1	32
Monuron	8.426	199.0 → 72.0	21	199.0 → 126.0	29
Propoxycarbazone sodium	8.494	421.1 → 180.0	15	421.1 → 138.0	30
Cinosulfuron	8.524	414.2 → 183.1	16	414.2 → 215.1	14
Dichlorvos	8.577	221.0 → 109.0	17	221.0 → 79.0	29
Azamethiphos	8.587	325.0 → 182.9	12	325.0 → 111.9	40
Oxasulfuron	8.620	407.0 → 150.1	20	407.0 → 107.1	50
Mephosfolan	8.720	270.0 → 140.0	25	270.0 → 196.0	15
Metribuzin	8.721	215.0 → 187.1	20	215.0 → 84.1	25
Thifensulfuron-methyl	8.766	388.0 → 167.1	15	388.0 → 205.0	
Propoxur	8.802	210.1 → 111.1	15	210.1 → 168.1	10
Simazine	8.803	202.1 → 68.0	40	202.1 → 132.0	22
Bromacil	8.806	261.0 → 205.0	20	261.0 → 187.9	40
Pirimicarb-desmethyl-formamido	8.853	253.2 → 71.9	20	253.2 → 225.1	8
Bendiocarb	8.857	224.2 → 167.2	6	224.2 → 109.2	17
Nicosulfuron	8.877	411.1 → 182.1	21	411.1 → 213.1	17
Carbofuran	8.948	222.1 → 165.1	10	222.1 → 123.1	20
Formetanate	8.952	222.1 → 165.1	15	222.1 → 65.1	59
Hexazinone	8.991	253.2 → 171.1	20	253.2 → 71.1	40
Imazamethabenz methyl	9.004	289.0 → 144.4	44	289.0 → 161.2	30
Ofurace	9.045	282.0 → 254.0	8	282.0 → 178.0	20
Metsulfuron-methyl	9.057	382.0 → 167.1	15	382.0 → 199.0	20
Karbutylate	9.069	297.2 → 181.0	15	297.2 → 280.0	3
Thiazafluron	9.074	241.0 → 184.0	13	241.0 → 74.0	43
Pyracarbolid	9.123	218.1 → 125.0	21	218.1 → 96.9	33
DMST	9.144	215.0 → 106.0	13	215.0 → 151.0	5
Malaoxon	9.172	315.1 → 99.0	25	315.1 → 127.0	9
Simetryn	9.254	214.1 → 124.2	22	214.1 → 144.0	22
Fenamiphos sulfoxide	9.261	320.0 → 233.1	24	320.0 → 171.0	22
Tebuthiuron	9.267	229.1 → 172.1	17	229.1 → 116.0	29

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Desmetryn	9.298	214.1 → 172.1	16	214.1 → 82.0	32
Terbuthylazine-desethyl	9.332	202.0 → 146.0	16	202.0 → 104.0	30
Fenthion oxon sulfone	9.390	295.1 → 78.0	50	295.1 → 104.0	30
Fenthionsulfoxide	9.391	294.9 → 108.9	36	294.9 → 280.0	18
Metosulam	9.405	418.0 → 175.0	32	418.0 → 140.0	50
Carbaryl	9.426	202.0 → 145.0	10	202.0 → 127.1	30
Fenamiphos sulfone	9.494	336.0 → 266.0	20	336.0 → 308.1	14
Fenfuram	9.507	202.2 → 109.1	24	202.2 → 120.1	16
Chlorsulfuron	9.597	358.0 → 167.1	15	358.0 → 141.1	20
Monolinuron	9.603	215.0 → 126.0	19	215.0 → 148.0	13
Amidosulfuron	9.621	370.0 → 261.1	15	370.0 → 218.1	25
Bromoxynil (Brominal)	9.672	276.0 → 81.0	37	278.0 → 81.0	37
Cyprofuram	9.741	280.0 → 69.0	16	280.0 → 41.0	50
Fenthion sulfone	9.743	310.9 → 124.9	19	310.9 → 108.8	29
Ethiofencarb	9.755	226.0 → 107.0	18	226.0 → 164.0	4
Foramsulfuron	9.795	453.1 → 182.1	25	453.1 → 139.1	50
Secbumeton	9.917	226.2 → 170.1	21	226.2 → 67.9	55
Cyantraniliprole	9.923	475.4 → 286.0	18	475.4 → 444.0	20
Fosthiazate	9.965	284.0 → 104.1	25	284.0 → 228.1	10
Procymidone	9.968	301.0 → 284.0	4		
Prometon	9.968	226.2 → 142.1	24	226.2 → 184.0	21
Thiodicarb	10.036	355.0 → 88.1	10	355.0 → 108.1	10
Chlorotoluron	10.053	213.1 → 72.0	25	213.1 → 140.0	25
Phorate sulfoxide	10.099	277.0 → 199.0	7	277.0 → 143.0	21
Disulfoton sulfoxide	10.107	291.1 → 185.0	11	291.1 → 213.1	5
Metobromuron	10.111	259.0 → 148.0	15	259.0 → 170.0	20
Disulfoton sulfone	10.290	306.9 → 125.0	16	306.9 → 153.0	8
Isoprocarb	10.292	194.0 → 136.9	6	194.0 → 95.1	12
Paraoxon	10.295	276.1 → 94.0	40	276.1 → 248.0	10
Famphur (Famophos)	10.304	326.0 → 217.0	20	326.0 → 281.0	10
Methabenzthiazuron	10.307	222.0 → 165.0	10	222.0 → 150.0	35
Phorate sulfone	10.309	293.0 → 171.0	9	293.0 → 246.9	1
Atrazine	10.340	216.1 → 174.2	20	216.1 → 68.0	40
Flutriafol	10.436	302.0 → 70.1	15	302.0 → 123.0	30
Mesosulfuron-methyl	10.464	504.1 → 182.1	25	504.1 → 139.1	50
Trifloxysulfuron	10.481	438.1 → 182.0	20	438.1 → 257.0	20
Metazachlor	10.517	278.0 → 134.1	20	278.0 → 210.1	10
Tribenuron-methyl	10.534	396.0 → 155.1	10	396.0 → 181.1	20
Propachlor	10.546	212.1 → 170.0	10	212.1 → 94.1	40
Lenacil	10.555	235.2 → 153.1	15	235.2 → 136.0	35
DEET	10.578	192.1 → 91.1	37	192.1 → 119.0	16
Isoproturon	10.581	207.0 → 72.0	23	207.0 → 46.0	19
Azimsulfuron	10.589	425.0 → 182.0	14	425.0 → 156.0	42
Buturon	10.602	237.0 → 84.0	16	237.0 → 126.0	32
Pirimiphos-methyl-n-desethyl	10.624	278.0 → 246.0	18	278.0 → 125.0	26
Trimethacarb	10.639	194.1 → 137.0	9	194.1 → 122.1	28

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Fensulfothion	10.684	308.8 → 281.0	13	308.8 → 235.1	23
Isoxaflutole	10.699	359.8 → 250.9	20	359.8 → 220.0	40
Metalaxyl	10.739	280.1 → 220.2	10	280.1 → 160.1	25
Ioxynil	10.744	369.8 → 126.8	37	369.8 → 215.0	35
Forchlorfenuron	10.751	248.1 → 129.0	16	248.1 → 92.9	40
Difenoxuron	10.801	287.0 → 72.0	24	287.0 → 123.0	22
Heptenophos	10.804	251.0 → 127.0	15	251.0 → 125.0	25
Ametryn	10.811	228.1 → 186.1	16	228.1 → 68.2	44
Azaconazole	10.812	300.0 → 158.9	32	300.0 → 230.8	16
Cycluron	10.840	199.2 → 72.1	28	199.2 → 88.9	17
Norflurazon	10.886	304.3 → 284.0	25	304.3 → 160.0	35
Fensulfothion sulfone	10.922	324.9 → 268.8	14	324.9 → 191.0	28
Dimethachlor	11.025	256.0 → 224.0	15	256.0 → 148.0	30
Methoprotryne	11.043	272.2 → 198.0	24	272.2 → 169.9	33
Diphenamid	11.052	240.1 → 134.0	20	240.1 → 167.0	25
Desmedipham	11.103	318.1 → 182.2	20	318.1 → 136.1	10
Climbazole	11.129	293.1 → 69.0	24	293.1 → 197.0	16
Pyrimethanil	11.136	200.1 → 82.1	30	200.1 → 107.1	25
Azinphos-methyl (Guthion)	11.220	318.0 → 261.0	10	318.0 → 132.1	13
Flazasulfuron	11.225	407.9 → 182.1	20	407.9 → 139.1	45
Benoxacor	11.234	260.2 → 149.0	20	260.2 → 134.1	36
Clomazone	11.288	240.0 → 125.1	20	240.0 → 89.1	50
Phenmedipham	11.295	318.1 → 168.1	9	318.1 → 136.0	25
Phosmet	11.321	317.9 → 160.0	10	317.9 → 133.0	40
Chlorantraniliprole	11.327	483.9 → 285.9	10	483.9 → 452.9	20
Dimefuron	11.395	339.0 → 72.2	35	339.0 → 167.1	23
Bensulfuron-methyl	11.406	411.0 → 149.0	22	411.0 → 182.2	20
Fenobucarb	11.514	208.1 → 95.1	10	208.1 → 152.1	5
Fenpropimorph	11.580	304.4 → 147.3	33	304.4 → 117.2	67
Linuron	11.582	249.0 → 160.0	20	249.0 → 182.1	15
Terbufos sulfone	11.585	321.1 → 171.0	11	321.1 → 115.1	33
Terbufos sulfoxyde	11.625	305.1 → 187.0	9	305.1 → 96.8	49
Propanil	11.636	218.1 → 127.1	30	218.1 → 161.9	16
Ethofumesat	11.685	304.0 → 287.1	5	304.0 → 121.1	25
Diethofencarb	11.697	268.1 → 226.0	10	268.1 → 124.0	35
Furalaxyl	11.713	302.1 → 95.0	27	302.1 → 242.1	15
Azoxystrobin	11.748	404.0 → 372.2	15	404.0 → 344.0	25
Flurtamone	11.766	334.0 → 247.0	29	334.0 → 178.0	53
Siduron	11.784	233.3 → 137.2	18	233.3 → 94.0	30
Methiocarb	11.795	226.1 → 121.1	20	226.1 → 169.1	10
Chlorbromuron	11.881	293.0 → 182.0	15	293.0 → 203.9	21
Halofenozide	11.892	329.1 → 120.9	20	329.1 → 76.9	40
Ethiprole	11.909	397.1 → 255.0	41	397.1 → 351.0	21
Dimethenamide	11.922	276.1 → 244.1	10	276.1 → 168.1	20
Fenamidon	11.923	312.1 → 92.1	30	312.1 → 236.2	15
Terbuthylazine	11.943	230.1 → 174.1	18	230.1 → 104.1	40

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Dimethomorph	11.948	388.0 → 301.1	20	388.0 → 165.1	35
Promecarb	12.058	208.1 → 109.1	15	208.1 → 151.0	10
Boscalid (Nicobifen)	12.078	343.0 → 307.1	17	343.0 → 271.0	33
Imazosulfuron	12.082	412.9 → 152.9	10	412.9 → 156.0	22
Bispyribac	12.104	431.0 → 275.1	10	431.0 → 413.1	15
Prometryn	12.151	242.1 → 158.1	26	242.1 → 200.2	20
Pyrifenox	12.165	295.0 → 93.0	29	295.0 → 66.1	60
Mandipropamid	12.175	411.9 → 328.1	15	411.9 → 356.1	10
Paclobutrazol	12.190	294.1 → 70.1	20	294.1 → 125.0	40
Pronamide	12.204	256.0 → 190.0	15	256.0 → 44.0	40
Propyzamide	12.204	256.0 → 190.0	20	256.0 → 173.0	30
Triflusulfuron-methyl	12.207	493.0 → 264.0	22	493.1 → 96.1	60
Flutolanil	12.214	324.1 → 262.1	16	324.1 → 65.0	48
Isoxaben	12.256	333.2 → 165.0	16	333.2 → 150.0	48
Fluopicolide	12.266	382.9 → 172.9	25	382.9 → 144.9	50
Isocarbophos	12.282	291.1 → 188.9	25	291.1 → 231.1	9
Isoprothiolane	12.282	291.1 → 188.8	20	291.1 → 231.0	8
Flurprimidol	12.294	313.1 → 270.1	28	313.1 → 269.1	40
Mepronil	12.337	270.1 → 91.1	40	270.1 → 228.1	10
Ethoxysulfuron	12.399	398.9 → 217.9	28	398.9 → 261.0	14
Triadimefon	12.406	294.1 → 69.1	25	294.1 → 197.1	15
Benthiavalicarb-isopropyl	12.410	382.1 → 180.0	39	382.1 → 116.1	23
Myclobutanil	12.457	289.1 → 70.1	15	289.1 → 125.0	35
Pyridafenthion	12.539	341.0 → 189.0	20	341.0 → 92.1	40
Mefenacet	12.577	299.2 → 148.0	13	299.2 → 120.1	31
Chloroxuron	12.585	291.0 → 72.1	20	291.0 → 164.0	15
Dimethylvinphos	12.599	331.0 → 127.0	10	331.0 → 205.0	20
Triazophos	12.607	314.0 → 162.1	20	314.0 → 119.1	40
Halosulfuron-methyl	12.615	435.0 → 182.1	20	435.0 → 139.0	50
Isazofos	12.615	314.0 → 162.2	16	314.0 → 120.0	30
Bifenazate	12.637	301.1 → 198.2	5	301.1 → 170.1	20
Cyproconazole	12.691	292.1 → 70.1	20	292.1 → 125.1	35
Fluopyram	12.694	397.1 → 173.0	32	397.1 → 208.0	22
Mepanipyrim	12.696	224.0 → 106.1	30	224.0 → 209.2	21
Tepraloxydim	12.766	342.1 → 250.2	15	342.1 → 166.1	25
Trietazin	12.807	230.1 → 99.0	25	230.1 → 202.1	20
Fenchlorphos oxon	12.827	305.0 → 108.9	22	305.0 → 257.8	24
Triazamate	12.834	315.1 → 72.0	20	315.1 → 198.1	10
Butafenacil	12.851	492.3 → 180.0	46	492.3 → 331.0	26
Fenhexamid	12.853	302.0 → 97.2	25	302.0 → 55.1	45
Tetraconazole	12.887	372.0 → 159.0	35	372.0 → 70.1	25
Flufenacet	12.894	364.0 → 152.1	20	364.0 → 194.2	10
Mecarbam	12.896	330.0 → 227.0	10	330.0 → 97.1	45
Triticonazole	12.941	318.1 → 70.1	15	318.1 → 125.1	45
Ethoprophos (Ethoprop)	12.973	243.0 → 97.0	35	243.0 → 131.0	20
Napropamide	12.990	272.2 → 58.1	28	272.2 → 129.0	12

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Pethoxamid	12.991	296.1 → 131.1	20	296.1 → 91.0	48
Bupirimate	13.011	317.1 → 166.1	25	317.1 → 108.1	30
Cyazofamid	13.051	325.0 → 108.1	13	325.0 → 44.1	36
Epoxyconazol	13.066	330.0 → 121.1	20	330.0 → 101.1	50
Prothioconazole-desthio	13.099	312.0 → 69.9	23	312.0 → 124.8	41
Tebutam	13.153	234.2 → 91.0	28	234.2 → 65.0	50
Metolachlor	13.164	284.1 → 252.2	15	284.1 → 176.2	25
Dipropetryn	13.173	256.1 → 144.1	32	256.1 → 214.1	20
Fenbuconazole	13.174	337.1 → 70.1	20	337.1 → 125.1	40
Diflubenzuron	13.199	311.0 → 158.0	15	311.0 → 141.0	40
Uniconazole-P	13.221	292.1 → 70.0	24	292.1 → 125.0	36
Cyprodinil	13.226	226.1 → 93.1	45	226.1 → 77.1	60
Fipronil	13.289	435.0 → 330.0	17	435.0 → 250.0	28
Flusilazole	13.297	316.0 → 247.2	20	316.0 → 165.1	30
Fenamiphos	13.322	304.1 → 217.1	25	304.1 → 202.0	40
Fenoxycarb	13.363	302.1 → 88.1	20	302.1 → 116.1	10
Picoxystrobin	13.366	368.1 → 145.1	25	368.1 → 205.1	10
Rotenone	13.367	395.0 → 213.1	25	395.0 → 192.1	25
Silthiofam	13.462	268.1 → 252.1	5	268.1 → 73.0	28
Tetrachlorvinphos (Dietreen)	13.463	364.9 → 127.0	16	364.9 → 203.9	40
Neburon	13.473	275.0 → 57.0	27	275.0 → 88.0	17
Dimoxystrobin	13.496	327.1 → 205.1	5	327.1 → 116.0	20
Phenthoate	13.501	321.0 → 79.1	53	321.0 → 247.0	9
Quinalphos	13.502	299.0 → 163.0	25	299.0 → 147.0	25
Isoxadifen-ethyl	13.512	296.0 → 232.0	18	296.0 → 204.0	30
Clodinafop-propargyl	13.522	350.1 → 91.1	40	350.1 → 222.0	40
Beflubutamid	13.575	356.0 → 91.0	30	356.0 → 162.1	25
Kresoxim-methyl	13.580	314.1 → 222.2	15	314.1 → 267.1	10
Carfentrazone-ethyl	13.589	412.0 → 346.1	25	412.0 → 366.1	20
Flubendiamide	13.600	681.0 → 254.0	30	681.0 → 273.7	15
Sulfotep	13.624	323.0 → 97.0	44	323.0 → 115.0	40
Penconazole	13.635	284.0 → 70.1	15	284.0 → 159.0	30
Fenthion	13.700	279.1 → 169.1	16	279.1 → 247.0	10
Propaphos	13.730	305.1 → 221.0	12	305.1 → 141.0	28
Tebuconazole	13.731	308.1 → 70.1	20	308.1 → 125.0	40
Ediphenphos	13.752	311.0 → 109.0	40	311.0 → 173.0	20
Carpropamid	13.777	334.0 → 103.0	51	334.0 → 139.0	23
Furmecyclox	13.821	252.1 → 170.1	12	252.1 → 110.0	26
Isomethiozin	13.848	269.1 → 200.0	15	269.1 → 172.0	25
Flamprop-isopropyl	13.861	364.1 → 105.0	20	364.1 → 77.0	40
Propiconazole	13.905	342.0 → 158.9	35	342.0 → 69.1	20
Zoxamide	13.908	336.0 → 187.0	25	336.0 → 159.0	50
Benalaxyl	13.910	326.1 → 148.1	20	326.1 → 294.2	10
Coumaphos	13.912	363.0 → 226.9	28	363.0 → 307.0	16
Diazinon	13.926	305.1 → 169.0	25	305.1 → 153.1	25
Chlorfenvinphos	13.938	359.0 → 155.1	13	359.0 → 170.0	45

Name	RT (min)	Quantifier		Qualifier	
		Transition	CE (ev)	Transition	CE (ev)
Bromuconazole	14.018	377.9 → 70.1	25	375.9 → 70.1	25
Prochloraz	14.025	376.0 → 308.0	10	376.0 → 266.0	15
Hexaconazole	14.035	314.0 → 70.1	20	314.0 → 159.0	35
Pyraclostrobin	14.106	388.0 → 194.1	10	388.0 → 163.1	25
Bromfenvinfos	14.111	404.9 → 155.0	10	404.9 → 98.9	40
Metconazole	14.117	320.1 → 70.1	25	320.1 → 125.1	45
Orbencarb	14.144	258.0 → 125.0	26	258.0 → 100.0	12
Pirimiphos methyl	14.158	306.2 → 67.0	50	306.2 → 108.0	35
Fenchlorazol-ethyl	14.208	404.0 → 358.0	26	404.0 → 288.0	40
Metrafenon	14.329	409.0 → 209.1	10	409.0 → 226.9	25
Pencycuron	14.397	329.1 → 125.0	30	329.1 → 218.1	15
Difenoconazole (mix of isomers)	14.485	406.0 → 251.1	25	406.0 → 337.1	15
EPN	14.539	324.0 → 156.9	28	324.0 → 296.1	14
Cadusafos	14.550	271.1 → 97.0	40	271.1 → 130.9	20
Haloxyfop-methyl	14.554	375.9 → 316.0	18	375.9 → 288.0	30
Piperophos	14.662	354.1 → 255.0	12	354.1 → 170.7	24
Trifloxystrobin	14.665	409.1 → 186.1	15	409.1 → 145.0	50
Clethodim	14.908	360.1 → 164.1	20	360.1 → 268.2	10
Prosulfocarb	14.915	252.1 → 91.1	25	252.1 → 128.2	10
Fenoxaprop-ethyl	15.029	362.1 → 288.0	26	362.1 → 91.1	34
Profenofos	15.033	374.9 → 304.9	20	374.9 → 347.0	10
Quizalofop-ethyl	15.073	373.1 → 299.1	16	373.1 → 271.2	24
Furathiocarb	15.227	383.1 → 195.1	20	383.1 → 252.1	10
Sethoxydim	15.309	328.0 → 178.1	20	328.0 → 282.2	10
Pirimifos-ethyl	15.360	334.1 → 198.1	22	334.1 → 182.1	24
Fluazinam	15.365	462.9 → 415.9	18	462.9 → 398.0	14
Quinoxyfen	15.610	308.0 → 197.0	39	308.0 → 162.0	50
Chlorpyrifos (Dursban)	15.655	349.9 → 96.9	35	351.9 → 96.9	40
Tralkoxydim	15.795	330.1 → 284.2	10	330.1 → 138.1	20
Tiocarbazil	16.003	280.2 → 91.1	38	280.2 → 100.0	14
Butralin	16.098	296.2 → 240.0	11	296.2 → 222.0	23
Profoxydim	16.505	466.0 → 280.2	16	468.0 → 280.0	12
Cinidon-ethyl	17.254	394.1 → 107.1	34	394.1 → 135.0	20
Etofenprox	17.256	394.2 → 177.2	10	394.2 → 107.1	45
Pyridalyl	17.664	490.0 → 109.0	36	490.0 → 183.0	16

extraction with the Bond Elut QuEChERS AOAC extraction kit followed by cleanup with the Agilent Captiva EMR-GPD kit. This workflow provided excellent linearity, recovery, and reproducibility.

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