Improved LC/MS/MS Pesticide Multiresidue Analysis Using Triggered MRM and Online Dilution

Application Note

Food Safety

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Abstract

This application note describes the development and validation of a large pesticide multiresidue LC/MS/MS method using Agilent 1290 Infinity II LC systems coupled to Agilent 6490 triple quadrupole LC/MS instruments. The method enables the analysis of about 450 globally important pesticides in a short analysis time (analyte elution in less than 10 minutes). The MS/MS acquisition method uses triggered multiple reaction monitoring (tMRM), which provides increased confidence in analyte identification through triggered acquisition of additional MRMs when one of the primary MRMs exceeds a set abundance threshold. The mobile phase gradient was optimized to spread the analytes evenly throughout the elution window, with special attention paid to the separation of critical pairs. The LC system uses an online dilution setup, ensuring excellent peak shapes of early eluting (more polar) analytes. As a result, acetonitrile extracts (prepared using a QuEChERS-based extraction) are injected directly without a need for dilution with an aqueous buffer/solution prior to the injection. The method was validated in three different routine laboratories in multiple food commodity types/matrices, with 0.01 mg/kg method validated limit of quantitation (LOQ) achieved for the majority analyte-matrix combinations.

Agilent Technologies

Introduction

Multiresidue methods, capable of simultaneous analysis of a larger number of analytes, provide the most practical approach to routine pesticide residue monitoring in food, feed, dietary supplements, and similar sample types. In addition to the economic benefits (cost, time, and labor efficiency), large multiresidue methods and careful selection of the included analytes can also address challenges associated with global trade (global sample origin due to global sourcing of raw materials and global distribution of products) and different regulatory issues in different countries when it comes to pesticide use and misuse, regulatory limits, or pesticide residue definitions. Modern multiresidue methods typically employ tandem mass spectrometry using triple quadrupole instruments coupled to both gas chromatography and liquid chromatography (GC/MS/MS and LC/MS/MS) to cover a wide range of both GC- and LC/MS/MS amenable pesticides. High-end triple quadrupole instruments provide sensitivity, selectivity, and speed for the determination of a large number of compounds at low concentration levels, even in highly complex matrices.

When a pesticide residue is detected in a sample, the first step is identification. Using MS/MS, two overlapping precursor-to-product ion transitions (multiple reaction monitoring, MRM) within a certain ion ratio and retention time tolerance are typically required for analyte identification. The widely accepted SANTE guidelines (SANTE/11945/2015) for analytical quality control and method validation procedures for pesticide residue analysis in food and feed [1] recommend the following identification criteria for GC/MS/MS and LC/MS/MS methods: retention time within ± 0.1 minutes, ≥ 2 product ions, and ± 30 % maximum relative tolerance for ion ratios (as compared to the retention times and ion ratios obtained for the given analyte in concurrently analyzed standards).

In routine practice, especially when analyzing highly complex samples, the minimum identification criteria may not be enough to prevent potentially false positive or false negative results. Therefore, additional information is beneficial for improved identification confidence and also fast decision making on whether to accept/reject the given result. For compounds amenable to both GC/MS/MS and LC/MS/MS analysis, it is helpful to include these analytes on both analytical platforms, and take advantage of orthogonal selectivity of GC/MS/MS and LC/MS/MS techniques for a high degree of identification confidence. There are compounds, however, that can be analyzed only on one platform, or for which the second platform provides inferior sensitivity or other poorer performance characteristics. This is the case for many modern pesticides that are more polar and thermally labile, and thus more suitable for LC/MS/MS analysis. To obtain additional MS/MS information without compromising the number of analytes that could be included in the LC/MS/MS method, the Agilent 6400 Series triple quadrupole LC/MS instruments offer so-called triggered MRM (tMRM) functions.

In tMRM, up to 10 MRMs can be acquired for each analyte, and combined into a product ion spectrum (at optimum collision energies for each product ion), which is used for library matching of selected pesticides, as shown in Figure 1. Using the tMRM function, some of the transitions (primary transitions) are acquired during the entire analyte acquisition window. The acquisition of the additional transitions is triggered (and performed for a defined number of scans) if one of the primary transitions exceeds the set abundance threshold [2,3].

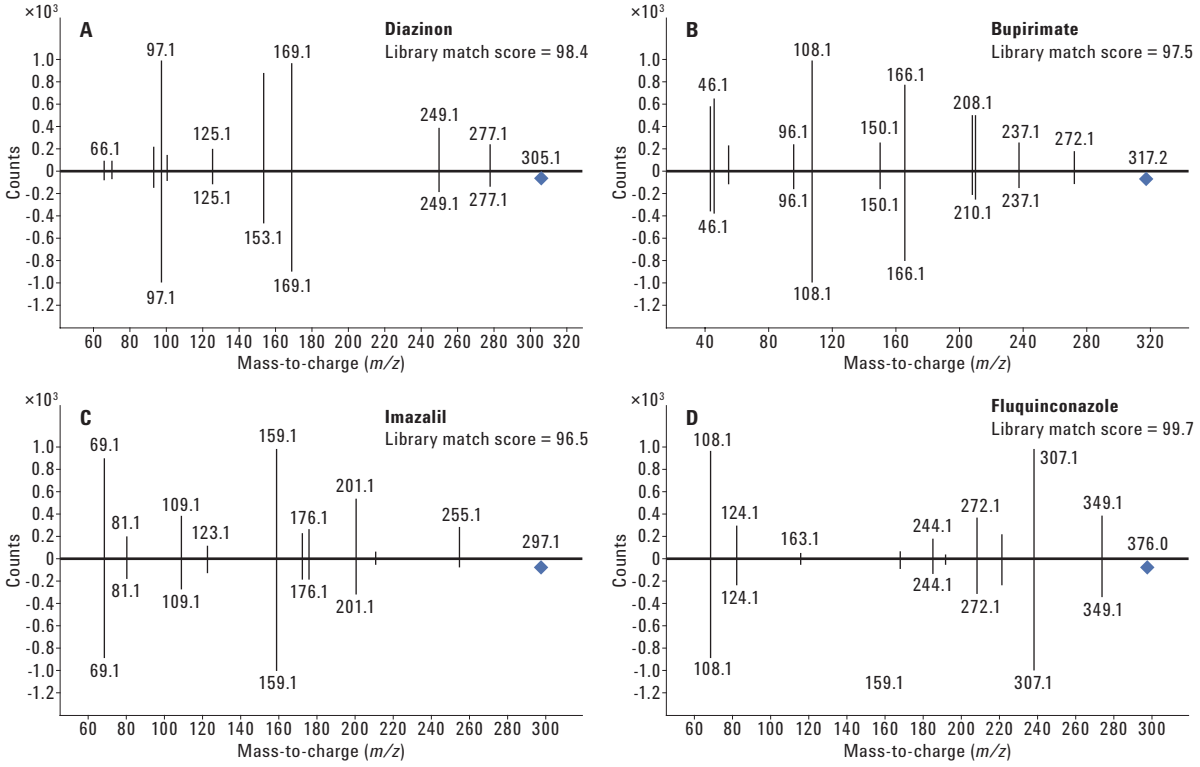


Figure 1. Examples of triggered MRM spectra and their matching against a reference library obtained using 10 MRMs for selected pesticides.

This application note describes the development and validation of a pesticide multiresidue LC/MS/MS method for the analysis of approximately 450 globally relevant pesticides using Agilent 1290 Infinity II LC systems coupled to Agilent 6490 triple quadrupole LC/MS instruments. The method is completely compatible with the Agilent 1290 Infinity II LC and an Agilent 6495 triple quadrupole LC/MS. The analytes are compounds amenable to a QuEChERS-based extraction and LC/MS/MS analysis, and represent priority pesticides included in regulatory monitoring testing programs in the US, Canada, EU, and Asia. Special attention was paid to the inclusion of pesticides specifically listed in certain regulations or guidelines, such as in the EU infant formula directive 141/2006/EC, the USDA National Organic Program, or US and European Pharmacopoeia pesticide monographs.

This method enables the analysis of a large number of analytes using a relatively short separation time (analyte elution in less than 10 minutes) and uses tMRM for increased identification confidence, using two to three primary MRMs, and typically four or more total MRMs, resulting in > 2,000 MRMs in the method. In addition, it improves retention and peak shape of early eluting, more polar analytes, which are notorious for having poor peak shapes when injected in extracts with a higher content of organic solvents, such as in QuEChERS acetonitrile extracts. This was achieved by using a special online dilution setup (a serial combination of two high-pressure mixers), enabling effective mixing of the injected sample with the initial highly aqueous mobile phase before reaching the column.

The method development was carried out at multiple laboratory sites. The final method was assembled at one location, and then transferred onto multiple instruments in three pesticide testing laboratories in the US, EU, and Asia, followed by method validation in multiple matrices using the SANTE method validation guidelines and criteria [1].

Experimental

Pesticide standards

A composite standard solution, containing all the analytes listed in Table 1 (pages 12–22) , was prepared at 1 µg/mL in acetonitrile containing 1 % acetic acid. To prepare this composite solution, the Agilent LC/MS standard mixes 1 to 8 at 100 µg/mL in acetonitrile (p/n 5190-0551) were combined with several custom mixes. The composite solution was then used for the preparation of solvent-based and matrix-matched standards. All standard solutions were stored at –20 °C.

Sample preparation

Sample preparation was based on the AOAC Int. Official method 2007.01 [4] using the acetate buffer QuEChERS extraction and partition steps but without any cleanup. High-moisture (10 g), low-moisture/low-fat (5 g), and low-moisture/high-fat and complex samples (1 g) were extracted using 10 mL of acetonitrile with 1 % acetic acid (10 mL of water was added to low-moisture samples) by shaking for 30 minutes. An internal standard mixture (100 µL of 1 µg/mL of the internal standards listed in Table 1) was added to the samples prior to extraction. After the initial shaking, 4 g of anhydrous magnesium sulfate and 1 g of sodium acetate were added to the sample tubes, followed by immediate shaking/vortexing for 1 minute. After centrifugation at >1,500 rcf for 5 minutes, an aliquot (400 µL) of the upper acetonitrile layer was placed in an autosampler vial together with 40 µL of a quality control (QC) standard containing 0.1 µg/mL triphenyl phosphate (TPP) in acetonitrile with 1 % acetic acid.

Matrix-matched standards (typically at concentrations corresponding to 0.001 to 0.050 µg/mL in the extract) were prepared by extracting blank matrices, and adding 40 µL of an appropriate standard solution to the 400 µL blank extract aliquot instead of the QC solution.

For trueness and precision (recovery and relative standard deviation, RSD) evaluation, blank matrix samples were spiked at 0.01, 0.02, or 0.05 mg/kg in five replicates during the method validation.

LC/MS/MS conditions

LC/MS/MS analyses were conducted using 1290 Infinity II LC systems (1,200 bar) coupled to 6490 triple quadrupole LC/MS instruments in three different laboratories. All systems used the same LC and MS conditions, listed in Table 2. Agilent MassHunter software was used for data acquisition and processing.

Table 2. Instrument Conditions

UHPLC parameters

Parameter	Value					
Analytical column	Agilent ZORBAX Eclipse Plus C18, Rapid Resolution HD, 2.1 × 100 mm, 1.8 µm					
Guard column	Agilent ZORBAX Eclipse Plus C18, 2.1 × 5 mm, 1.8 µm					
Online dilution setup	see Figure 2					
Column temperature	40 °C (G1316C TCC)					
Mobile phase A	10 mM ammonium formate in water-methanol (98:2, v/v) + 0.1 % formic acid					
Mobile phase B	10 mM ammonium formate in methanol-water (99:1, v/v) + 0.1 % formic acid					
Injection volume	2 µL (G4226A autosampler)					
Binary pump (G4220A) gradient and flow	Time (min)	%A	%B			Flow (mL/min)
	0.00	100	0			0.100
	0.20	100	0			0.100
	0.21	100	0			0.500
	0.50	50	50			0.500
	2.50	45	55			0.500
	5.50	25	75			0.500
	7.50	15	85			0.500
	8.30	0	100			0.500
	12.00	0	100			0.500
	12.10	100	0			0.500
	14.80	100	0			0.500
	14.90	100	0			0.100
Quaternary pump (G4204A) gradient and flow	Time (min)	%A	%B	%C	%D	Flow (mL/min)
	0.00	100	0	0	0	0.500
	0.20	100	0	0	0	0.500
	0.40	100	0	0	0	0.000
	14.80	100	0	0	0	0.000
	14.90	100	0	0	0	0.500

MS/MS parameters

Parameter	Value
Ionization mode	Positive ESI with Agilent Jet Stream (AJS)
Scan type	Triggered MRM (with three repeats)
Cycle time	650 ms
Stop time	15 minutes
Divert valve program	At 0 minutes to waste, at 1 minute to MS, at 10 minutes to waste
MS1/MS2 resolution	Unit
Gas temperature	180 °C
Gas flow	20 L/min
Nebulizer	40 psi
Sheath gas temperature	225 °C
Sheath gas flow	11 L/min
Capillary voltage	4,500 V
Nozzle voltage	0 V
iFunnel RF high/low	150/60

Results and Discussion

Optimization of MS/MS conditions

The MS/MS method development involved optimization and selection of MS/MS transitions (typically, 10 MRMs per analyte) using Agilent MassHunter Optimizer software, followed by a detailed review of the collected information. MassHunter Optimizer is a versatile tool for automated optimization of MRM conditions, including selection of precursor and product ions, and optimization of collision energies (CE) [5]. Practical considerations for routine optimization of pesticides and other compounds using MassHunter Optimizer are discussed in detail in a separate document [6].

Optimization of UHPLC conditions and online dilution

The aim of the UHPLC optimization was to achieve optimum analyte separation and detection within the relatively short separation time of less than 10 minutes. In addition, we wanted to improve retention and peak shape of early eluting, more polar analytes (such as cyromazine, methamidophos, acephate, and so forth), which are notorious for having poor peak shapes when injected in extracts with a higher content of organic solvents. Our ultimate goal was to be able to inject QuEChERS acetonitrile extracts directly, without any pre-injection dilution, while having sharp and well-focused peaks of the early eluting pesticides.

Figure 2 shows a typical situation that can be observed for early eluting pesticides when injected in acetonitrile in multiresidue methods. The early eluting peaks exhibit peak splitting and broadening. The most polar analytes usually show an unretained portion eluting at the dead time. This is caused by a breakthrough of molecules surrounded by the strong injection solvent. A lower injection volume can improve the situation, but usually not solve it completely. This option provides lower sensitivity due to the decreased sample volume introduced into the system. Another option is to dilute the sample extract and calibration standards before the injection using water or an aqueous buffer. This is a common practice but, unfortunately, the typically recommended dilution factors, such as 1:2 extract dilution, do not fully solve the peak splitting/retention problem. Higher dilution factors would be needed, but they can lead to stability and solubility issues. Moreover, the pre-injection dilution requires an additional step in the sample preparation method.

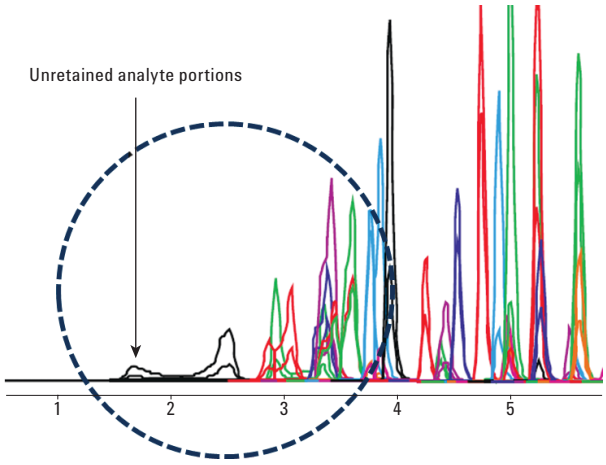
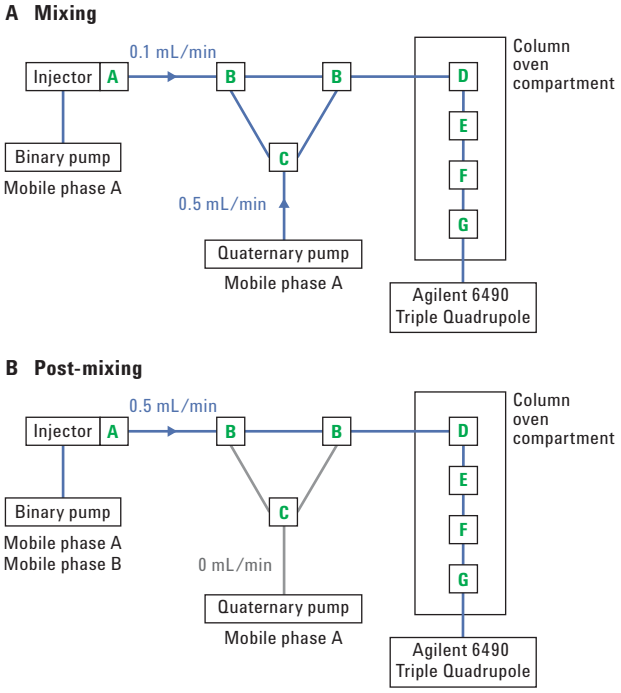


Figure 2. Illustration of problematic peak shape and retention of early eluting, more polar pesticides when injected in acetonitrile in other multiresidue LC/MS/MS methods [3].

We decided to use online dilution and mixing to improve the chromatography of early eluting compounds. Figure 3 provides the online dilution setup (a serial combination of two high-pressure mixers) used in the final method. This setup enables highly effective mixing of the injected sample with the initial highly aqueous mobile phase A before reaching the column, resulting in excellent peak shapes and retention of early eluting analytes (Figure 4). During the mixing stage, the method uses only mobile phase A. The sample is introduced at a lower flow rate of 0.1 mL/min using a binary pump, while the quaternary pump (a second high-pressure pump) flow rate is at 0.5 mL/min for more effective mixing with the aqueous mobile phase. After the mixing step, the quaternary pump flow is stopped, and the binary pump gradient starts. This online dilution design proved to be robust and easily transferable onto multiple systems in multiple locations. However, it requires the use of a second high-pressure pump (a quaternary pump in our case). To eliminate the second pump, it is possible to use a 6-port high-pressure valve and a T-piece to split the binary pump flow between the injector and the online dilution (2-mixer) system (Figure 5). This setup requires more precise timing and tubing consideration as compared to the two-pump option.



Components

A 2 µm in-line direct connect SS filter (Analytical Sales & Services, p/n 48812) threaded directly to the injector valve

B 25 µL high-pressure static mixer (Resolution Systems, p/n 402-0025HP)

C Valco SS mixing tee 1/16 inch 0.25 mm bore (Resolution Systems, PN ZT1C or Sigma-Aldrich, p/n 58626)

D Agilent 0.3 µm in-line filter (p/n 5067-4638)

E Heat exchanger (p/n G1316-80002)

F UHPLC (1,200 bar) guard column Agilent ZORBAX Eclipse Plus C18, 2.1 × 5 mm, 1.8 µm (p/n 821725-901)

G UHPLC (1,200 bar) column Agilent ZORBAX RRHD Eclipse Plus C18, 2.1 × 100 mm, 1.8 µm (p/n 959758-902)

Figure 3. Online dilution setup used in the LC/MS/MS method during (A) mixing of the injected sample with mobile phase A (initial 0.2 minutes), and (B) post-mixing when the binary pump gradient starts.

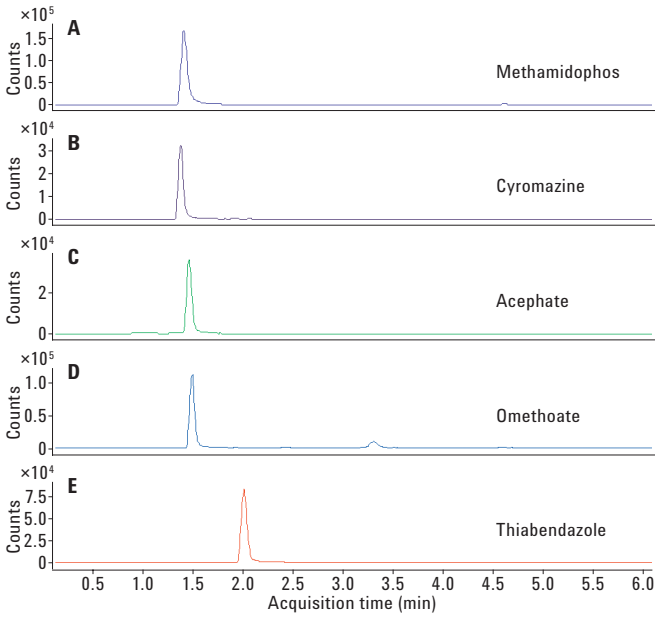
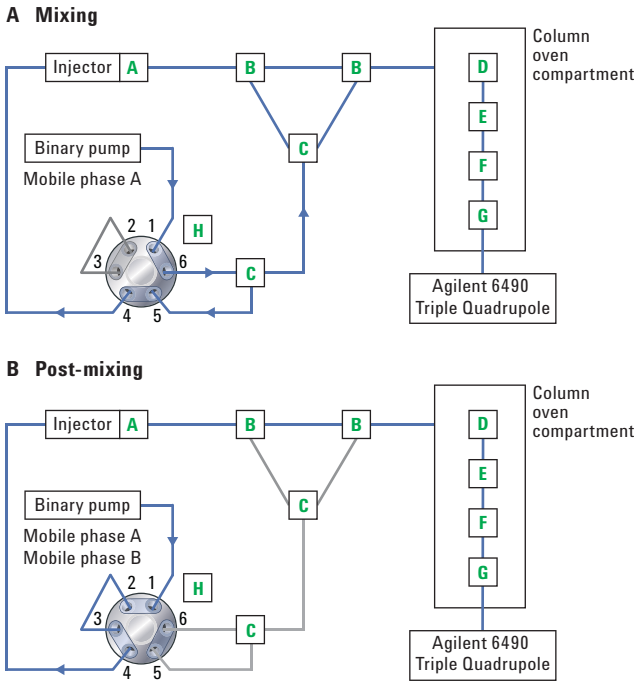


Figure 4. Peak shape of early eluting pesticides methamidophos, cyromazine, acephate, and omethoate injected in 3 µL of acetonitrile using the online dilution system depicted in Figure 2 (Note: thiabendazole was added to the picture to show the peak shape of this not as early eluting but often tailing analyte).



Components

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H 6-port, 2-position valve (1,200 bar)

Figure 5. Alternative on-line dilution setup without the use of the second high-pressure pump. Arrows indicate the mobile phase flow direction during (A) mixing of the injected sample with mobile phase when the binary pump flow is split between the injector and the 2-mixer system and (B) post-mixing when the binary pump gradient starts. Components: A–G the same as in Figure 2; H: 6-port, 2-position valve (1,200 bar).

Final LC/MS/MS method optimization

The final method optimization involved mainly selection of the method MRMs for each analyte and optimization of the tMRM conditions, LC gradient (analyte separation), MS source conditions, and injection volume.

The initial MRM optimization usually provided 10 MRMs per analytes. These MRMs were then ranked based on their sensitivity and also selectivity, which was evaluated in multiple challenging matrices. Two (in some cases three) top-ranked MRMs were included in the tMRM draft method as the primary MRMs (that is, to be collected throughout the entire analyte acquisition window). The draft method was then supplemented with triggered MRMs to create a total of four MRMs per compound in the majority of cases. The distribution of MRMs throughout the run was then evaluated using histograms. This approach permitted optimization of the final mobile phase gradient to spread the analytes and MRMs evenly throughout the run. Special attention was paid to the separation of critical pairs to make sure that those compounds could be resolved using MS/MS and/or chromatography. Using the optimized separation conditions, further triggered MRMs were added to some compounds for the final method. In some cases this meant as many as 6–7 total MRMs per analyte (see Table 1). Only two MRMs were used for internal standards. The total MRMs for individual analytes depended on several factors, including the actual number of viable transitions or amenability to the GC/MS/MS analysis (more MRMs were added for compounds amenable only to LC/MS/MS). Figure 6 shows the chromatographic separation and also histograms (obtained in the MassHunter acquisition software) illustrating the distribution of 968 primary MRMs and 2,070 total MRMs.

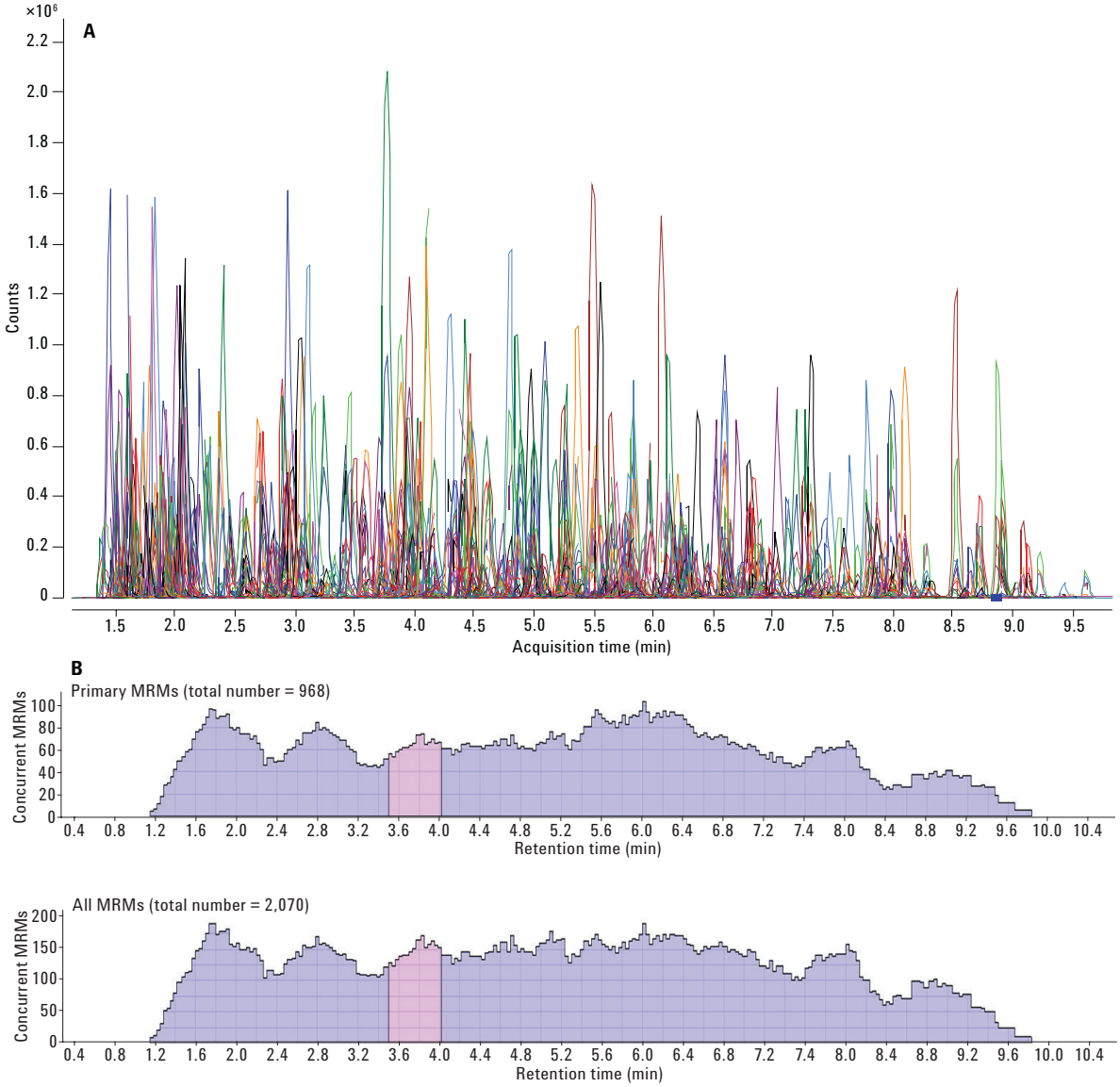

Figure 6. Extracted ion chromatograms of the analytes included in the method, and MRM histograms showing distribution of the analytes including their primary MRMs and all MRMs.

Using the final method MRMs, different cycle times were tested to evaluate repeatability of quantification (peak areas) at different settings. The cycle time parameter affects the number of data points across a peak and dictates minimum dwell time for the MRM acquisition. A cycle time of 650 ms was selected for the final method, providing a minimum primary MRM dwell time of 5.22 ms, and at least seven to eight data points above baseline for good analyte quantitation. This translated to good repeatability obtained in the method validation throughout the chromatographic run, as demonstrated in Figure 7.

Source conditions and injection volume were fine-tuned using the final method LC gradient and MRM program. We initially targeted 3 µL as the injection volume for undiluted QuEChERS extracts to replace a previously used 10 µL injection of three-fold diluted extracts analyzed on a different LC/MS/MS system. However, the sensitivity of the 6490 triple quadrupole LC/MS allowed us to use a lower injection volume of 2 µL, which has the benefit of a reduced matrix introduction into the system.

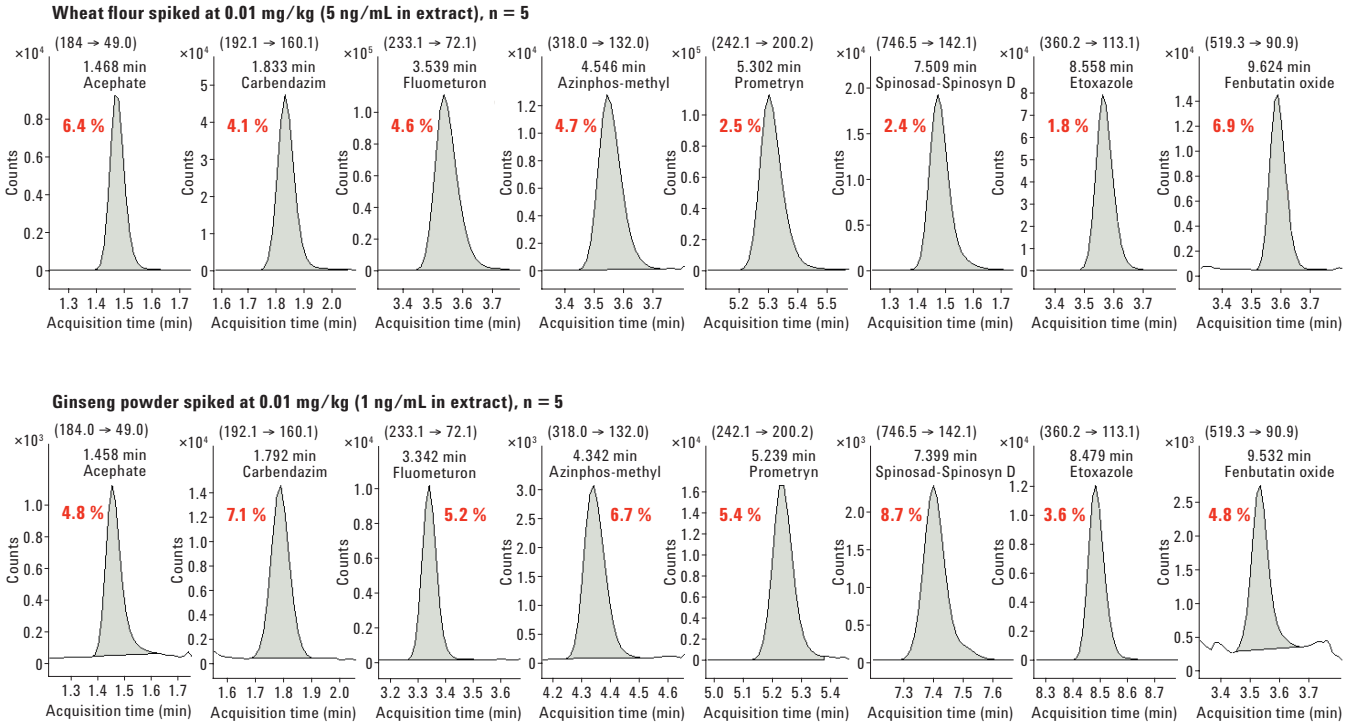

Figure 7. Chromatograms of quantitation MRMs and repeatability results (% RSD, five replicates) obtained during the method validation in wheat flour and ginseng powder for selected analytes from different pesticide classes eluting throughout the chromatographic run.

Interlaboratory method transfer and validation

The method development, especially the MRM optimization, was done in four different laboratories. The final method was assembled at one site, then transferred onto multiple identically configured 1290 Infinity II LC systems with 6490 triple quadrupole LC/MS instruments in three different pesticide routine testing laboratories in the US, Europe, and Asia, which then conducted the method validation. The method transfer mainly involved verification or an update of the analyte retention times using MassHunter software.

The method was validated in multiple commodity types/matrices using the SANTE method validation guidelines and criteria [1]. A method-validated limit of quantitation (LOQ) of 0.01 mg/kg was achieved for the majority analyte-matrix combinations. The evaluated matrices included representative matrices from the following SANTE commodity groups:

- High water content
- High water content, high acid content
- High sugar content, low water content
- High oil content, low water content
- High starch/protein, low water/fat
- Difficult/unique commodities
- Milk and milk products.

Examples of the validation results are provided in the supplemental information to this application note [7], which shows recoveries and RSDs of pesticides included in Agilent LC/MS mixes one to eight (p/n 5190-0551), obtained during the method validation in tomato, orange juice, spinach, and wheat flour.

Analyte identification using triggered MRM

The tMRM function provides additional information beyond the minimum identification criteria, providing increased identification confidence. It also serves as a useful tool for eliminating false positive results and effectively dealing with suspect results. Figure 8 gives an example of a suspect result for a pesticide, fenhexamid, in a highly complex botanical extract sample. The retention time in the sample matches the retention time of the analyte in the reference standard analyzed in the same sample batch. The qualifier transition *m/z* 302.1 → 97.1 is present in the sample at the same retention time, but the ion ratio is not within the tolerance. However, this is a highly complex sample where potential matrix interferences could affect the ion ratio. Therefore, having the additional MRM information is helpful for fast decision making and dismissing this as suspect because the additional tMRMs do not match, with one of them (*m/z* 302.1 → 143.1) actually missing.

The same botanical extract sample contained an herbicide, imazathepyr. Figure 9 shows that, in this case, there were five well matching MRMs, providing confidence in the identification of imazathepyr in this complex sample.

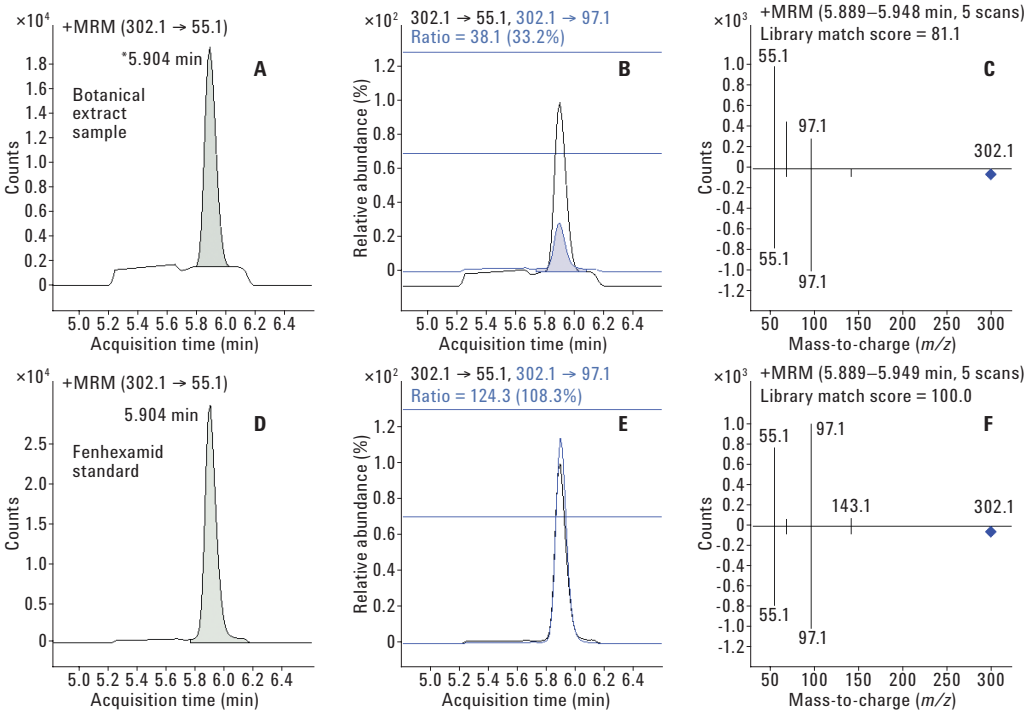

Figure 8. Example of a suspect result for fenhexamid in a botanical extract sample, comparing its quantitation MRM (A), overlay of quantitation and qualification MRMs (B), and tMRM library match (C) in the sample with those obtained for a fenhexamid reference standard analyzed in the same sample batch (D, E, and F, respectively). The suspect result was dismissed due to the missing m/z 302.1 → 143.1 transition, and two additional MRMs with an incorrect ion ratio in the sample.

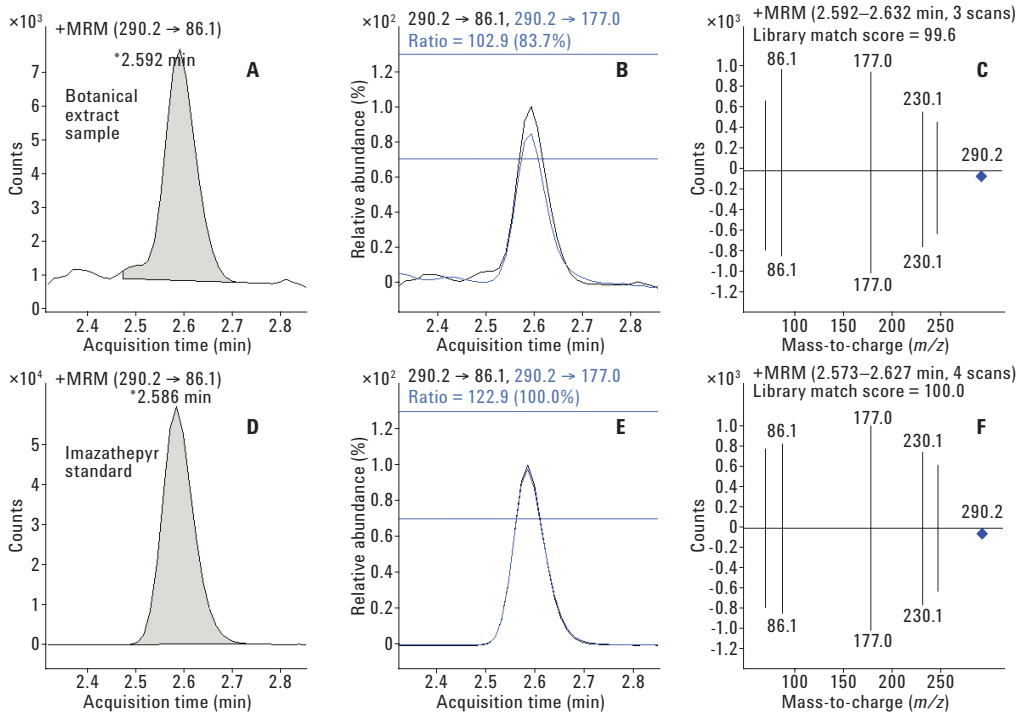

Figure 9. Example of positive identification of imazathepyr in a botanical extract sample, comparing its quantification MRM (A), overlay of quantitation and qualification MRMs (B), and tMRM library match (C) in the sample with those obtained for a imazathepyr reference standard analyzed in the same sample batch (D, E, and F, respectively). A high identification confidence was achieved due to five matching MRMs (two primary and three triggered).

Conclusions

This LC/MS/MS method provides fast and reliable analysis of about 450 globally important pesticides in various food commodities. It uses the tMRM function for increased identification confidence and effective dealing with suspect results. Robust online dilution setup provides excellent peak shapes and retention of early eluting (more polar) analytes, which are notorious troublemakers in other multiresidue pesticide LC/MS/MS methods. The method was successfully transferred and validated in three different laboratories using Agilent 1290 Infinity II LC systems coupled to Agilent 6490 triple quadrupole LC/MS instruments.

View the full validated results:

Validation Results for LC/MS/MS Pesticide Multiresidue Analysis using Triggered MRM and Online Dilution

Acknowledgements

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Table 1. List of Compounds Included in the Method Together with Their Chemical Abstract Service (CAS) Numbers, Retention Times (RT), Primary Transitions, Collision Energies (CE), and Total Number of Transitions in the tMRM Program. For Compounds Provided in Agilent LC/MS mixes 1–8 (p/n 5190-0551), the Respective Mix Number is Aso Listed

Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Abamectin - Avermectin B1a	71751-41-2	7	9.09	890.5 → 305.1 (28); 890.5 → 307.1 (16); 890.5 → 567.4 (12)	5
Acephate	30560-19-1	1	1.50	184.0 → 143.0 (4); 184.0 → 49.0 (20)	4
Acetamiprid	135410-20-7	5	1.96	223.1 → 125.9 (16); 223.1 → 89.9 (36)	4
Acetochlor	34256-82-1		5.89	270.1 → 59.2 (28); 270.1 → 148.2 (20); 270.1 → 224.2 (12)	4
Acibenzolar-S-methyl	135158-54-2		4.80	211.0 → 135.9 (32); 211.0 → 139.9 (24)	5
Aclonifen	74070-46-5		6.26	265.0 → 182.2 (28); 265.0 → 218.1 (24)	4
Acrinathrin	101007-06-1		8.91	559.2 → 208.0 (16); 559.2 → 181.0 (32); 559.2 → 82.8 (14)	4
Alachlor	15972-60-8		5.89	270.1 → 45.0 (32); 270.1 → 238.0 (12); 270.1 → 162.3 (20)	4
Alanycarb	83130-01-2	5	6.52	400.1 → 238.1 (8); 400.1 → 91.1 (56)	4
Aldicarb	116-06-3	5	2.42	208.1 → 116.0 (8); 208.1 → 89.0 (12)	5
Aldicarb sulfone (Aldoxycarb)	1646-88-4		1.57	240.1 → 76.2 (12); 240.1 → 148.2 (16)	4
Aldicarb sulfoxide	1646-87-3		1.54	207.1 → 89.0 (12); 207.1 → 65.0 (20)	4
Allethrin	584-79-2		8.04	303.2 → 135.0 (8); 303.2 → 107.0 (20)	4
Ametryn	834-12-8		4.46	228.1 → 186.2 (16); 228.1 → 68.0 (52)	5
Amidosulfuron	120923-37-7	4	3.24	370.1 → 218.1 (24); 370.1 → 69.1 (56)	5
Aminocarb	2032-59-9	4	1.60	209.1 → 137.0 (24); 209.1 → 122.0 (48)	4
Amitraz	33089-61-1		8.85	294.2 → 163.0 (12); 294.2 → 122.0 (32)	6
Amitraz metabolite DMF	60397-77-5		2.66	150.1 → 107.1 (20); 150.1 → 106.1 (40)	5
Amitraz metabolite DMPF	33089-74-6		1.72	163.1 → 122.1 (16); 163.1 → 106.1 (48)	4
Anilofos	64249-01-0		6.57	368.0 → 198.9 (12); 368.0 → 124.9 (44)	4
Atrazine	1912-24-9		3.91	216.1 → 174.0 (16); 216.1 → 68.1 (36)	5
Azaconazole	60207-31-0	1	4.21	300.0 → 159.1 (44); 300.0 → 231.1 (20)	5
Azamethiphos	35575-96-3	2	2.75	325.0 → 112.1 (40); 325.0 → 76.1 (60)	4
Azinphos-ethyl	2642-71-9	1	5.81	346.1 → 132.0 (16); 346.1 → 160.1 (4); 346.1 → 289.1 (4)	4
Azinphos-methyl	86-50-0	1	4.51	318.0 → 125.0 (24); 318.0 → 260.9 (4); 318.0 → 132.0 (16)	5
Azoxystrobin	131860-33-8	5	4.94	404.1 → 372.0 (12); 404.1 → 329.1 (36)	5
Beflubutamid	113614-08-7	8	6.41	356.1 → 91.1 (40); 356.1 → 65.1 (68)	4
Benalaxyl	71626-11-4	2	6.63	326.2 → 148.2 (24); 326.2 → 91.2 (52)	4
Bendiocarb	22781-23-3		2.90	224.1 → 109.0 (12); 224.1 → 167.0 (4)	4
Benfuracarb	82560-54-1	4	7.72	411.2 → 195.1 (36); 411.2 → 252.1 (12)	5
Benoxacor	98730-04-2		4.55	260.0 → 149.0 (16); 260.0 → 134.0 (36)	5
Bensulide	741-58-2		6.30	398.1 → 77.0 (60); 398.1 → 157.8 (24)	4
Bentazone	25057-89-0		2.42	241.1 → 198.9 (8); 241.1 → 80.0 (56)	4
Benzoximate	29104-30-1	7	6.95	364.1 → 199.0 (8); 364.1 → 105.1 (36)	5
Bifenazate	149877-41-8	8	5.63	301.2 → 198.1 (4); 301.2 → 170.1 (24)	4
Bifenthrin	82657-04-3	2	9.27	440.2 → 181.2 (20); 440.2 → 166.2 (52)	4
Bispyribac	125401-92-5	7	5.17	431.1 → 275.1 (12); 431.1 → 118.9 (48)	5
Bitertanol	55179-31-2	3	6.91	338.2 → 70.3 (4); 338.2 → 269.3 (4)	5
Bixafen	581809-46-3		6.31	414.0 → 265.9 (28); 414.0 → 394.1 (16)	4
Boscalid	188425-85-6	4	5.20	343.0 → 307.0 (20); 343.0 → 140.0 (20)	5
Bromacil	314-40-9		2.97	261.0 → 204.9 (12); 261.0 → 187.8 (32)	4
Bromuconazole I	116255-48-2	2	5.56	378.0 → 159.1 (44); 378.0 → 70.1 (20)	2
Bromuconazole II	116255-48-2	2	6.25	378.0 → 159.1 (40); 378.0 → 70.1 (24)	2
Bupirimate	41483-43-6	2	5.99	317.2 → 166.1 (18); 317.2 → 108.1 (28)	4
Buprofezin	69327-76-0	1	7.87	306.2 → 201.1 (12); 306.2 → 116.0 (12)	5

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Butachlor	23184-66-9		8.04	312.2 → 57.0 (24); 312.2 → 238.0 (8)	5
Butafenacil	134605-64-4		5.83	492.1 → 179.9 (52); 492.1 → 330.9 (24)	4
Butocarboxim	34681-10-2	4	2.37	213.1 → 75.1 (12); 213.1 → 47.1 (48)	3
Butocarboxim sulfoxide	34681-24-8		1.51	207.1 → 74.9 (12); 207.1 → 87.9 (8)	4
Butoxycarboxim (butocarboxim sulfone)	34681-23-7		1.57	240.1 → 106.0 (4); 240.1 → 44.1 (24)	4
Butylate	2008-41-5		7.56	218.2 → 57.1 (12); 218.2 → 156.1 (8); 218.2 → 100.1 (12)	4
Cadusafos	95465-99-9		7.14	271.1 → 97.0 (40); 271.1 → 158.9 (12)	5
Carbaryl	63-25-2	6	3.24	202.1 → 145.1 (4); 202.1 → 127.0 (28)	5
Carbendazim	10605-21-7	5	1.87	192.1 → 160.1 (16); 192.1 → 132.1 (36)	4
Carbetamide	16118-49-3		2.63	237.1 → 118.0 (12); 237.1 → 72.0 (36)	5
Carbofuran	1563-66-2	8	2.96	222.1 → 123.0 (20); 222.1 → 165.1 (8)	4
Carbofuran-3-hydroxy-	16655-82-6		1.94	238.1 → 163.2 (12); 238.1 → 181.0 (4)	4
Carbosulfan	55285-14-8	6	9.14	381.2 → 118.0 (20); 381.2 → 160.1 (12)	6
Carboxin	5234-68-4	5	3.23	236.1 → 143.1 (12); 236.1 → 87.1 (28)	5
Carfentrazone-ethyl	128639-02-1	4	6.39	412.1 → 346.1 (24); 412.1 → 366.1 (16)	4
Chlorantraniliprole	500008-45-7	8	4.59	484 → 452.9 (20); 484 → 286.1 (20)	5
Chlorbromuron	13360-45-7		5.03	293.0 → 181.9 (12); 293.0 → 203.8 (16)	5
Chlordimeform	6164-98-3		1.78	197.1 → 46.2 (20); 197.1 → 116.9 (28)	4
Chlorfenvinphos I	470-90-6	2	6.67	359.0 → 155.1 (12); 359.0 → 99.1 (36)	4
Chlorfenvinphos II	470-90-6	2	6.92	359.0 → 155.1 (12); 359.0 → 99.1 (36)	4
Chlorfluazuron	71422-67-8		8.76	540.0 → 382.9 (28); 540.0 → 158.0 (24)	6
Chloridazon (Pyrazon)	1698-60-8	4	2.05	222.0 → 104.1 (28); 222.0 → 92.1 (36)	4
Chlorimuron-ethyl (Classic)	90982-32-4		5.28	415.1 → 185.9 (24); 415.1 → 184.9 (28)	5
Chlorotoluron (Chlortoluron)	15545-48-9	7	3.69	213.1 → 72.0 (20); 213.1 → 46.1 (16)	5
Chloroxuron	1982-47-4	7	5.59	291.1 → 72.0 (20); 291.1 → 46.1 (20)	4
Chlorpyrifos	2921-88-2	2	8.21	349.9 → 97.0 (40); 349.9 → 197.8 (28)	5
Chlorpyrifos-methyl	5598-13-0	2	7.07	321.9 → 47.1 (48); 321.9 → 125.0 (20)	2
Chlorsulfuron	64902-72-3	4	3.16	358.0 → 141.1 (24); 358.0 → 167.1 (20)	4
Clethodim I	99129-21-2	3	5.48	360.1 → 164.1 (16); 360.1 → 240.1 (12)	4
Clethodim II	99129-21-2	3	7.51	360.1 → 164.1 (16); 360.1 → 166.1 (32)	5
Clodinafop-propargyl	105512-06-9		6.35	350.1 → 265.9 (12); 350.1 → 90.9 (36)	4
Clofentezine	74115-24-5	4	6.82	303.0 → 138.1 (12); 303.0 → 102.1 (44)	5
Clomazone	81777-89-1	8	4.59	240.1 → 125.1 (32); 240.1 → 89.1 (68)	5
Cloquintocet-mexyl	99607-70-2		8.01	336.1 → 237.9 (16); 336.1 → 178.9 (36)	5
Clothianidin	210880-92-5		1.86	250.0 → 132.1 (16); 250.0 → 169.2 (12)	4
Coumaphos	56-72-4	2	6.64	363.0 → 227.1 (28); 363.0 → 307.1 (16)	4
Cyanazine	21725-46-2		2.64	241.1 → 214.2 (16); 241.1 → 103.9 (28)	5
Cyanofenphos	13067-93-1		6.48	304.1 → 156.9 (20); 304.1 → 119.9 (20); 304.1 → 62.9 (44)	3
Cyazofamid	120116-88-3	4	5.96	325.1 → 108.1 (20); 325.1 → 44.1 (36)	4
Cycloate	1134-23-2	1	7.13	216.1 → 83.1 (12); 216.1 → 55.1 (36)	5
Cycloxydim	101205-02-1		7.46	326.2 → 180.0 (24); 326.2 → 100.9 (24)	5
Cycluron	2163-69-1	7	4.24	199.2 → 89.1 (12); 199.2 → 69.1 (20)	5
Cyflufenamid	180409-60-3		6.92	413.1 → 222.9 (20); 413.1 → 202.9 (40)	5
Cyhexatin	91465-08-6		9.02	365.0 → 201.0 (16); 365.0 → 81.2 (28)	4

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Cymiazole	61676-87-7	1	1.99	219.1 → 171.2 (28); 219.1 → 100.0 (30)	4
Cymoxanil	57966-95-7	4	2.14	199.1 → 128.1 (8); 199.1 → 111.1 (16)	4
Cyproconazole I	94361-06-5	1	5.65	292.1 → 70.1 (48); 292.1 → 125.1 (40)	3
Cyproconazole II	94361-06-5	1	6.07	292.1 → 70.1 (48); 292.1 → 125.1 (40)	3
Cyprodinil	121552-61-2	8	6.17	226.1 → 93.0 (36); 226.1 → 77.1 (56)	4
Cyromazine	66215-27-8		1.41	167.1 → 85.0 (16); 167.1 → 68.0 (40)	4
DEET (Diethyltoluamide)	134-62-3	4	4.03	192.1 → 119.1 (20); 192.1 → 91.1 (40)	5
Demeton-S (disulfoton oxon)	126-75-0		4.67	259.1 → 89.0 (4); 259.1 → 61.0 (44)	2
Demeton-S-methyl	919-86-8		3.05	231.0 → 89.0 (8); 231.0 → 61.0 (40)	2
Demeton-S-methyl sulfone	17040-19-6		1.66	263.0 → 109.1 (32); 263.0 → 169.0 (12)	4
Desmedipham	13684-56-5	8	4.42	318.1 → 182.1 (16); 318.1 → 136.1 (36)	5
Dialifos (Dialifor)	10311-84-9		7.06	394.0 → 207.9 (20); 394.0 → 186.9 (8)	5
Diazinon	333-41-5	2	6.65	305.1 → 97.1 (36); 305.1 → 169.1 (20)	4
Diazinon oxon	962-58-3		4.56	289.1 → 135.1 (28); 289.1 → 233.0 (20)	5
Dichlofluanid	1085-98-9		5.73	333.0 → 123.0 (32); 333.0 → 224.0 (16); 350.0 → 123.0 (32)	5
Dichlorvos	62-73-7	2	2.85	221.0 → 109.1 (16); 221.0 → 79.1 (28)	4
Diclobutrazol	75736-33-3		6.36	328.1 → 69.9 (36); 328.1 → 158.9 (40)	4
Diclocymet I	139920-32-4		5.92	313.1 → 172.9 (16); 313.1 → 101.9 (52)	4
Diclocymet II	139920-32-4		6.15	313.1 → 172.9 (16); 313.1 → 101.9 (52)	4
Dicrotophos	141-66-2		1.75	238.1 → 112.2 (12); 238.1 → 72.0 (32)	4
Diethofencarb	87130-20-9	6	4.89	268.2 → 124.0 (32); 268.2 → 226.1 (4)	5
Difenoconazole	119446-68-3	3	7.13	406.1 → 251.1 (24); 406.1 → 188.1 (48)	5
Diflubenzuron	35367-38-5	4	6.08	311.0 → 158.1 (24); 311.0 → 141.1 (56)	4
Diflufenican	83164-33-4	1	7.31	395.1 → 266.0 (28); 395.1 → 246.0 (40)	5
Dimethachlor	50563-36-5	1	4.38	256.1 → 224.1 (24); 256.1 → 148.1 (36)	5
Dimethametryn	22936-75-0		6.09	256.2 → 95.9 (28); 256.2 → 90.9 (32)	4
Dimethenamid	87674-68-8		5.03	276.1 → 244.0 (16); 276.1 → 168.1 (28)	5
Dimethoate	60-51-5	8	2.00	230.0 → 125.0 (24); 230.0 → 47.0 (56)	4
Dimethomorph I	110488-70-5	5	5.06	388.1 → 301.1 (24); 388.1 → 165.1 (36)	5
Dimethomorph II	110488-70-5	5	5.37	388.1 → 301.1 (24); 388.1 → 165.1 (36)	5
Dimetilan	644-64-4		2.03	241.1 → 71.9 (24); 241.1 → 196.0 (8)	3
Dimoxystrobin	149961-52-4	1	6.32	327.2 → 205.1 (12); 327.2 → 116.1 (40)	4
Diniconazole	83657-24-3	2	7.01	326.1 → 70.0 (36); 328.1 → 70.1 (36)	4
Dinitramine	29091-05-2		6.78	323.1 → 289.3 (16); 323.1 → 194.9 (44)	4
Dinotefuran	165252-70-0	7	1.55	203.1 → 129.1 (12); 203.1 → 114.0 (12)	4
Dioxacarb	6988-21-2	7	1.99	224.1 → 123.1 (20); 224.1 → 167.1 (12)	4
Diphenamid	957-51-7		4.38	240.1 → 134.0 (28); 240.1 → 91.0 (48)	5
Dipropetryn	4147-51-7		6.12	256.2 → 213.9 (20); 256.2 → 101.9 (48)	4
Disulfoton	298-04-4	1	7.00	275.1 → 89.0 (8); 275.1 → 61.0 (40)	2
Disulfoton sulfone	2497-06-5		3.81	307.0 → 96.9 (36); 307.0 → 125.1 (20)	5
Disulfoton sulfoxide	2497-07-6		3.67	291.0 → 185.0 (12); 291.0 → 96.8 (44)	5
Diuron	330-54-1	5	4.11	233.0 → 72.0 (20); 233.0 → 46.0 (16); 235.0 → 72.1 (20)	4
DMSA (Dimethylphenylsulfamide)	4710-17-2		2.41	201.1 → 92.0 (16); 201.1 → 65.0 (36)	4
DMST (Dimethylaminosulfotoluidide)	66840-71-9		3.08	215.1 → 77.0 (52); 215.1 → 51.1 (60)	3

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Dodemorph I	1593-77-7		4.40	282.3 → 116.0 (16); 282.3 → 98.0 (24)	5
Dodemorph II	1593-77-7		4.60	282.3 → 116.0 (16); 282.3 → 98.0 (24)	5
Dodine	2439-10-3		6.77	228.3 → 59.9 (24); 228.3 → 56.9 (24)	5
Doramectin	117704-25-3		9.27	916.5 → 331.2 (24); 916.5 → 113.1 (52)	4
Emamectin B1a benzoate	117704-25-3		8.20	886.5 → 157.9 (44); 886.5 → 81.9 (72)	5
Emamectin B1b benzoate	117704-25-3		7.87	872.5 → 157.9 (40); 872.5 → 81.9 (56)	4
Epoxiconazole	133855-98-8	2	5.96	330.1 → 121.1 (24); 330.1 → 101.1 (48)	4
Eprinomectin B1a	123997-26-2		9.00	914.5 → 186.1 (24); 914.5 → 153.9 (44)	5
Ethaboxam	162650-77-3		3.71	321 → 183.1 (24); 321 → 200.1 (28)	5
Ethidimuron (Sulfadiazole)	30043-49-3	8	1.85	265.1 → 208.0 (12); 265.1 → 113.9 (20)	4
Ethiofencarb	29973-13-5		3.48	226.1 → 107.2 (12); 226.1 → 77.1 (56)	6
Ethiofencarb sulfone	53380-23-7		1.80	275.1 → 106.9 (20); 275.1 → 200.9 (8)	4
Ethiofencarb sulfoxide	53380-22-6		1.82	242.1 → 106.9 (16); 242.1 → 163.9 (8)	4
Ethion	563-12-2	2	8.10	385.0 → 199.1 (12); 385.0 → 97.1 (52)	5
Ethiprole	181587-01-9		5.08	397.0 → 351.1 (20); 397.0 → 255.1 (44)	5
Ethirimol	23947-60-6	4	2.80	210.2 → 98.1 (32); 210.2 → 140.1 (28)	4
Ethofumesate	26225-79-6	4	4.88	287.1 → 121.1 (16); 287.1 → 161.1 (20)	5
Ethoprophos (Ethoprop)	13194-48-4	2	5.88	243.1 → 97.1 (32); 243.1 → 131.1 (20)	4
Ethoxyquin	91-53-2	8	4.96	218.2 → 160.2 (36); 218.2 → 174.0 (32)	5
Etofenprox	80844-07-1	3	9.23	394.2 → 177.1 (16); 394.2 → 107.0 (44)	6
Etoxazole	153233-91-1		8.54	360.2 → 141.0 (32); 360.2 → 113.1 (60)	6
Famoxadone	131807-57-3	4	6.70	392.1 → 331.0 (8); 392.1 → 93.0 (44)	5
Fenamidone	161326-34-7	5	5.06	312.1 → 92.1 (24); 312.1 → 236.2 (8)	5
Fenamiphos	22224-92-6	1	6.18	304.1 → 217.0 (24); 304.1 → 202.0 (40)	4
Fenamiphos sulfone	31972-44-8		3.13	336.1 → 308.1 (12); 336.1 → 265.8 (12)	4
Fenamiphos sulfoxide	31972-43-7		2.97	320.1 → 108.0 (48); 320.1 → 171.0 (24)	4
Fenarimol	60168-88-9	2	5.79	331.0 → 81.1 (28); 331.0 → 139.1 (36)	4
Fenazaquin	120928-09-8	5	8.90	307.2 → 57.1 (28); 307.2 → 161.1 (14)	6
Fenbuconazole	114369-43-6	2	6.08	337.1 → 125.1 (40); 337.1 → 70.1 (28)	4
Fenbutatin oxide	13356-08-6		9.62	519.3 → 90.9 (76); 519.3 → 196.9 (56); 517.3 → 90.9 (72); 517.3 → 194.9 (56)	6
Fenchlorphos oxon	3983-45-7		5.75	304.9 → 109.1 (20); 306.9 → 109.0 (20)	4
Fenhexamid	126833-17-8	3	5.79	302.1 → 97.1 (28); 302.1 → 55.1 (48)	4
Fenobucarb	3766-81-2	5	4.77	208.1 → 95.1 (12); 208.1 → 77.1 (48)	5
Fenoxanil I	115852-48-7		6.22	329.1 → 86.0 (24); 329.1 → 189.0 (24)	4
Fenoxanil II	115852-48-7		6.22	329.1 → 86.0 (24); 329.1 → 189.0 (24)	4
Fenoxycarb	72490-01-8	6	6.21	302.1 → 88.0 (20); 302.1 → 116.2 (8)	4
Fenpropathrin	39515-41-8		8.65	350.2 → 125.1 (12); 350.2 → 55.1 (44)	2
Fenpropidin	67306-00-7	5	4.49	274.3 → 147.1 (28); 274.3 → 86.1 (28)	5
Fenpropimorph	67564-91-4		4.99	304.3 → 147.2 (32); 304.3 → 117.1 (64)	5
Fenpyroximate	111812-58-9	5	8.72	422.2 → 366.1 (16); 422.2 → 135.1 (36)	6
Fensulfothion	115-90-2		4.07	309.0 → 157.0 (28); 309.0 → 173.0 (24)	5
Fensulfothion oxon	6552-21-2		2.23	293.1 → 94.0 (52); 293.1 → 140.0 (44)	5
Fensulfothion oxon sulfone	6132-17-8		2.32	309.1 → 253.0 (16); 309.1 → 175.0 (28)	5
Fensulfothion sulfone	14255-72-2		4.27	325.0 → 268.9 (12); 325.0 → 191.0 (24)	5

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Fenthion	55-38-9		6.47	279.0 → 169.0 (16); 279.0 → 105.2 (24)	4
Fenthion oxon	6552-12-1		4.52	263.1 → 231.2 (16); 263.1 → 216.0 (24)	5
Fenthion oxon sulfone	14086-35-2		1.97	295.0 → 217.1 (16); 295.0 → 104.2 (24)	4
Fenthion oxon sulfoxide	6552-13-2		1.91	279.1 → 104.1 (32); 279.1 → 264.2 (16)	4
Fenthion sulfone	3761-42-0		3.34	311.0 → 125.0 (24); 311.0 → 109.1 (32)	5
Fenthion sulfoxide	3761-41-9		3.10	295.0 → 109.1 (36); 295.0 → 280.1 (16)	4
Fentin	76-87-9		4.31	351.0 → 197.0 (32); 351.0 → 120.0 (60); 349.0 → 195.0 (32)	4
Fentrazamide	158237-07-1		6.58	350.1 → 83.0 (24); 350.1 → 154.1 (12)	4
Fenuron	101-42-8	7	2.01	165.1 → 72.0 (24); 165.1 → 46.1 (8)	4
Fipronil	120068-37-3	4	6.20	454.0 → 368.1 (26); 454.0 → 255.0 (44)	4
Flazasulfuron	104040-78-0	4	4.50	408.1 → 182.1 (24); 408.1 → 83.1 (60)	5
Flonicamid	158062-67-0	6	1.69	230.1 → 203.1 (16); 230.1 → 174.1 (16)	4
Fluazifop-butyl	69806-50-4		7.80	384.1 → 282.2 (20); 384.1 → 328.2 (16)	5
Flubendiamide	272451-65-7	7	6.47	683.0 → 408.0 (8); 683.0 → 273.9 (40)	3
Flucarbazone-sodium	181274-17-9		2.04	414.0 → 129.9 (24); 414.0 → 114.9 (56)	4
Fludioxonil	131341-86-1	2	5.06	266.1 → 229.1 (8); 266.1 → 158.1 (36)	5
Flufenacet	142459-58-3	1	5.85	364.1 → 152.0 (20); 364.1 → 194.1 (8)	4
Flufenoxuron	101463-69-8	4	8.53	489.1 → 158.1 (16); 489.1 → 141.1 (56)	4
Flumethrin	69770-45-2		9.15	527.1 → 267.0 (12); 527.1 → 238.9 (24); 527.1 → 202.9 (36)	5
Flumetsulam	98967-40-9	8	1.84	326.1 → 129.1 (36); 326.1 → 109.1 (68)	4
Flumioxazin	103361-09-7	6	4.61	355.1 → 299.1 (32); 355.1 → 107.0 (36)	5
Fluometuron	2164-17-2	8	3.55	233.1 → 72.1 (24); 233.1 → 46.1 (16)	4
Fluopicolide	239110-15-7	1	5.34	383.0 → 173.1 (36); 383.0 → 109.1 (68)	5
Fluopyram	658066-35-4		5.70	397.1 → 207.9 (24); 397.1 → 144.9 (60)	4
Fluoxastrobin	361377-29-9	8	5.82	459.1 → 427.1 (16); 459.1 → 188.1 (44)	4
Fluquinconazole	136426-54-5	2	5.71	376.0 → 108.1 (52); 376.0 → 307.1 (28)	4
Fluridone	59756-60-4		4.69	330.1 → 309.0 (40); 330.1 → 310.0 (32)	5
Flusilazole	85509-19-9	2	6.18	316.1 → 165.1 (28); 316.1 → 247.1 (16)	4
Flutolanil	66332-96-5		5.31	324.1 → 242.0 (28); 324.1 → 262.0 (20)	5
Flutriafol	76674-21-0	8	3.90	302.1 → 70.1 (12); 302.1 → 123.1 (32)	5
Foramsulfuron	173159-57-4	3	3.34	453.1 → 182.2 (28); 453.1 → 83.1 (68)	4
Forchlorfenuron	68157-60-8	7	4.16	248.1 → 129.0 (16); 248.1 → 93.1 (40)	5
Formetanate hydrochloride	23422-53-9		1.47	222.1 → 165.1 (12); 222.1 → 46.2 (28)	4
Formothion	2540-82-1		2.52	258.0 → 124.9 (24); 258.0 → 198.9 (8)	6
Fosthiazate	98886-44-3	1	3.58	284.1 → 104.1 (24); 284.1 → 228.1 (8)	5
Fuberidazole	3878-19-1	4	2.15	185.1 → 156.0 (28); 185.1 → 65.0 (48)	5
Furalaxyl	57646-30-7	7	4.88	302.1 → 95.1 (40); 302.1 → 242.1 (12)	4
Furathiocarb	65907-30-4	6	7.82	383.2 → 195.0 (24); 383.2 → 252.0 (8)	5
Griseofulvin	126-07-8		3.89	353.1 → 164.9 (16); 353.1 → 214.9 (24)	5
Halofenozide	112226-61-6	8	5.04	331.1 → 104.9 (16); 331.1 → 138.9 (20)	5
Halosulfuron-methyl	100784-20-1	8	5.45	435.1 → 182.1 (24); 435.1 → 83.1 (56)	4
Haloxyfop	69806-34-4		6.16	362.0 → 287.9 (32); 362.0 → 90.9 (28)	4
Haloxyfop-methyl	69806-40-2		7.22	376.1 → 316.0 (16); 376.1 → 90.9 (40)	5
Hexaconazole	79983-71-4	2	6.73	314.1 → 70.1 (24); 314.1 → 159.1 (40)	5
Hexaflumuron	86479-06-3	7	7.40	461.0 → 158.1 (20); 461.0 → 141.1 (48)	4

Table 1. List of Compounds Included in the Method Together with Their Chemical Abstract Service (CAS) Numbers, Retention Times (RT), Primary Transitions, Collision Energies (CE), and Total Number of Transitions in the tMRM Program (continued). For Compounds Provided in Agilent LC/MS mixes 1–8 (p/n 5190-0551), the Respective Mix Number is Aso Listed

Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Hexazinone	51235-04-2		3.00	253.2 → 171.1 (12); 253.2 → 71.0 (36)	4
Hexythiazox	78587-05-0	4	8.29	353.1 → 228.0 (16); 353.1 → 168.0 (28)	6
Hydramethylnon	67485-29-4	7	7.33	495.2 → 323.2 (32); 495.2 → 151.1 (56)	5
Hydroprene-S-	65733-18-8		9.58	267.2 → 94.9 (24); 267.2 → 55.1 (40)	4
Imazalil	35554-44-0	2	3.78	297.1 → 159.1 (24); 297.1 → 201.1 (16)	5
Imazamethabenz-methyl	81405-85-8		3.02	289.2 → 143.9 (40); 289.2 → 85.9 (24)	4
Imazethapyr	81335-77-5		2.55	290.2 → 177.0 (28); 290.2 → 86.1 (28)	5
Imidacloprid	138261-41-3	5	1.82	256.1 → 209.0 (16); 256.1 → 175.0 (28)	4
Indoxacarb	144171-61-9	3	7.33	528.1 → 203.1 (36); 528.1 → 150.1 (32)	5
Ipconazole	125225-28-7	2	7.41	334.2 → 70.1 (24); 334.2 → 125.1 (60)	4
Iprodione	36734-19-7		6.10	330.0 → 244.9 (16); 332.0 → 246.9 (16)	2
Iprovalicarb	140923-17-7	5	5.73	321.2 → 119.0 (20); 321.2 → 91.0 (60)	4
Isocarbamid	30979-48-7		2.20	186.1 → 86.9 (16); 186.1 → 129.9 (12)	4
Isofenphos	25311-71-1		6.97	346.1 → 216.9 (24); 346.1 → 245.0 (8)	5
Isofenphos-methyl	99675-03-3	1	6.43	332.1 → 231.1 (16); 332.1 → 120.9 (44)	4
Isoprocarb	2631-40-5		3.87	194.1 → 95.1 (12); 194.1 → 137.0 (4)	5
Isoprothiolane	50512-35-1	1	5.33	291.1 → 85.1 (60); 291.1 → 231.1 (12); 291.1 → 145.1 (40)	5
Isoproturon	34123-59-6		4.05	207.1 → 72.1 (24); 207.1 → 46.1 (24)	5
Isoxaben	82558-50-7	4	5.33	333.2 → 165.0 (20); 333.2 → 107.1 (60)	5
Isoxadifen-ethyl	163520-33-0		6.32	296.1 → 203.9 (24); 296.1 → 231.9 (12)	4
Isoxaflutole	141112-29-0	3	4.11	360.1 → 250.9 (12); 360.1 → 220.1 (44)	5
Isoxathion	18854-01-8		6.82	314.1 → 104.9 (36); 314.1 → 96.9 (56)	5
ISTD/QC - Atrazine-d5	163165-75-1		3.87	221.1 → 101.1 (20); 221.1 → 179.0 (20)	2
ISTD/QC - BDMC	672-99-1		5.18	258.0 → 122.1 (28); 258.0 → 201.0 (8)	2
ISTD/QC - Chlorpyrifos-d10	285138-81-0		8.15	360.0 → 99.1 (32); 360.0 → 199.1 (16)	2
ISTD/QC - Fentin-d15	358731-94-9		4.18	366.0 → 202.0 (32); 366.0 → 119.9 (60)	2
ISTD/QC - Imidacloprid-d4	1015855-75-0		1.82	260.1 → 213.0 (16); 260.1 → 179.1 (24)	2
ISTD/QC - Simazine-d10	220621-39-6		2.90	212.1 → 105.0 (32); 212.1 → 76.2 (28)	2
ISTD/QC - Triphenyl phosphate (TPP)	115-86-6		6.73	327.1 → 215.0 (44); 327.1 → 152.1 (44)	2
Ivermectin B1a	70288-86-7	7	9.46	892.5 → 307.2 (24); 892.5 → 569.3 (12)	4
Kresoxim-methyl	143390-89-0	4	6.38	314.1 → 223.0 (15); 314.1 → 116.0 (32)	4
Lactofen	77501-63-4		7.92	479.1 → 343.9 (28); 479.1 → 222.9 (52)	5
Lenacil	2164-08-1	1	4.03	235.1 → 153.1 (20); 235.1 → 136.1 (36)	5
Linuron	330-55-2	4	4.81	249.0 → 160.0 (20); 249.0 → 182.1 (12)	5
Lufenuron	103055-07-8	4	8.15	511.0 → 158.1 (20); 511.0 → 141.1 (44)	4
Malaoxon	1634-78-2	3	2.99	315.1 → 99.1 (36); 315.1 → 127.2 (12)	4
Malathion	121-75-5	3	5.33	331.1 → 127.1 (8); 331.1 → 125.1 (36)	5
Mandipropamid	374726-62-2	4	5.28	412.1 → 328.1 (16); 412.1 → 125.1 (44)	5
Mecarbam	2595-54-2	3	5.84	330.1 → 97.0 (40); 330.1 → 227.0 (8); 330.1 → 199.0 (12)	4
Mepanipyrim	110235-47-7	3	5.65	224.1 → 106.0 (24); 224.1 → 104.1 (32)	4
Mepanipyrim-2-hydroxypropyl	204571-52-8		4.03	244.2 → 200.1 (16); 244.2 → 226.0 (20)	5
Mephosfolan	950-10-7		2.79	270.0 → 139.9 (24); 270.0 → 195.9 (12)	5
Mesosulfuron-methyl	208465-21-8	6	3.87	504.1 → 182.1 (28); 504.1 → 83.1 (68)	5
Metaflumizone	139968-49-3	4	7.99	507.1 → 178.0 (36); 507.1 → 116.0 (52)	5

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Metalaxyl	139968-49-3	3	4.12	280.2 → 220.1 (12); 280.2 → 160.2 (24)	5
Metamitron	41394-05-2	4	2.03	203.1 → 104.1 (24); 203.1 → 77.1 (24)	4
Metazachlor	67129-08-2	3	3.99	278.1 → 134.1 (28); 278.1 → 210.1 (8)	5
Metconazole	125116-23-6	2	6.81	320.1 → 70.1 (36); 320.1 → 125.1 (48)	4
Methabenzthiazuron	18691-97-9	5	3.86	222.1 → 165 (16); 222.1 → 150 (36)	5
Methamidophos	10265-92-6	1	1.45	142.0 → 47.1 (28); 142.0 → 94.0 (12); 142.0 → 125.1 (10)	4
Methidathion	950-37-8	3	4.34	303.0 → 85.1 (24); 303.0 → 145.1 (8)	3
Methiocarb	2032-65-7	7	4.97	226.1 → 121.0 (16); 226.1 → 169.2 (6)	5
Methiocarb sulfone	2179-25-1		1.98	275.1 → 122.2 (28); 275.1 → 201.2 (12)	4
Methiocarb sulfoxide	2635-10-1		1.85	242.1 → 122.2 (32); 242.1 → 170.1 (24)	4
Methomyl	16752-77-5	5	1.68	163.1 → 88.0 (8); 163.1 → 58.2 (20)	4
Methoprotryne	841-06-5	7	4.56	272.2 → 198.0 (24); 272.2 → 170.0 (28)	5
Methoxyfenozide	161050-58-4	5	5.47	369.2 → 149.1 (16); 369.2 → 91.1 (60)	4
Metobromuron	3060-89-7	8	3.75	259.0 → 169.9 (20); 259.0 → 91.1 (56)	5
Metolachlor	51218-45-2	3	6.01	284.1 → 176.2 (24); 284.1 → 134.1 (32)	4
Metolcarb	1129-41-5		2.62	166.1 → 109.1 (8); 166.1 → 94.0 (36); 166.1 → 91.1 (24)	5
Metosulam	139528-85-1		3.07	418.0 → 174.9 (24); 418.0 → 139.9 (60)	4
Metoxuron	19937-59-8		2.42	229.1 → 71.9 (20); 229.1 → 46.2 (20)	4
Metrafenone	220899-03-6	4	7.01	409.1 → 209.1 (28); 409.1 → 227.0 (24)	5
Metribuzin	21087-64-9	4	2.99	215.1 → 49.1 (28); 215.1 → 84.1 (20)	4
Metsulfuron-methyl	74223-64-6	4	2.84	382.1 → 167.0 (16); 382.1 → 56.0 (48)	4
Mevinphos I	7786-34-7	3	1.94	225.0 → 127.1 (20); 225.0 → 193.1 (8)	4
Mevinphos II	7786-34-7	3	2.18	225.0 → 127.1 (16); 225.0 → 193.1 (8)	4
Mexacarbate	315-18-4	7	3.20	223.1 → 136.1 (44); 223.1 → 151.1 (28)	5
MGK 264 I	113-48-4		7.17	276.2 → 210.0 (12); 276.2 → 97.9 (24)	3
MGK 264 II	113-48-4		7.61	276.2 → 210.0 (12); 276.2 → 97.9 (24)	3
Molinate	2212-67-1	3	5.39	188.1 → 126.1 (8); 188.1 → 55.1 (28)	2
Monocrotophos	6923-22-4	4	1.70	224.1 → 127.1 (16); 224.1 → 98.1 (12)	4
Monolinuron	1746-81-2		3.42	215.1 → 125.9 (16); 215.1 → 98.9 (44)	6
Moxidectin	113507-06-5	7	9.27	640.4 → 528.0 (4); 640.4 → 199.1 (28); 640.4 → 81.1 (60); 640.4 → 98.1 (60); 640.4 → 478.1 (8)	5
Myclobutanil	88671-89-0	1	5.48	289.1 → 70.2 (24); 289.1 → 125.1 (40)	4
Naled (Dibrom)	300-76-5		4.28	380.8 → 126.9 (12); 382.8 → 127.0 (12); 380.8 → 108.9 (44)	5
Napropamide	15299-99-7		5.89	272.2 → 129.0 (16); 272.2 → 171.1 (20)	4
Naptalam	132-66-1		2.93	292.1 → 148.9 (40); 292.1 → 255.9 (40); 292.1 → 64.9 (60)	4
Neburon	555-37-3		6.28	275.1 → 88.0 (12); 275.1 → 57.1 (20)	4
Nicosulfuron	111991-09-4	4	2.79	411.1 → 182.1 (28); 411.1 → 106.1 (44)	5
Nitenpyram	150824-47-8	7	1.61	271.1 → 225.1 (8); 271.1 → 126.1 (36)	4
Norflurazon	27314-13-2		4.27	304.1 → 284.0 (24); 304.1 → 88.1 (52)	5
Norflurazon-desmethyl	23576-24-1		3.67	290.0 → 269.9 (28); 290.0 → 145.0 (48)	5
Novaluron	116714-46-6	4	7.55	493.0 → 158.0 (20); 493.0 → 141.0 (52)	4
Nuarimol	63284-71-9		4.93	315.1 → 251.9 (20); 315.1 → 138.9 (44)	5
Ofurace	58810-48-3		2.97	282.1 → 160.0 (36); 282.1 → 148.0 (40)	4
Omethoate	1113-02-6	6	1.52	214.0 → 125.0 (24); 214.0 → 183.0 (8)	4
Oxadiazon	19666-30-9	3	8.01	345.1 → 220.1 (20); 345.1 → 185.1 (28)	5

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Oxadixyl	77732-09-3	3	2.51	279.1 → 219.1 (8); 279.1 → 132.1 (32)	6
Oxamyl	23135-22-0	5	1.59	237.1 → 72.1 (12); 237.1 → 90.1 (12)	4
Oxamyl oxime	30558-43-1		1.54	163.1 → 72.1 (16); 163.1 → 47.1 (28)	4
Oxasulfuron	144651-06-9	4	2.66	407.1 → 150.1 (20); 407.1 → 107.0 (56)	4
Oxycarboxin	5259-88-1		2.13	268.1 → 174.9 (24); 268.1 → 146.9 (32)	4
Oxydemeton-methyl	301-12-2		1.63	247.0 → 169.0 (12); 247.0 → 125.0 (22)	4
Paclobutrazol	76738-62-0	3	5.27	294.1 → 70.1 (16); 294.1 → 125.1 (48)	4
Paraoxon	311-45-5		3.80	276.1 → 94.0 (40); 276.1 → 220.0 (16)	5
Paraoxon-methyl	950-35-6		2.47	248.0 → 202.1 (16); 248.0 → 90.1 (28)	5
Penconazole	66246-88-6	3	6.40	284.1 → 70.1 (24); 284.1 → 123.1 (52)	4
Pencycuron	66063-05-6	6	7.05	329.1 → 125.2 (24); 329.1 → 89.1 (64)	5
Pendimethalin	40487-42-1	3	8.27	282.1 → 212.0 (8); 282.1 → 194.0 (16)	3
Penoxsulam	219714-96-2		3.38	484.1 → 194.9 (36); 484.1 → 164.0 (36)	6
Phenmedipham	13684-63-4	4	4.57	318.1 → 93.0 (56); 318.1 → 136.0 (24); 318.1 → 168.0 (12)	5
Phenthoate	2597-03-7	3	6.32	321.0 → 247.1 (8); 321.0 → 163.1 (12)	4
Phorate sulfone	2588-04-7		3.82	293.0 → 171.0 (8); 293.0 → 96.8 (44)	5
Phorate sulfoxide	2588-03-6		3.66	277.0 → 96.9 (44); 277.0 → 143.0 (20)	5
Phosalone	2310-17-0	3	6.89	368.0 → 182.1 (12); 368.0 → 110.9 (56)	5
Phosmet	732-11-6	6	4.60	318.0 → 159.9 (16); 318.0 → 133.0 (40)	5
Phosmet oxon	3735-33-9		2.44	302.0 → 160.0 (24); 302.0 → 77.0 (56); 302.0 → 133.1 (40)	5
Phosphamidon I	13171-21-6	3	2.49	300.1 → 127.0 (16); 300.1 → 174.0 (12)	5
Phosphamidon II	13171-21-6	3	2.60	300.1 → 127.0 (16); 300.1 → 174.0 (12)	2
Phoxim	14816-18-3	4	6.77	299.1 → 77.1 (32); 299.1 → 129.1 (16)	5
Picolinafen	137641-05-5	3	7.90	377.1 → 238.1 (28); 377.1 → 145.1 (68)	5
Picoxystrobin	117428-22-5	5	6.24	368.1 → 145.1 (24); 368.1 → 205.1 (12)	4
Piperonyl butoxide	51-03-6		8.05	356.2 → 119.1 (44); 356.2 → 177.1 (32)	5
Piperophos	24151-93-7		7.29	354.1 → 170.9 (28); 354.1 → 212.9 (16)	5
Pirimicarb	23103-98-2	3	3.12	239.1 → 72.1 (20); 239.1 → 182.3 (16)	4
Pirimicarb-desmethyl	30614-22-3		2.05	225.1 → 72.0 (24); 225.1 → 168.1 (12)	4
Pirimiphos-methyl	29232-93-7	3	6.85	306.1 → 108.0 (36); 306.1 → 164.1 (28)	5
Prallethrin	23031-36-9		7.26	301.2 → 133.0 (12); 301.2 → 105.0 (20)	5
Pretilachlor	51218-49-6		7.45	312.2 → 176.0 (32); 312.2 → 251.9 (16)	5
Primisulfuron-methyl	86209-51-0		5.39	469.1 → 253.9 (20); 469.1 → 198.9 (24)	5
Prochloraz	67747-09-5	1	6.76	376.0 → 307.9 (12); 376.0 → 70.1 (20)	5
Prodiamine	29091-21-2		7.95	351.1 → 249.9 (32); 351.1 → 266.9 (20)	5
Profenofos	41198-08-7	3	7.60	375.0 → 304.8 (20); 373.0 → 302.8 (20); 373.0 → 96.9 (44)	7
Promecarb	2631-37-0	7	5.16	208.1 → 109.0 (12); 208.1 → 151.0 (4)	5
Prometon	1610-18-0	4	3.93	226.2 → 184.1 (16); 226.2 → 142.1 (20)	5
Prometryn	7287-19-6		5.39	242.1 → 158.1 (24); 242.1 → 200.2 (16)	5
Propamocarb	24579-73-5	5	1.54	189.2 → 102.0 (16); 189.2 → 74.0 (24)	4
Propanil	709-98-8		4.98	218.0 → 127.2 (24); 218.0 → 162.0 (14); 218.0 → 57.1 (20)	5
Propaquizafop	111479-05-1	4	7.92	444.1 → 100.1 (24); 444.1 → 56.1 (36)	5
Propargite	2312-35-8	4	8.55	368.1 → 175.1 (16); 368.1 → 57.1 (24)	5
Propetamphos (Safrotin)	31218-83-4	3	5.52	282.1 → 138.1 (20); 282.1 → 156.1 (8)	4
Propham	122-42-9	3	3.79	180.1 → 120.0 (16); 180.1 → 92.1 (28)	2

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Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Propiconazole	60207-90-1	2	6.64	342.1 → 69.1 (20); 342.1 → 159.1 (44)	4
Propoxur	114-26-1	6	2.91	210.1 → 111.1 (12); 210.1 → 65.1 (40)	4
Propyzamide (Pronamide)	23950-58-5	3	5.31	256.0 → 173.1 (28); 256.0 → 190.1 (16)	5
Proquinazid	189278-12-4	1	8.75	373.0 → 330.9 (12); 373.0 → 288.9 (24)	6
Prosulfocarb	52888-80-9	4	7.49	252.1 → 91.1 (24); 252.1 → 65.1 (64)	5
Prothioconazole-desthio	120983-64-4		5.98	312.1 → 70.1 (28); 312.1 → 125.1 (32)	4
Pymetrozine	123312-89-0	7	1.55	218.1 → 105.0 (24); 218.1 → 78.0 (48)	4
Pyracarbolid	24691-76-7	7	3.11	218.1 → 125.1 (20); 218.1 → 97.1 (28)	4
Pyraclostrobin	175013-18-0	5	6.82	388.1 → 194.2 (8); 388.1 → 162.9 (20)	5
Pyraflufen-ethyl	129630-19-9		6.62	413.0 → 338.9 (20); 413.0 → 252.9 (32)	4
Pyrazophos	13457-18-6		6.95	374.1 → 222.1 (24); 374.1 → 194.1 (32)	5
Pyrethrum - Cinerin I	13457-18-6		8.62	317.2 → 107.0 (20); 317.2 → 149.1 (8)	6
Pyrethrum - Cinerin II	13457-18-6		7.25	361.2 → 107.1 (24); 361.2 → 149.1 (8)	5
Pyrethrum - Jasmolin I	13457-18-6		8.92	331.2 → 163.2 (8); 331.2 → 107.0 (24)	6
Pyrethrum - Jasmolin II	13457-18-6		7.86	375.2 → 163.1 (8); 375.2 → 107.1 (36); 375.2 → 77.1 (60)	5
Pyrethrum - Pyrethrin I	13457-18-6		8.66	329.2 → 161.1 (8); 329.2 → 133.1 (16)	6
Pyrethrum - Pyrethrin II	13457-18-6		7.38	373.2 → 161.1 (8); 373.2 → 133.1 (24)	5
Pyridaben	96489-71-3	5	8.93	365.2 → 147.1 (28); 365.2 → 309.1 (12)	6
Pyridalyl	179101-81-6		9.44	490.0 → 108.9 (40); 490.0 → 182.9 (20)	6
Pyridaphenthion	119-12-0		5.56	341.1 → 188.9 (28); 341.1 → 91.9 (48)	4
Pyridate	55512-33-9	5	9.10	379.1 → 207.0 (12); 379.1 → 351.1 (8)	6
Pyrifenox I	88283-41-4		5.40	295.0 → 92.9 (28); 295.0 → 91.9 (76)	4
Pyrifenox II	88283-41-4		5.70	295.0 → 92.9 (28); 295.0 → 91.9 (76)	4
Pyrimethanil	53112-28-0	6	4.68	200.1 → 107.2 (24); 200.1 → 82.0 (28)	5
Pyriproxyfen	95737-68-1	5	8.10	322.2 → 96.1 (20); 322.2 → 78.1 (56)	5
Pyroquilon	57369-32-1		2.81	174.1 → 117.0 (36); 174.1 → 132.0 (28)	5
Pyroxsulam	422556-08-9		2.85	435.1 → 194.9 (28); 435.1 → 193.9 (36)	4
Quinalphos	95737-68-2	3	6.29	299.1 → 97.1 (40); 299.1 → 163.1 (28)	4
Quinmerac	90717-03-6	7	2.03	222.0 → 203.9 (20); 222.0 → 141.0 (44)	4
Quinoclamine	2797-51-5	4	2.71	208.0 → 105.1 (28); 208.0 → 77.1 (40)	5
Quinoxyfen	124495-18-7	3	8.14	308.0 → 197.1 (40); 308.0 → 162.1 (56)	5
Quizalofop	82-68-8		5.93	345.1 → 298.9 (16); 345.1 → 272.9 (24)	4
Quizalofop-ethyl	76578-14-8		7.66	373.1 → 299.0 (20); 373.1 → 90.9 (36)	5
Resmethrin	10453-86-8		9.04	339.2 → 171.1 (12); 339.2 → 128.1 (52)	6
Rimsulfuron	122931-48-0	4	3.31	432.1 → 182.1 (32); 432.1 → 325.1 (16)	5
Rotenone	83-79-4	7	6.20	395.2 → 213.0 (24); 395.2 → 192.0 (20)	4
Schradan (Octamethylpyrophosphoramide)	152-16-9		2.10	287.1 → 135.0 (32); 287.1 → 241.9 (16)	4
Secbumeton	26259-45-0	7	4.11	226.2 → 170.1 (16); 226.2 → 113.9 (24)	5
Sethoxydim I	74051-80-2		5.27	328.2 → 178.0 (20); 328.2 → 282.3 (8)	5
Sethoxydim II	74051-80-2		7.84	328.2 → 178.0 (20); 328.2 → 282.3 (8)	5
Siduron	1982-49-6		4.97	233.2 → 94.0 (40); 233.2 → 55.1 (48)	5
Silthiofam	175217-20-6	4	6.28	268.1 → 139.1 (20); 268.1 → 73.1 (36)	4
Simazine	122-34-9		2.98	202.1 → 96.1 (24); 202.1 → 104.1 (30)	4
Simeconazole	149508-90-7		5.84	294.2 → 70.0 (24); 294.2 → 134.9 (28)	4

Table 1. List of Compounds Included in the Method Together with Their Chemical Abstract Service (CAS) Numbers, Retention Times (RT), Primary Transitions, Collision Energies (CE), and Total Number of Transitions in the tMRM Program (continued). For Compounds Provided in Agilent LC/MS mixes 1–8 (p/n 5190-0551), the Respective Mix Number is Aso Listed

Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Simetryn	1014-70-6		3.47	214.1 → 68.1 (40); 214.1 → 124.1 (20)	6
Spinetoram - Spinosyn J	187166-40-1		7.56	748.5 → 142.1 (36); 748.5 → 98.1 (72)	5
Spinetoram - Spinosyn L	187166-40-1		7.99	760.5 → 142.1 (36); 760.5 → 98.1 (72)	5
Spinosad - Spinosyn A	168316-95-8	7	7.03	732.5 → 142.0 (32); 732.5 → 98.3 (52)	5
Spinosad - Spinosyn D	168316-95-8	7	7.47	746.5 → 142.1 (32); 746.5 → 98.4 (60)	5
Spirodiclofen	148477-71-8	1	8.76	411.1 → 313.1 (8); 411.1 → 71.1 (32)	6
Spiromesifen	283594-90-1	6	8.52	388.2 → 273.0 (8); 388.2 → 255.0 (28)	6
Spiromesifen enol	148476-30-6		4.77	273.2 → 186.9 (16); 273.2 → 67.0 (40)	5
Spirotetramat	203313-25-1	6	5.85	374.2 → 216.1 (40); 374.2 → 302.2 (20)	4
Spiroxamine I	118134-30-8	1	4.97	298.3 → 144.1 (20); 298.3 → 100.1 (36)	5
Spiroxamine II	118134-30-8	1	5.07	298.3 → 144.1 (20); 298.3 → 100.1 (36)	5
Sulfentrazone	122836-35-5	6	3.17	404.0 → 306.9 (28); 404.0 → 273.1 (40)	4
Sulprofos	35400-43-2		8.33	323.0 → 218.8 (12); 323.0 → 139.2 (32)	6
Tebuconazole	107534-96-3	2	6.49	308.1 → 70.0 (20); 308.1 → 124.9 (52)	4
Tebufenozide	112410-23-8	5	6.25	353.2 → 133.1 (20); 353.2 → 105.1 (52)	4
Tebufenpyrad	119168-77-3	3	7.86	334.1 → 145.0 (28); 334.1 → 117.0 (40)	5
Tebupirimfos	96182-53-5		7.95	319.1 → 153.1 (32); 319.1 → 276.9 (12)	5
Tebuthiuron	34014-18-1	7	3.15	229.1 → 172.1 (12); 229.1 → 116.0 (24)	4
Teflubenzuron	83121-18-0	4	7.89	381.0 → 141.0 (48); 381.0 → 158.0 (16)	5
Temephos	3383-96-8	7	8.02	467.0 → 125.0 (44); 467.0 → 418.9 (20)	5
Tepraloxydim I	149979-41-9	3	3.34	342.2 → 250.0 (8); 342.2 → 166.0 (16)	5
Tepraloxydim II	149979-41-9	3	5.70	342.2 → 250.0 (8); 342.2 → 166.0 (16)	4
Terbufos	13071-79-9	3	7.82	289.1 → 103.1 (4); 289.1 → 57.0 (24); 289.1 → 232.9 (0)	4
Terbufos sulfone	56070-16-7		4.80	338.1 → 171.0 (12); 338.1 → 97.1 (60)	5
Terbufos sulfoxide	10548-10-4		4.83	305.1 → 187.1 (6); 305.1 → 96.8 (52)	5
Terbumeton	33693-04-8		4.15	226.2 → 170.1 (20); 226.2 → 114.2 (26)	5
Terbuthylazine	5915-41-3		5.07	230.1 → 174.1 (16); 230.1 → 96.1 (32)	5
Terbutryn	886-50-0		5.68	242.1 → 186.2 (20); 242.1 → 71.1 (36)	4
Tetrachlorvinphos	961-11-5		6.27	366.9 → 127.0 (16); 364.9 → 127.0 (16)	2
Tetraconazole	112281-77-3	2	5.85	372.0 → 70.1 (24); 372.0 → 159.1 (44)	4
Thiabendazole	148-79-8	5	2.07	202.0 → 131.0 (40); 202.0 → 175.0 (28)	4
Thiabendazole-5-hydroxy-	948-71-0		1.68	218.0 → 190.9 (28); 218.0 → 147.0 (36)	4
Thiacloprid	111988-49-9	5	2.12	253.0 → 126.1 (24); 253.0 → 90.1 (48)	4
Thiamethoxam	153719-23-4	5	1.68	292.0 → 211.0 (20); 292.0 → 131.9 (44)	5
Thiazopyr	117718-60-2		6.49	397.1 → 377.0 (24); 397.1 → 335.0 (36)	4
Thidiazuron	51707-55-2	7	2.93	221.0 → 101.9 (12); 221.0 → 93.9 (8)	4
Thifensulfuron-methyl	79277-27-3	4	2.71	388.0 → 166.9 (16); 388.0 → 56.0 (44); 388.0 → 140.9 (20)	4
Thiobencarb (Benthiocarb)	28249-77-6		6.93	258.1 → 124.9 (16); 258.1 → 88.9 (64)	5
Thiodicarb	59669-26-0	5	3.50	355.0 → 88.1 (24); 355.0 → 108.1 (12)	6
Thiofanox	39196-18-4	5	3.62	241.0 → 184.0 (8); 241.0 → 57.0 (20); 241.0 → 98.0 (8)	4
Thiofanox sulfone	39184-59-3		1.89	268.1 → 57.1 (12); 268.1 → 75.9 (8)	4
Thiofanox sulfoxide	39184-27-5		1.84	235.1 → 103.9 (12); 235.1 → 56.9 (12)	4
Thionazin (Zinophos)	297-97-2		3.99	249.0 → 97.0 (24); 249.0 → 192.9 (12)	5
Thiophanate-methyl	23564-05-8		2.86	343.1 → 151.1 (16); 343.1 → 93.1 (56)	4
Tolfenpyrad	129558-76-5		7.99	384.2 → 197.0 (28); 384.2 → 116.9 (40)	5

Table 1. List of Compounds Included in the Method Together with Their Chemical Abstract Service (CAS) Numbers, Retention Times (RT), Primary Transitions, Collision Energies (CE), and Total Number of Transitions in the tMRM Program (continued). For Compounds Provided in Agilent LC/MS mixes 1–8 (p/n 5190-0551), the Respective Mix Number is Aso Listed

Compound	CAS	Agilent Mix No.	RT (min)	Primary transition (CE)	No. of transitions
Tolylfluanid	731-27-1	3	6.44	347.0 → 137.0 (36); 347.0 → 237.9 (8)	4
Topramezone	210631-68-8		1.68	364.1 → 334.0 (12); 364.1 → 235.9 (24)	4
Tralkoxydim	87820-88-0	1	8.30	330.2 → 284.2 (12); 330.2 → 96.1 (32)	6
Triadimefon	43121-43-3	3	5.43	294.1 → 197.0 (12); 294.1 → 69.0 (20)	4
Triadimenol	55219-65-3	6	5.61	296.1 → 70.0 (12); 298.1 → 70.0 (12); 296.1 → 99.2 (12)	4
Triasulfuron	82097-50-5	4	2.73	402.1 → 141.1 (36); 402.1 → 167.0 (36)	5
Triazophos	24017-47-8	3	5.62	314.1 → 162.1 (20); 314.1 → 97.1 (36)	4
Tribenuron-methyl	101200-48-0	4	3.93	396.1 → 155.1 (28); 396.1 → 181.1 (28)	5
Tribufos (DEF)	78-48-8		8.93	315.1 → 57.1 (32); 315.1 → 169.0 (14)	6
Trichlorfon (Metrifonate)	52-68-6	6	2.01	256.9 → 109.0 (12); 256.9 → 220.9 (8)	4
Tricyclazole	41814-78-2	2	2.31	190.0 → 136.1 (28); 190.0 → 163.1 (20)	5
Trietazine	1912-26-1	6	5.72	230.1 → 99.0 (24); 230.1 → 132.0 (20)	4
Trifloxystrobin	141517-21-7	5	7.33	409.1 → 186.1 (20); 409.1 → 145.1 (56)	5
Trifloxysulfuron (sodium)	199119-58-9		3.91	438.07 → 182.1 (24); 438.07 → 139.1 (56)	5
Triflumizole	68694-11-1	3	7.34	346.1 → 73.0 (16); 346.1 → 55.0 (12)	5
Triflumuron	64628-44-0	4	6.86	359.0 → 156.1 (16); 359.0 → 139.0 (40)	5
Triforine	26644-46-2		4.54	434.9 → 389.9 (12); 434.9 → 97.9 (44)	5
Trimethacarb	2655-15-4	6	4.10	194.1 → 137.1 (12); 194.1 → 122.1 (32)	5
Triticonazole	131983-72-7	2	5.87	318.1 → 70.1 (16); 320.1 → 70.1 (16); 318.1 → 125.1 (40)	4
Uniconazole	83657-17-4	2	6.07	292.1 → 70.1 (20); 294.1 → 70.0 (20); 292.1 → 125.1 (28)	4
Vamidothion	2275-23-2	2	1.92	288.1 → 146.1 (8); 288.1 → 118.1 (28)	4
Zoxamide	156052-68-5	6	6.63	336.0 → 186.9 (28); 336.0 → 158.9 (52)	4

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