Application Note: 51878

Non-targeted Screening and Accurate Mass Confirmation of 510 Pesticides on the High Resolution Exactive Benchtop LC/MS Orbitrap Mass Spectrometer

Allen Zhang, James S. Chang, Christine Gu, Mark Sanders, Thermo Fisher Scientific, San Jose, CA, USA

Key Words

- Exactive
- High Mass Accuracy
- High Resolution
- Orbitrap Technology
- Pesticide Analysis

Overview

As agricultural trade grows and food safety concerns mount, stricter pesticide regulations are being enforced around the world. Increased pesticide testing and reductions in maximum permissible residue levels have driven demand for fast, sensitive and cost-effective analytical methods for high-throughput screening of multi-class pesticides in food. Detection of 510 pesticides at low ppb levels was achieved within 12 minutes using the Thermo Scientific Exactive benchtop LC/MS system powered by Orbitrap technology. The high resolving power of the Thermo Scientific Orbitrap platform enables accurate mass confirmation of all compounds, including isobaric pesticides. Accurate, robust, easy to use and cost-efficient, the Exactive™ LC/MS is ideally suited for routine, comprehensive screening of targeted and non-targeted pesticides at or below the 0.01 mg/kg (10 ppb) default limit set by EU and Japanese legislation.

Introduction

In 2007, the United States Environmental Protection Agency (EPA) completed a ten-year reassessment of 9,721 pesticide tolerances to meet more stringent safety standards and recommended the revocation or modification of thousands of uses of pesticides in food.[1] China published national standard GB 2763-2005 in 2005, which established 478 maximum residue levels (MRLs) for 136 pesticides.[2] Japan's Positive List System, introduced in 2006, established MRLs for hundreds of agricultural chemicals, including approximately 400 pesticides, in food and set a uniform limit of 10 ppb to chemicals for which MRLs have not been determined.[3] Regulation (EC) No. 396/2005 of the European Parliament, implemented in 2008, harmonized all pesticide MRLs for European Union (EU) member states and set default limits of 0.01 mg/kg for all pesticide/commodity combinations for which no MRLs have been set.[4] A pesticide safety review of about 1,000 active substances on the market was mandated by EU Directive 91/414/EEC and, upon completion in 2009, led to the approval of only about 250 substances, effectively setting the permissible levels of over 700 de-listed pesticides to the default limit.[5] The EU and Japanese regulations are among the most stringent in the world and have fueled the need for faster and more sensitive analytical methods for cost-efficient, high-throughput screening of multi-class pesticide residues.

Pesticides in food were traditionally monitored and quantified using gas chromatography (GC) coupled with either selective detectors (e.g. electron capture) or mass spectrometry (MS). GC/MS continues to be widely used in pesticide analysis because it is highly selective, provides confirmation of multiple classes of pesticides in a single analytical run, and is relatively inexpensive and easy to operate. However, GC/MS cannot detect polar, thermally unstable or low volatility compounds without derivatization. Recent improvements in liquid chromatography (LC) throughput and MS detection capabilities have led to a surge in the use of LC/MS-based techniques for screening, confirmation and quantitation of ultra-trace levels of multi-class pesticide residues, including those that are not GC-amenable. LC-triple quadrupole tandem MS (LC/MS/MS) enables highly selective and sensitive quantification and confirmation of hundreds of target pesticides in a single run, but this approach requires extensive compound-dependent parameter optimization and cannot be used to screen for untargeted pesticides. Full scan approaches using high performance time-of-flight (TOF) or Orbitrap™ mass spectrometers coupled to ultra-high pressure LC (U-HPLC) facilitate rapid and sensitive screening and detection of LC-amenable pesticide residues present in a sample. The superior resolving power of the Orbitrap mass spectrometer (up to 100,000 FWHM) compared to TOF instruments (10,000–20,000) ensures the high mass accuracy required for complex sample analysis.[6] High resolution LC/MS instrumentation, however, can be cost-prohibitive for many routine monitoring laboratories.

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The Thermo Scientific Exactive benchtop LC/MS Orbitrap mass spectrometer was designed for accurate and reliable screening of complex samples in a wide range of demanding high-throughput applications. Built on Orbitrap mass analyzer technology, the Exactive delivers exceptional mass resolution (up to 100,000) to ensure highly accurate mass measurements and to enable confident discrimination of co-eluting, isobaric compounds in complex samples.[6,7] A wide in-scan dynamic range (3-4 orders of magnitude) facilitates the detection of trace levels of compounds in the presence of highly abundant matrix interferences. High scan speeds and polarity switching ensure full compatibility with U-HPLC and high-throughput methods. Cost-effective and easy to operate, the Exactive is an ideal tool for compliance monitoring in regulatory labs. In this note, we demonstrate rapid screening and accurate mass confirmation of 510 pesticides at low ppb levels using U-HPLC coupled to a high resolution Exactive benchtop Orbitrap mass spectrometer. Full scan U-HPLC-single stage Orbitrap MS can be used to screen a virtually limitless number of pesticides and, unlike MS/MS methods, does not require compound-dependent parameter optimization.

Materials and Methods

Sample Preparation

Pesticide standards were obtained from the U.S. Food and Drug Administration (FDA). A stock solution of a mixture of 510 pesticides was prepared at a concentration of 3 mg/L. Calibration solutions, with concentrations of 1-250 ppb, were prepared by serial dilution of the stock solution in 50:50 (v/v) acetonitrile/water.

Spiked spinach samples were prepared for analysis using a modified QuEChERS method (Figure 1). QuEChERS, an acronym for Quick, Easy, Cheap, Effective, Rugged, and Safe, is a sample preparation procedure used to extract pesticides from food.[8] Malathion D6 was used as an internal standard for calibration.

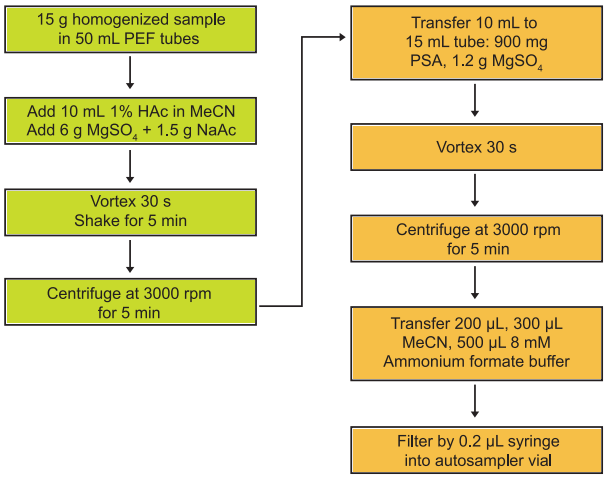


Figure 1: Schematic of the modified QuEChERS workflow used to extract pesticides from spinach matrices

Experimental Conditions

Instrumentation

LC/MS analysis was performed using a Thermo Scientific Accela U-HPLC system. With a CTC Analytics PAL autosampler coupled to an Exactive benchtop Orbitrap mass spectrometer (Figure2). Data acquisition was performed using Thermo Scientific Xcaliber software. Thermo Scientific Pathfinder software was used for data processing.

Figure 2: LC/MS analysis was performed using an Accela™ U-HPLC system coupled to an Exactive benchtop Orbitrap mass spectrometer

LC Parameters

Column:	Thermo Scientific Hypersil GOLD aQ C18 column (100 x 2.1 mm, 1.9 µm particle size)		
Mobile Phase:	A: Water with 0.1% formic acid and 4 mM ammonium formate B: Methanol with 0.1% formic acid and 4 mM ammonium formate		
Flow Rate:	300 µL/min		
Column Temperature:	ambient		
Sample Injection Volume:	10 µL		
Gradient:	Time (min)	%A	%B
	0	100	0
	1	100	0
	8	0	100
	12	0	100
	12.5	100	0
	14	100	0

MS Parameters

Full mass scan positive/negative ion mode (mass range = 100 to 1500)	
Resolution:	50,000
Automatic Gain Control (AGC) Target Value:	10e6
Heated Electrospray Ionization Source Conditions:	
Spray Voltage:	2200 V
Capillary Temperature:	280 °C
Sheath Gas:	32 au
Auxiliary Gas:	7 au
Vaporizer Temperature:	200 °C

Results and Discussion

U-HPLC improves chromatographic resolution, speed and sensitivity, and when coupled to MS, facilitates rapid, high-throughput analysis of challenging samples. Using U-HPLC-single stage Orbitrap MS, a mixture of 510 pesticides representing a broad spectrum of chemical classes was separated and detected within 12 minutes (Table 1). High resolution (50,000) and high mass accuracy (< 5 ppm without internal calibration for most compounds) enabled identification of all analytes (Table 1). Separation of isobaric pesticides was achieved only at the high resolving powers provided by Orbitrap MS, as demonstrated in Figure 3. Excellent linearity in detector response was observed over the range of 1-250 ppb, with correlation coefficients greater than 0.99 for the majority of pesticides (Table 1). Chromatograms and calibration curves for eight representative pesticides are shown in Figure 4. For the concentration range studied (1-250 ppb), limits of quantitation (LOQs) were estimated from triplicate injections (CV < 15%) of standard solutions at concentration levels corresponding to a signal-to-noise ratio of 10. As shown in Table 1, LOQs ranged from 1-50 ppb, and for 499 pesticides, LOQs were at or below 10 ppb, the MRL imposed by EU and Japanese regulations.

To evaluate the applicability of this technique to complex food samples, U-HPLC-single stage Orbitrap MS was used to screen for pesticides extracted from a spiked spinach matrix. An extraction procedure based on fast and efficient QuEChERS methodology was used to facilitate rapid high-throughput multiresidue analysis. Table 2 summarizes this and mass spectral data obtained for a representative set of extracted pesticides. Extracted ion chromatograms and calibration curves for six pesticides extracted from the spiked spinach matrix are depicted in Figure 5. The detection and quantitation capabilities of this method were assessed using the EPA method detection limit (MDL) procedure.[9] For all pesticides, limits of detection (LODs) and LOQs were lower than 1 ppb (Table 2).

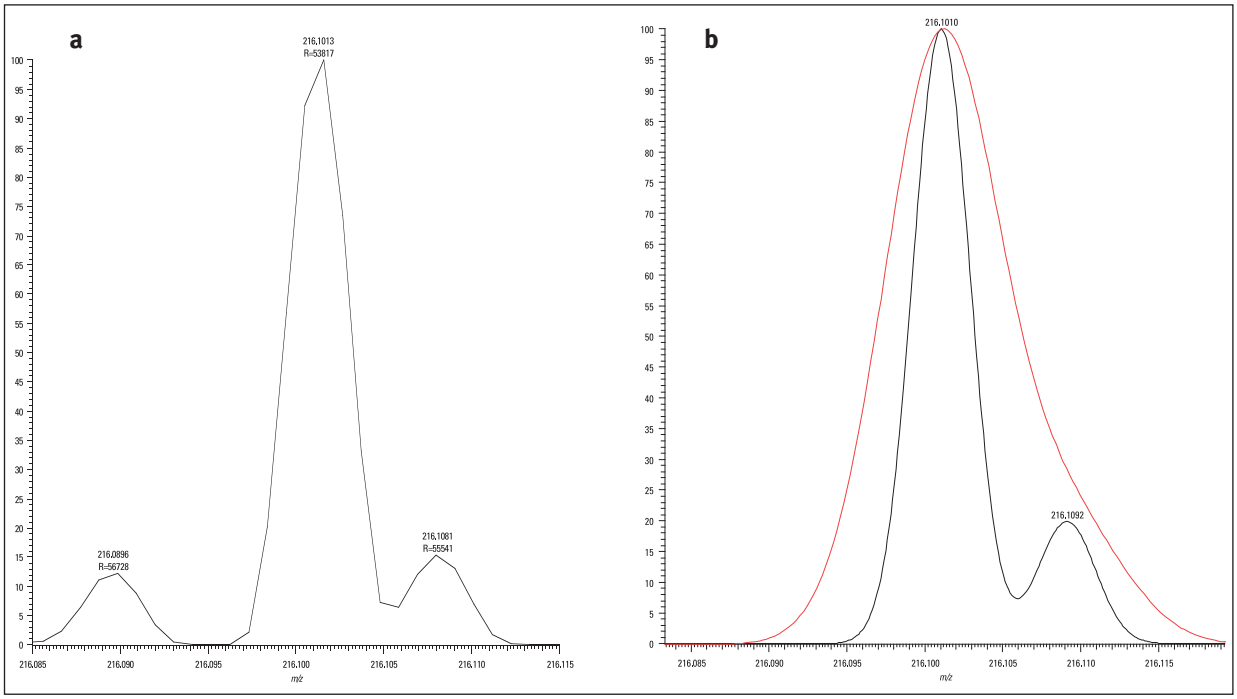


Figure 3: The high resolving power of the Exactive benchtop Orbitrap mass spectrometer enabled separation of the $[M+H]^+$ ion of atrazine (m/z = 216.1012) from the $[M+NH_4]^+$ ion of cymoxanil (m/z = 216.1088). (a) Mass spectra of the two isobaric pesticides at a resolution of 50,000. (b) Simulated mass spectra of the isobaric pesticides at resolutions of 25,000 (red line) and 50,000 (black line).

LC/MS data for Pesticide Standards *(Table 1)*

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Abamectin B1a	C48H72O14	+	890.526	890.5261	0	10	0.9898
Abamectin B1b	C47H70O14	+	876.5104	876.5138	3.8	10	0.9315
Acephate	C4H10NO3PS	+	184.0192	184.0193	0.8	1	0.9994
Acequinocyl	C24H32O4	+	402.2639	402.2638	0.2	1	0.9886
Acetamiprid	C10H11C N4	+	223.0745	223.0747	0.7	1	0.9989
Acibenzolar S-methyl	C8H6N2OS2	+	210.9994	211.0004	4.4	10	0.9936
Acifluorfen	C14H7ClF3NO5	-	359.9892	359.9896	1.1	1	0.9961
Aclonifen	C12H9ClN2O3	+	282.064	282.065	3.6	25	0.9812
Acrinathrin	C26H21F6NO5	+	559.1662	559.1664	0.3	1	0.9931
Akton	C12H14Cl3O3PS	+	374.954	374.9536	1	25	0.9859
Alachlor	C14H20C NO2	+	270.1255	270.1255	0.3	1	0.9890
Alanycarb	C17H25N3O4S2	+	400.1359	400.1369	2.5	1	0.9049
Aldicarb	C7H14N2O2S	+	208.1114	208.1116	0.6	1	0.9989
Aldicarb sulfone	C7H14N2O4S	+	223.0747	223.0747	0.3	1	0.9987
Aldicarb sulfoxide	C7H14N2O3S	+	207.0798	207.0798	0.1	1	0.9998
Allethrin	C19H26O3	+	303.1955	303.1957	0.6	1	0.9983
Allidochlor	C8H12ClNO	+	174.068	174.068	0	1	0.9936
Ametryn	C9H17N5S	+	228.1277	228.1278	0.4	1	0.9979
Amicarbazone	C10H19N5O2	+	242.1612	242.1612	0.1	1	0.9986
Aminocarb	C11H16N2O2	+	209.1285	209.1285	0.3	1	0.9997
Aminopyralid	C6H4Cl2N2O2	-	204.9577	204.9571	2.9	1	0.9629
Amitraz	C19H23N3	+	294.1965	294.1965	0.1	1	0.9725
Ancymidol	C15H16N2O2	+	257.1285	257.1284	0.4	1	0.9954
Anilazine	C9H5Cl3N4	-	272.9507	272.9572	2.4	1	0.9653
Anilofos	C13H19C NO3PS2	+	368.0305	368.0304	0.3	1	0.9986
Anilofos	C13H19C NO3PS2	+	368.0305	368.0304	0.3	1	0.9971
Antimycin A	C28H40N2O9	-	547.2661	547.2668	1.2	1	0.9928
Aramite	C15H23ClO4S	+	352.1344	352.1345	0.4	1	0.9946
Aspon	C12H28O5P2S2	+	379.0926	379.0927	0.1	1	0.9853
Asulam	C8H10N2O4S	+	248.07	248.07	0	1	0.9986
Atrazine	C8H14ClN5	+	216.1011	216.1012	0.8	1	0.9991
Azaconazole	C12H11Cl2N3O2	+	300.0301	300.0302	0.1	1	0.9940
Azadirachtin	C35H44O16	+	738.2968	738.2968	0	1	0.9904
Azafenidrin	C15H13Cl2N3O2	+	338.0458	338.0458	0	1	0.9932
Azamethiphos	C9H10ClN2O5PS	+	324.9809	324.981	0.2	1	0.9991
Azinphos methyl oxon	C10H12N3O4PS	+	302.0359	302.0359	0.1	1	0.9969
Azinphos-ethyl	C12H16N3O3PS2	+	346.0444	346.0443	0.1	1	0.9906
Azinphos-methyl	C10H12N3O3PS2	+	318.0131	318.0129	0.3	1	0.9957
Azoxystrobin	C22H17N3O5	+	404.1241	404.124	0.2	1	0.9948
Barban	C11H9Cl2NO2	+	275.0349	275.0355	2.4	10	0.9953
Benalaxyl	C20H23NO3	+	326.1751	326.175	0.4	1	0.9986
Benazolin	C9H6C NO3S	+	243.983	243.9827	1.2	1	0.9863
Bendiocarb	C11H13NO4	+	224.0917	224.0919	0.8	1	0.9993
Benfluralin	C13H16F3N3O4	+	353.1431	353.143	0.2	1	0.9883
Benfuracarb	C20H30N2O5S	+	428.2214	428.2211	0.6	1	0.9956
Benodanil	C13H10INO	+	323.988	323.9879	0.4	1	0.9925
Benoxacor	C11H11Cl2NO2	+	260.024	260.024	0.1	10	0.9989
Bensulide	C14H24NO4PS3	+	415.0943	415.0944	0.1	1	0.9872
Bentazone	C10H12N2O3S	+	241.0641	241.0643	0.5	1	0.9982
Benthiavalicarb	C15H18FN3O3S	+	340.1126	340.114	4.2	1	0.9047
Benzoximate	C18H18C NO5	+	364.0946	364.0944	0.7	1	0.9965
Bifenazate	C17H20N2O3	+	301.1547	301.1546	0.1	1	0.9892
Bifenox	C14H9Cl2NO5	+	359.0196	359.0193	0.8	10	0.9668
Bifenthrin	C23H22C F3O2	+	423.1333	423.1322	2.6	10	0.9729
Binapacryl	C15H18N2O6	+	340.1503	340.1496	2.2	10	0.9688
Bispyribac-sodium	C19H17N4NaO8	+	453.1017	453.1018	0.1	10	0.9843
Bitertanol	C20H23N3O2	+	338.1863	338.1861	0.5	1	0.9916
Boscalid	C18H12Cl2N2O	+	343.04	343.0399	0.1	1	0.9797
Brodifacoum	C31H23BrO3	-	521.0758	521.0755	0.5	1	0.9905

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Bromadiolone	C30H23BrO4	-	525.0707	525.0706	0.1	1	0.9879
Bromoxynil	C7H3Br2NO	-	273.8509	273.8506	1	1	0.9990
Bromuconazole(cis-)	C13H12BrCl2N3O	+	375.9614	375.9613	0	1	0.9961
Bromuconazole(trans-)	C13H12BrCl2N3O	+	375.9614	375.9613	0	1	0.9912
Bufencarb	C13H19NO2	+	222.1489	222.149	0.6	1	0.9965
Bupirimate	C13H24N4O3S	+	317.1642	317.1641	0.2	1	0.9978
Buprofezin	C16H23N3OS	+	306.1635	306.1632	0.7	1	0.9974
Butachlor	C17H26ClNO2	+	329.199	329.1989	0.3	10	0.9928
Butafenacil	C20H18ClF3N2O6	+	492.1144	492.1144	0.1	1	0.9981
Butocarboxim	C7H14N2O2S	+	208.1114	208.1116	0.6	1	0.9971
Butoxycarboxim	C7H14N2O4S	+	223.0747	223.0747	0.3	1	0.9990
Butralin	C14H21N3O4	+	296.1605	296.1604	0.4	1	0.9983
Butylate	C11H23NOS	+	218.1573	218.1575	0.9	1	0.9993
Cadusafos	C10H23O2PS2	+	271.095	271.0948	0.8	1	0.9874
Carbaryl	C12H11NO2	+	202.0863	202.0855	3.9	1	0.9923
Carbendazim	C9H9N3O2	+	192.0768	192.0767	0.4	1	0.9986
Carbetamide	C12H16N2O3	+	237.1234	237.1235	0.6	1	0.9982
Carbofuran	C12H15NO3	+	222.1125	222.1126	0.4	1	0.9980
Carbofuran, 3OH-	C12H15NO4	+	255.1339	255.1338	0.5	1	0.9986
Carboxin	C12H13NO2S	+	236.074	236.074	0.3	1	0.9972
Carfentrazone-ethyl	C15H14Cl2F3N3O3	+	429.0703	429.0702	0.1	1	0.9957
Carpropamid	C15H18Cl3NO	+	334.0527	334.0526	0.1	1	0.9982
Chinomethionate	C10H6N2OS2	+	252.026	252.0267	2.7	10	0.9963
Chlorantraniliprole	C18H14BrCl2N5O2	+	481.9781	481.978	0.1	1	0.9718
Chlorbromuron	C9H10BrClN2O2	+	292.9687	292.9688	0.2	1	0.9958
Chlorbufam	C11H10ClNO2	+	241.0738	241.073	3.5	1	0.9864
Chlordimeform	C10H13ClN2	+	197.084	197.084	0.1	10	0.9973
Chlorfenvinphos	C12H14Cl3O4P	+	358.9768	358.9767	0.2	1	0.9976
Chlorfluazuron	C20H9Cl3F5N3O3	+	556.9968	556.9968	0.1	1	0.9963
Chloroxuron	C15H15ClN2O2	+	291.0895	291.0893	0.8	1	0.9978
Chlorpropham	C10H12ClNO2	+	214.0629	214.0632	1.3	10	0.9910
Chlorpyrifos	C9H11Cl3NO3PS	+	349.9336	349.9336	0	1	0.9951
Chlorpyrifos oxon	C9H11Cl3NO4P	+	333.9564	333.9564	0.1	1	0.9903
Chlorpyrifos-methyl	C7H7Cl3NO3PS	+	321.9023	321.9022	0.1	25	0.9763
Chlorthiamid	C7H5Cl2NS	+	222.9858	222.9852	2.8	10	0.9857
Chlorthion	C8H9C NO5PS	+	314.9966	314.9971	1.6	25	0.9812
Chlorthiophos	C11H15Cl2O3PS2	+	360.965	360.9643	1.9	25	0.9632
Chlortoluron	C10H13ClN2O	+	213.0789	213.079	0.6	1	0.9976
Clethodim	C17H26ClNO3S	+	360.1395	360.1395	0.2	1	0.9923
Clofentezine	C14H8Cl2N4	+	320.0464	320.045	4.5	10	0.9935
Clothianidin	C6H8C N5O2S	+	250.016	250.016	0.2	1	0.9916
Coumaphos	C14H16ClO5PS	+	363.0217	363.0217	0.1	1	0.9983
Coumaphos oxon	C14H16ClO6P	+	347.0446	347.0446	0	1	0.9951
Crotoxyphos	C14H19O6P	+	332.1258	332.1255	0.7	1	0.9982
Crufomate	C12H19ClNO3P	+	309.1129	309.112	3.1	1	0.9914
Cumyluron	C17H19ClN2O	+	303.1259	303.1258	0.2	1	0.9989
Cyanazine	C9H13ClN6	+	241.0963	241.0963	0.2	1	0.9951
Cyazofamid	C13H13ClN4O2S	+	342.0786	342.077	4.6	1	0.9895
Cyclanilide	C11H9Cl2NO3	-	271.9887	271.9891	1.8	1	0.9991
Cycloate	C11H21NOS	+	216.1417	216.1418	0.4	1	0.9913
Cyclohexamide	C15H23NO4	+	299.1965	299.1966	0.3	1	0.9977
Cycluron	C11H22N2O	+	199.1805	199.1805	0.1	1	0.9922
Cyflufenamid	C20H17F5N2O2	+	413.1283	413.1282	0.2	1	0.9977
Cyfluthrin	C22H18Cl2FNO3	+	451.0986	451.098	1.3	10	0.7124
Cyhalothrin	C23H19ClF3NO3	+	467.1344	467.1339	1	1	0.9859
Cymoxanil	C7H10N4O3	+	216.1091	216.1088	1.3	1	0.9885
Cypermethin	C22H19Cl2NO3	+	433.108	433.108	0	10	0.9859
Cyphenothrin	C24H25NO3	+	393.2173	393.2173	0	1	0.9959
Cyproconazole	C15H18ClN3O	+	292.1211	292.1211	0.2	1	0.9978

LC/MS data for Pesticide Standards *(Table 1 continued)*

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Cyprodinil	C14H15N3	+	226.1339	226.1339	0.3	1	0.9967
Cyprosulfamide	C18H18N2O5S	+	375.1009	375.1009	0.1	1	0.9977
Cyromazine	C6H10N6	+	167.104	167.1039	0.2	1	0.9445
Daimuron	C17H20N2O	+	269.1648	269.1646	0.7	1	0.9992
Dazomet	C5H10N2S2	+	163.0358	163.0358	0.1	1	0.9451
DEF (Tribufos)	C12H27OPS3	+	315.1034	315.1033	0.3	1	0.9840
Deltamethrin	C22H19Br2NO3	+	521.007	521.0073	0.5	1	0.9986
Demeton S-methyl	C6H15O3PS2	+	231.0273	231.0275	0.9	1	0.9966
Demeton S-sulfone	C6H15O5PS2	+	263.0171	263.0173	0.8	10	0.9914
Demeton-O	C8H19O3PS2	+	259.0586	259.0586	0.1	1	0.9960
Demeton-S (Disulfoton oxon)	C8H19O3PS2	+	259.0586	259.0586	0.1	1	0.9960
Desmedipham	C16H16N2O4	+	318.1448	318.1448	0	1	0.9975
Desmetryn	C8H15N5S	+	214.1121	214.1122	0.6	1	0.9986
Dialifor	C14H17C NO4PS2	+	411.0363	411.0363	0.1	1	0.9984
Diallate	C10H17Cl2NOS	+	270.0481	270.0482	0.5	1	0.9636
Diamidafos (Nellite)	C8H13N2O2P	+	201.0787	201.0787	0	1	0.9986
Diazinon	C12H21N2O3PS	+	305.1083	305.1081	0.9	1	0.9983
Diazinon hydroxy	C12H21N2O4PS	+	321.1032	321.1031	0.6	1	0.9985
Diazinon oxon	C12H21N2O4P	+	289.1312	289.1311	0.2	1	0.9385
Dicapthon	C8H9C NO5PS	+	314.9966	314.9971	1.6	25	0.9812
Dichlofluanid	C9H11Cl2FN2O2S2	+	349.9961	349.9961	0.2	1	0.9930
Dichlorfenthion	C10H13Cl2O3PS	+	314.9773	314.9768	1.5	10	0.9966
Dichlormid	C8H11Cl2NO	+	208.0291	208.0292	0.6	1	0.9923
Dichlorvos	C4H7Cl2O4P	+	220.9532	220.9533	0.4	10	0.9920
Diclobutrazol	C15H19Cl2N3O	+	328.0978	328.0978	0.1	1	0.9949
Dicrotophos	C8H16NO5P	+	238.0839	238.0839	0.2	1	0.9991
Diethofencarb	C14H21NO4	+	268.1543	268.1543	0.1	1	0.9994
Difenacoum	C31H24O3	+	445.1798	445.1798	0.1	1	0.9972
Difenoconazole	C19H17Cl2N3O3	+	406.072	406.0719	0.3	1	0.9914
Diflenoxuron	C16H18N2O3	+	287.139	287.1389	0.6	1	0.9938
Diflubenzuron	C14H9ClF2N2O2	-	309.0248	309.0246	0.6	1	0.9985
Dimepiperate	C15H21NOS	+	264.1417	264.1429	4.9	1	0.9994
Dimethachlor	C13H18C NO2	+	256.1099	256.1098	0.3	1	0.9921
Dimethametryn	C11H21N5S	+	256.159	256.1588	0.8	1	0.9983
Dimethenamid	C12H18C NO2S	+	276.082	276.0818	0.5	1	0.9977
Dimethoate	C5H12NO3PS2	+	230.0069	230.007	0.3	1	0.9993
Dimethomorph	C21H22C NO4	+	388.131	388.131	0	1	0.9970
Dimethylvinphos. Z-	C10H10Cl3O4P	+	330.9455	330.9455	0.1	1	0.9950
Dimetilan	C10H16N4O3	+	241.1295	241.1295	0.1	1	0.9990
Dimoxystrobin	C19H22N2O3	+	327.1703	327.1702	0.4	1	0.9905
Diniconazole	C15H17Cl2N3O	+	326.0821	326.0821	0.2	1	0.9899
Dinotefuran	C7H14N4O3	+	203.1139	203.1139	0.1	1	0.9957
Dioxacarb	C11H13NO4	+	224.0917	224.0919	0.8	1	0.9978
Dioxathion	C12H26O6P2S4	+	474.0426	474.0426	0	1	0.9900
Diphenamid	C16H17NO	+	240.1383	240.1383	0.1	1	0.9992
Diphenylamine	C12H11N	+	170.0964	170.0965	0.3	1	0.9952
Dipropetryn	C11H21N5S	+	256.159	256.1588	0.8	1	0.9983
Disulfoton	C8H19O2PS3	+	275.0358	275.0355	0.9	1	0.9935
Ditalimfos	C12H14NO4PS	+	300.0454	300.0452	0.6	1	0.9967
Dithianon	C14H4N2O2S2	+	314.0052	314.0064	3.6	10	0.9235
Dithiopyr	C15H16F5NO2S2	+	402.0615	402.0617	0.3	10	0.9866
Diuron	C9H10Cl2N2O	+	233.0243	233.0244	0.6	1	0.9947
DNOC	C7H6N2O5	-	197.0204	197.0205	1.5	1	0.9948
Dodemorph	C18H35NO	+	282.2791	282.279	0.6	1	0.9946
Doramectin	C50H74O14	+	916.5417	916.5418	0.1	10	0.9888
Edifenphos	C14H15O2PS2	+	311.0324	311.0322	0.6	1	0.9952
EPN	C14H14NO4PS	+	341.0719	341.0721	0.3	1	0.9983
Epoxiconazole	C17H13C FN3O	+	330.0804	330.0803	0.2	1	0.9953
Eprinomectin B1a	C50H75NO14	+	914.526	914.526	0	1	0.9852

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Eprinomectin B1b	C49H73NO14	+	900.5104	900.5131	3	10	0.9738
EPTC (eptam)	C9H19NOS	+	190.126	190.1261	0.2	1	0.9938
Esprocarb	C15H23NOS	+	266.1573	266.1572	0.4	1	0.9981
Etaconazol	C14H15Cl2N3O2	+	328.0614	328.0613	0.3	1	0.9980
Ethaboxam	C14H16N4OS2	+	321.0838	321.0839	0.3	1	0.9907
Ethalfluralin	C13H14F3N3O4	+	334.1009	334.0994	4.6	1	0.9845
Ethidimuron	C7H12N4O3S2	+	265.0424	265.0422	0.6	1	0.9805
Ethiofencarb	C11H15NO2S	+	226.0896	226.0898	0.8	1	0.9987
Ethiolate	C7H15NOS	+	162.0947	162.0947	0.2	1	0.9960
Ethion	C9H22O4P2S4	+	384.9949	384.9948	0.1	1	0.9914
Ethion monoxon	C9H22O5P2S3	+	369.0177	369.0177	0	1	0.9975
Ethiprole	C13H9Cl2F3N4OS	+	414.0165	414.0164	0.1	1	0.9817
Ethirimol	C11H19N3O	+	210.1601	210.1602	0.4	1	0.9984
Ethofumesate	C13H18O5S	+	304.1213	304.1213	0.1	1	0.9986
Ethoprop	C8H19O2PS2	+	243.0637	243.0637	0	1	0.9865
Ethoxyquin	C14H19NO	+	218.1539	218.1541	0.7	1	0.9967
Etobenzanid	C16H15Cl2NO3	+	340.0502	340.0502	0.1	1	0.9969
Etofenprox	C25H28O3	+	394.2377	394.2379	0.6	1	0.9928
Etoxazole	C21H23F2NO2	+	360.177	360.1769	0.1	1	0.9976
Etrimfos	C10H17N2O4PS	+	293.0719	293.0718	0.6	1	0.9982
Famoxadone	C22H18N2O4	+	392.1605	392.1603	0.4	1	0.9937
Famphur	C10H16NO5PS2	+	343.0546	343.0531	4.4	1	0.9973
Famphur oxon	C10H16NO6PS	+	327.0774	327.0775	0.2	1	0.9955
Fenamidone	C17H17N3OS	+	312.1165	312.1163	0.6	1	0.9986
Fenamiphos	C13H22NO3PS	+	304.1131	304.113	0.3	1	0.9944
Fenamiphos sulfone	C13H22NO5PS	+	336.1029	336.1029	0.1	1	0.9924
Fenamiphos sulfoxide	C13H22NO4PS	+	320.108	320.1079	0.2	1	0.9936
Fenarimol	C17H12Cl2N2O	+	331.04	331.0399	0.3	1	0.9825
Fenazaquin	C20H22N2O	+	307.1805	307.1805	0.1	1	0.9881
Fenbuconazole	C19H17ClN4	+	337.1215	337.1214	0.1	1	0.9970
Fenhexamid	C14H17Cl2NO2	+	302.0709	302.0709	0.2	1	0.9965
Fenitrothion	C9H12NO5PS	+	295.0512	295.0517	1.6	10	0.9971
Fenoxanil	C15H18Cl2N2O2	+	346.1084	346.1083	0.1	1	0.9914
Fenoxycarb	C17H19NO4	+	302.1387	302.1386	0.5	1	0.9943
Fenpiclonil	C11H6Cl2N2	+	254.0246	254.0246	0.3	1	0.9817
Fenpropathrin	C22H23NO3	+	350.1751	350.1759	2.4	1	0.9954
Fenpropimorph	C20H33NO	+	304.2635	304.2633	0.5	1	0.9919
Fenpyroximate	C24H27N3O4	+	422.2074	422.2074	0.2	1	0.9966
Fensulfothion	C11H17O4PS2	+	309.0379	309.0378	0.3	1	0.9969
Fenthion	C10H15O3PS2	+	279.0273	279.0286	4.5	1	0.9941
Fenthion oxon	C10H15O4PS	+	263.0501	263.0501	0.1	1	0.9975
Fenthion sulfone	C10H15O5PS2	+	328.0437	328.0439	0.6	1	0.9993
Fenthion sulfoxide	C10H15O4PS2	+	295.0222	295.022	0.6	1	0.9957
Fenuron	C9H12N2O	+	165.1022	165.1022	0.4	1	0.9998
Fenvalerate	C25H22ClNO3	+	437.1627	437.1629	0.7	10	0.9919
Fipronil	C12H4Cl2F6N4OS	-	434.9314	434.9316	0.4	1	0.9968
Flonicamid	C9H6F3N3O	-	228.039	228.0384	2.6	1	0.9989
Florasulam	C12H8F3N5O3S	+	360.0373	360.0374	0.2	1	0.9956
Fluazinam	C13H4Cl2F6N4O4	-	462.9441	462.945	1.9	1	0.9946
Flubendiamide	C23H22F7IN2O4S	-	681.016	681.0154	0.9	1	0.9917
Flucarbazone	C12H11F3N4O6S	+	414.069	414.069	0	1	0.9924
Fluchloralin	C12H13ClF3N3O4	+	373.0885	373.0894	2.4	10	0.9605
Flucythrinate	C26H23F2NO4	+	469.1933	469.1933	0.2	1	0.9932
Fludioxonil	C12H6F2N2O2	+	266.0736	266.0736	0.1	1	0.9749
Flufenacet	C14H13F4N3O2S	+	364.0737	364.0736	0.4	1	0.9980
Flufenoxuron	C21H11ClF6N2O3	+	489.0435	489.0436	0.1	1	0.9929
Flumetralin	C16H12ClF4N3O4	+	422.0525	422.0537	2.8	25	0.9917
Flumetsulam	C12H9F2N5O2S	+	326.0518	326.0516	0.6	1	0.9988
Flumioxazin	C19H15FN2O4	+	355.1089	355.1089	0	10	0.9677

LC/MS data for Pesticide Standards *(Table 1 continued)*

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Fluometuron	C10H11F3N2O	+	233.0896	233.0897	0.4	1	0.9983
Fluopicolide	C14H8Cl3F3N2O	+	382.9727	382.9728	0.2	1	0.9911
Fluorochloridone	C12H10Cl2F3NO	+	329.043	329.0431	0.4	1	0.9837
Fluorodifen	C13H7F3N2O5	+	346.0645	346.0652	2	10	0.9963
Fluoxastrobin	C21H16C FN4O5	+	459.0866	459.0865	0.3	1	0.9983
Fluquinconazole	C16H8Cl2FN5O	+	376.0163	376.0163	0	10	0.9939
Fluroxypyr	C7H5Cl2FN2O3	-	252.9588	252.9581	2.7	10	0.9928
Flusilazole	C16H15F2N3Si	+	316.1076	316.1076	0.1	1	0.9932
Flutolanil	C17H16F3NO2	+	341.1471	341.1471	0	1	0.9948
Flutriafol	C16H13F2N3O	+	302.11	302.11	0	1	0.9942
Fluvalinate ?	C26H22C F3N2O3	+	520.1609	520.1613	0.7	10	0.9968
Fonophos	C10H15OPS2	+	247.0375	247.0375	0.2	1	0.9165
Fonophos O-analog	C10H15O2PS	+	231.0603	231.0601	0.8	10	0.9526
Forchlorfenuron	C12H10C N3O	+	248.0585	248.0585	0.1	1	0.9967
Formasafen	C15H10C F3N2O6S	-	436.9827	436.9817	2.2	1	0.9972
Formetanate	C11H15N3O2	+	239.1503	239.1503	0.1	1	0.9981
Fosthiazate	C9H18NO3PS2	+	284.0539	284.0538	0.2	1	0.9958
Fuberidazole	C11H8N2O	+	185.0709	185.0708	0.9	1	0.9972
Furalaxyl	C17H19NO4	+	302.1387	302.1386	0.5	1	0.9943
Furathiocarb	C18H26N2O5S	+	383.1635	383.1635	0.1	1	0.9980
Griseofulvin	C17H17ClO6	+	353.0786	353.0787	0.2	1	0.9968
Halofenozide	C18H19C N2O2	-	329.1062	329.1063	0.3	1	0.9984
Haloxyfop-methyl	C16H13C F3NO4	+	376.0558	376.0556	0.4	1	0.9965
Heptenophos	C9H12ClO4P	+	251.0235	251.0235	0.2	10	0.9983
Hexaconazole	C14H17Cl2N3O	+	314.0821	314.082	0.4	1	0.9947
Hexaflumuron	C16H8Cl2F6N2O3	-	458.9743	458.9745	0.4	1	0.9834
Hexazinone	C12H20N4O2	+	253.1659	253.1658	0.5	1	0.9975
Hexythiazox	C17H21C N2O2S	+	353.1085	353.1084	0.4	1	0.9807
Hydramethylnon	C25H24F6N4	+	495.1978	495.1976	0.3	1	0.9965
Imazalil	C14H14Cl2N2O	+	297.0556	297.0555	0.4	1	0.9960
Imazamox	C15H19N3O4	+	306.1448	306.1447	0.5	1	0.9962
Imazapyr	C13H15N3O3	+	262.1186	262.1185	0.3	1	0.9972
Imazaquin	C17H17N3O3	+	312.1343	312.1341	0.5	1	0.9970
Imibenconazole	C17H13Cl3N4S	+	410.9999	411	0.2	1	0.9909
Imidacloprid	C9H10ClN5O2	+	256.0596	256.0595	0.5	1	0.9983
Imiprothrin	C17H22N2O4	+	319.1652	319.1651	0.4	1	0.9663
Inabenifide	C19H15C N2O2	+	339.0895	339.0895	0	1	0.9974
Indanofan	C20H17ClO3	+	341.0939	341.0938	0.4	1	0.9824
Indoxacarb	C22H17C F3N3O7	+	528.078	528.0779	0.2	1	0.9922
Ioxynil	C7H3I2NO	-	369.8231	369.8237	0.2	1	0.9955
Ipconazole	C18H24C N3O	+	334.1681	334.1679	0.4	1	0.9968
Iprobenfos	C13H21O3PS	+	289.1022	289.1021	0.1	1	0.9977
Iprovalicarb	C18H28N2O3	+	321.2173	321.2171	0.4	1	0.9993
Isazophos	C9H17ClN3O3PS	+	314.049	314.0489	0.3	1	0.9988
Isocarbamid	C8H15N3O2	+	186.1237	186.1237	0	1	0.9967
Isocarbophos	C11H16NO4PS	+	307.0876	307.0876	0.1	1	0.9941
Isofenfos	C15H24NO4PS	+	346.1236	346.1236	0.2	1	0.9911
Isofenfos O-analog	C15H24NO5P	+	330.1465	330.1473	2.6	10	0.9344
Isoprocarb	C11H15NO2	+	194.1176	194.1177	0.8	1	0.9978
Isopropalin	C15H23N3O4	+	310.1761	310.1761	0.2	1	0.9932
Isoprothiolane	C12H18O4S2	+	291.0719	291.0718	0.6	1	0.9961
Isoproturon	C12H18N2O	+	207.1492	207.1492	0.2	1	0.9939
Isoxaben	C18H24N2O4	+	333.1809	333.1809	0.1	1	0.9982
Isoxadifen-ethyl	C18H17NO3	+	296.1281	296.1281	0	1	0.9968
Isoxaflutole	C15H12F3NO4S	+	377.0777	377.0779	0.4	1	0.9919
Isoxathion	C13H16NO4PS	+	314.061	314.0608	0.7	1	0.9895
Ivermectin B1a	C48H74O14	+	892.5417	892.5415	0.2	10	0.9915
Ivermectin B1b	C47H72O14	+	883.4814	883.4818	0.4	50	0.9695
Kresoxim-methyl	C18H19NO4	+	314.1387	314.1386	0.2	1	0.9969

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Lactofen	C19H15ClF3NO7	+	479.0827	479.0828	0.1	1	0.9883
Linuron	C9H10Cl2N2O2	+	249.0192	249.0191	0.3	1	0.9977
Lufenuron	C17H8Cl2F8N2O3	+	510.9857	510.9833	4.7	1	0.9808
Malathion	C10H19O6PS2	+	348.0699	348.07	0.4	1	0.9950
Malathion O-analog	C10H19O7PS	+	315.0662	315.0661	0.2	1	0.9948
Mandipropamid	C23H22ClNO4	+	412.131	412.131	0.1	1	0.9978
Mefenacet	C16H14N2O2S	+	299.0849	299.0848	0.4	1	0.9985
Mefluidide	C11H13F3N2O3S	+	328.0937	328.0937	0.1	1	0.9987
Mepanipyrim	C14H13N3	+	224.1182	224.1184	0.6	1	0.9887
Mephospholan	C8H16NO3PS2	+	270.0382	270.038	0.6	1	0.9915
Mepronil	C17H19NO2	+	270.1489	270.1487	0.4	1	0.9938
Mesotrione	C14H13NO7S	+	340.0486	340.0502	4.9	1	0.9952
Metaflumizone	C24H16F6N4O2	-	505.1105	505.1106	0.1	1	0.9745
Metalaxyl	C15H21NO4	+	280.1543	280.1542	0.6	1	0.9988
Metazachlor	C14H16ClN3O	+	278.1055	278.1054	0.3	1	0.9984
Metconazole	C17H22ClN3O	+	320.1524	320.1523	0.4	1	0.9881
Methabenzthiazuron	C10H11N3OS	+	222.0696	222.0698	0.9	1	0.9982
Methacrifos	C7H13O5PS	+	258.056	258.0559	0.1	1	0.9958
Methamidophos	C2H8NO2PS	+	142.0086	142.0087	0.4	1	0.9990
Methidathion	C6H11N2O4PS3	+	319.9957	319.9956	0.2	1	0.9971
Methiocarb	C11H15NO2S	+	226.0896	226.0898	0.8	1	0.9987
Methomyl	C5H10N2O2S	+	163.0536	163.0534	0.9	1	0.9991
Methoprotryne	C11H21N5OS	+	272.154	272.1537	1	1	0.9978
Methoxyfenozide	C22H28N2O3	+	369.2173	369.2172	0.2	1	0.9935
Metobromuron	C9H11BrN2O2	+	259.0077	259.0077	0.2	1	0.9948
Metofluthrin	C18H20F4O3	-	359.1276	359.1277	0.2	1	0.9887
Metolachlor	C15H22ClNO2	+	284.1412	284.1411	0.1	1	0.9981
Metominostrobin(E-)	C16H16N2O3	+	285.1234	285.1232	0.7	1	0.9957
Metosulam	C14H13Cl2N5O4S	+	418.0138	418.0137	0.3	1	0.9924
Metoxuron	C10H13ClN2O2	+	229.0738	229.074	0.6	1	0.9995
Metrafenone	C19H21BrO5	+	409.0645	409.0643	0.4	1	0.9963
Metribuzin	C8H14N4OS	+	215.0961	215.0963	0.7	1	0.9969
Mevinphos	C7H13O6P	+	242.0788	242.0788	0.1	1	0.9977
Mexacarbate	C12H18N2O2	+	223.1441	223.1443	0.7	1	0.9991
Milbemectin A3	C31H44O7	+	546.3425	546.3421	0.8	10	0.9819
Milbemectin A4	C32H46O7	+	560.3582	560.3584	0.4	1	0.9905
Molinate	C9H17NOS	+	188.1104	188.1104	0.2	1	0.9881
Monocrotophos	C7H14NO5P	+	224.0682	224.0685	1	1	0.9989
Monolinuron	C9H11ClN2O2	+	215.0582	215.0583	0.7	1	0.9977
Moxidectin	C37H53NO8	+	640.3844	640.3847	0.5	1	0.9966
Myclobutanil	C15H17ClN4	+	289.1215	289.1214	0.1	1	0.9940
Naled	C4H7Br2Cl2O4P	+	395.8164	395.8164	0.1	10	0.9908
Naphthol	C10H8O	+	145.0648	145.0648	0.2	1	0.9939
Napropamide	C17H21NO2	+	272.1645	272.1644	0.5	1	0.9933
Naptalam sodium	C18H12NNaO3	+	331.1053	331.1067	4.2	1	0.9931
Neburon	C12H16Cl2N2O	+	275.0713	275.0711	0.5	1	0.9941
Nitenpyram	C11H15ClN4O2	+	271.0956	271.0948	3.2	1	0.9876
Nitralin	C13H19N3O6S	+	346.1067	346.1083	4.6	1	0.9824
Nitrothal-isopropyl	C14H17NO6	+	313.1394	313.1385	3.5	10	0.8345
Norflurazon	C12H9ClF3N3O	+	304.0459	304.0458	0.3	1	0.9858
Novaluron	C17H9ClF8N2O4	-	491.005	491.0053	0.6	1	0.9902
Noviflumuron	C17H7Cl2F9N2O3	-	526.9617	526.9613	0.7	1	0.9759
Nuarimol	C17H12ClFN2O	+	315.0695	315.0693	0.5	1	0.9907
Octhilinone (2-Octyl-4-isothiazoline-3-one)	C11H19NOS	+	214.126	214.1262	0.8	1	0.9977
Ofurace	C14H16ClNO3	+	299.1157	299.1156	0.2	1	0.9974
Omethoate (Dimethoate oxon)	C5H12NO4PS	+	214.0297	214.0298	0.4	1	0.9997
Orbencarb	C12H16ClNOS	+	258.0714	258.0712	0.6	1	0.9969

LC/MS data for Pesticide Standards *(Table 1 continued)*

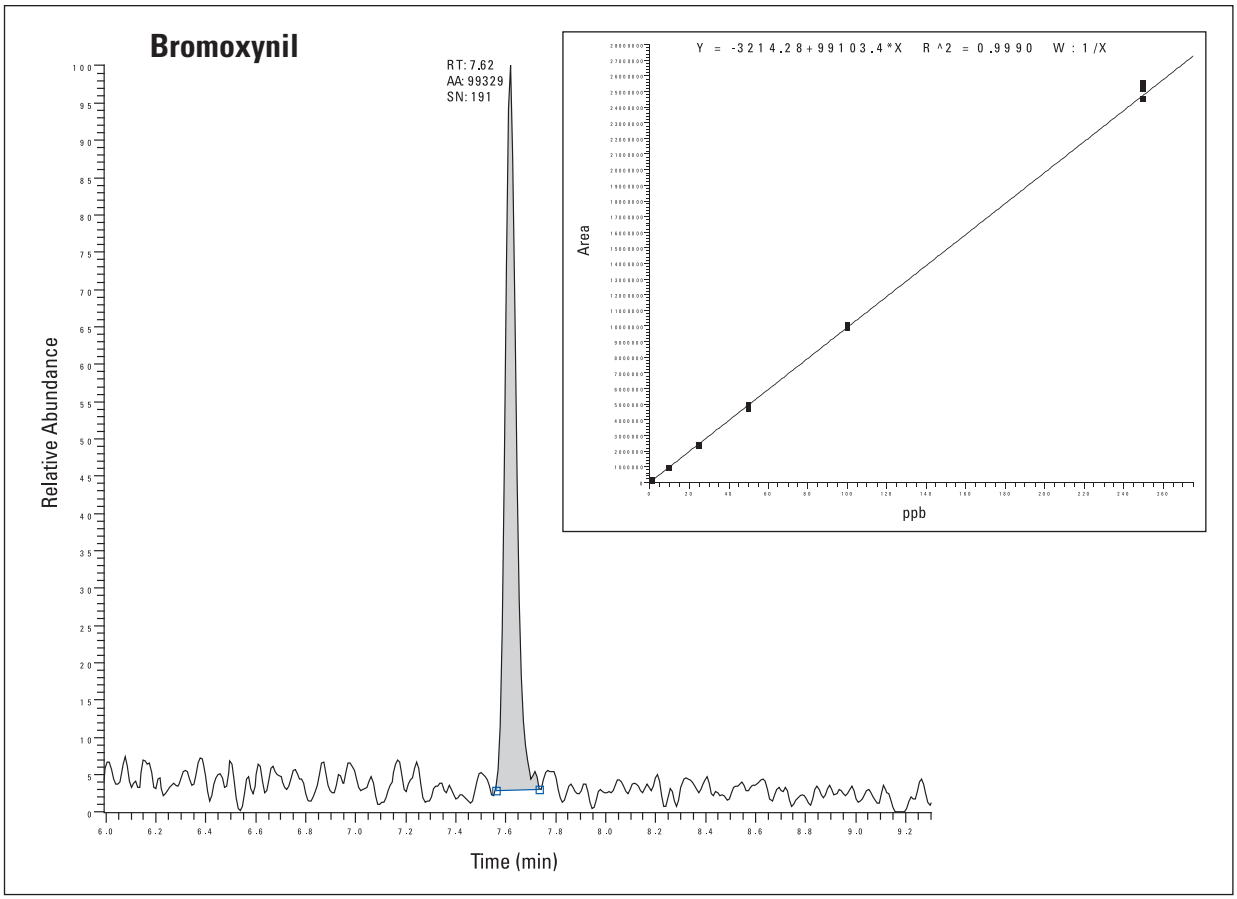
Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Oryzalin	C12H18N4O6S	-	345.0874	345.0876	0.5	1	0.9895
Oxadiazon	C15H18Cl2N2O3	+	362.1033	362.1032	0.1	1	0.9969
Oxadixyl	C14H18N2O4	+	279.1339	279.1339	0	1	0.9994
Oxamyl	C7H13N3O3S	+	237.1016	237.1017	0.5	1	0.9997
Paclobutrazol	C15H20C N3O	+	294.1368	294.1367	0.3	1	0.9955
Parathion	C10H14NO5PS	+	309.0669	309.0679	3.2	10	0.9645
Parathion methyl oxon	C8H10NO6P	+	265.0584	265.0585	0.5	10	0.9903
Parathion oxon	C10H14NO6P	+	293.0897	293.0896	0.3	1	0.9928
Pebulate	C10H21NOS	+	204.1417	204.1417	0.1	1	0.9929
Penconazole	C13H15Cl2N3	+	284.0716	284.0715	0.4	1	0.9931
Pencycuron	C19H21C N2O	+	329.1415	329.1414	0.5	1	0.9986
Pendimethalin	C13H19N3O4	+	282.1448	282.1448	0.2	10	0.9949
Penoxsulam	C16H14F5N5O5S	+	484.0709	484.071	0.3	1	0.9928
Penthiopyrad	C16H20F3N3OS	+	360.1352	360.1352	0.1	1	0.9935
Permethrin(cis-)	C21H20Cl2O3	+	408.1128	408.1129	0.2	1	0.9935
Permethrin(trans-)	C21H20Cl2O3	+	408.1128	408.1129	0.2	1	0.9935
Phenmedipham	C16H16N2O4	+	318.1448	318.1448	0	1	0.9975
Phenothrin	C23H26O3	+	368.222	368.2222	0.6	1	0.9944
Phenthoate	C12H17O4PS2	+	321.0379	321.0378	0.4	1	0.9929
Phenylphenol(o-)	C12H10O	+	188.107	188.107	0.2	1	0.9854
Phorate	C7H17O2PS3	+	261.0201	261.02	0.3	10	0.9812
Phorate oxon	C7H17O3PS	+	230.0974	230.0982	3.5	1	0.9973
Phorate oxon sulfone	C7H17O5PS2	+	277.0328	277.0327	0.5	1	0.9979
Phorate oxon sulfoxide	C7H17O4PS2	+	261.0379	261.0377	0.8	1	0.9995
Phorate sulfone	C7H17O4PS3	+	310.0365	310.0363	0.6	1	0.9951
Phorate sulfoxide	C7H17O4PS2	+	261.0379	261.0377	0.8	1	0.9995
Phosalone	C12H15C NO4PS2	+	385.0207	385.0206	0.3	1	0.9945
Phosmet	C11H12NO4PS2	+	318.0018	318.0018	0.1	1	0.9938
Phosphamidon	C10H19C NO5P	+	317.1028	317.1026	0.4	1	0.9936
Phoxim	C12H15N2O3PS	+	299.0614	299.0613	0.4	1	0.9963
Picloram	C6H3Cl3N2O2	+	240.9333	240.9331	0.7	10	0.9594
Picoxystrobin	C18H16F3NO4	+	368.1104	368.1104	0.1	1	0.9981
Pinoxaden	C23H32N2O4	+	401.2435	401.2434	0.3	1	0.9968
Piperonyl butoxide	C19H30O5	+	356.2432	356.2433	0.3	1	0.9872
Piperophos	C14H28NO3PS2	+	354.1321	354.132	0.3	1	0.9932
Pirimicarb	C11H18N4O2	+	239.1503	239.1503	0.1	1	0.9992
Pirimiphos-ethyl	C13H24N3O3PS	+	334.1349	334.1348	0.2	1	0.9977
Pirimiphos-methyl	C11H20N3O3PS	+	306.1036	306.1034	0.7	1	0.9952
Pretilachlor	C17H26C NO2	+	329.199	329.1989	0.3	1	0.9928
Probenazole	C10H9NO3S	+	224.0376	224.0378	0.9	1	0.9989
Prochloraz	C15H16Cl3N3O2	+	376.0381	376.0379	0.4	1	0.9933
Profenophos	C11H15BrClO3PS	+	372.9424	372.9424	0.1	1	0.9939
Prohexadione	C10H12O5	-	211.0612	211.0613	0.4	1	0.9936
Promecarb	C12H17NO2	+	208.1332	208.1333	0.4	1	0.9972
Prometon	C10H19N5O	+	226.1662	226.1664	0.7	1	0.9991
Prometryn	C10H19N5S	+	242.1434	242.1434	0.2	1	0.9985
Propachlor	C11H14C NO	+	212.0837	212.0839	0.8	1	0.9962
Propamocarb	C9H20N2O2	+	189.1598	189.1597	0.5	1	0.9992
Propanil	C9H9Cl2NO	-	215.9988	215.9987	0.4	1	0.9855
Propargite	C19H26O4S	+	368.189	368.1891	0.1	1	0.9961
Propazine	C9H16ClN5	+	230.1167	230.1168	0.5	1	0.9976
Propetamphos	C10H20NO4PS	+	299.1189	299.1188	0.3	1	0.9929
Propham	C10H13NO2	+	180.1019	180.1019	0.1	1	0.9131
Propiconazole	C15H17Cl2N3O2	+	342.0771	342.077	0.1	1	0.9885
Propisochlor	C15H22C NO2	+	284.1412	284.1411	0.1	1	0.9981
Propoxur	C11H15NO3	+	210.1125	210.1126	0.7	1	0.9949
Prothioconazole	C14H15Cl2N3OS	-	342.024	342.0245	1.4	1	0.9864
Prothoate	C9H20NO3PS2	+	286.0695	286.0693	0.8	1	0.9982
Pymetrozine	C10H11N5O	+	218.1036	218.1037	0.5	1	0.9985

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Pyracarbolid	C13H15NO2	+	218.1176	218.1177	0.6	1	0.9986
Pyraclofos	C14H18ClN2O3PS	+	361.0537	361.0537	0.1	1	0.9969
Pyraclostrobin	C19H18ClN3O4	+	388.1059	388.1057	0.5	1	0.9951
Pyraflufen-ethyl	C15H13Cl2F3N2O4	+	430.0543	430.0527	3.7	1	0.9833
Pyrasulfotole	C14H13F3N2O4S	-	361.0475	361.0476	0.2	1	0.9926
Pyrazone (Chloridazon)	C10H8ClN3O	+	239.0694	239.0687	3.1	50	0.9448
Pyrazophos	C14H20N3O5PS	+	374.0934	374.0933	0.3	1	0.9958
Pyridaben	C19H25ClN2OS	+	365.1449	365.145	0.3	1	0.9881
Pyridalyl	C18H14Cl4F3NO3	+	489.9753	489.9755	0.4	1	0.9958
Pyridaphenthion	C14H17N2O4PS	+	341.0719	341.0721	0.3	1	0.9938
Pyridate	C19H23ClN2O2S	+	379.1242	379.1242	0.2	1	0.9902
Pyrifenox	C14H12Cl2N2O	+	295.04	295.0397	0.7	1	0.9979
Pyrimethanil	C12H13N3	+	200.1182	200.1183	0.2	1	0.9977
Pyriproxyfen	C20H19NO3	+	322.1438	322.1438	0	1	0.9977
Pyroquilon	C11H11NO	+	174.0913	174.0913	0.5	1	0.9992
Pyroxsulam	C14H13F3N6O5S	+	435.0693	435.0693	0.1	1	0.9962
Quinalphos	C12H15N2O3PS	+	299.0614	299.0613	0.4	1	0.9963
Quinclamine	C10H6ClNO2	+	208.016	208.0158	1	1	0.9879
Quinoxyfen	C15H8Cl2FNO	+	308.004	308.0039	0.4	1	0.9980
Resmethrin	C22H26O3	+	339.1955	339.1955	0.1	1	0.9948
Rotenone	C23H22O6	+	395.1489	395.1489	0.1	1	0.9948
Saflufenacil	C17H17ClF4N4O5S	+	518.0883	518.0883	0	1	0.9868
Schradan	C8H24N4O3P2	+	287.1396	287.1389	2.7	1	0.9937
Secbumeton	C10H19N5O	+	226.1662	226.1664	0.7	1	0.9991
Sethoxydim	C17H29NO3S	+	328.1941	328.1939	0.5	1	0.9977
Siduron	C14H20N2O	+	233.1648	233.165	0.5	1	0.9996
Simazine	C7H12ClN5	+	202.0854	202.0855	0.3	1	0.9963
Simeconazole	C14H20FN3OSi	+	294.1432	294.1431	0.5	1	0.9949
Simetryn	C8H15N5S	+	214.1121	214.1122	0.6	1	0.9986
Spinetoram	C42H69NO10	+	748.4994	748.4992	0.3	1	0.9878
Spinetoram 1	C43H69NO10	+	760.4994	760.4995	0.1	1	0.9934
Spinosad A	C41H65NO10	+	732.4681	732.468	0.2	1	0.9960
Spinosad D	C42H67NO10	+	746.4838	746.4836	0.3	1	0.9932
Spirodiclofen	C21H24Cl2O4	+	428.139	428.1389	0.2	1	0.9991
Spiromefisen	C23H30O4	+	388.2482	388.2482	0	1	0.9934
Spirotetramat	C21H27NO5	+	374.1962	374.1963	0.3	1	0.9990
Spiroxamine	C18H35NO2	+	298.2741	298.2739	0.4	1	0.9910
Sulcotrione	C14H13ClO5S	+	346.0511	346.0519	2.6	10	0.9706
Sulfentrazone	C11H10Cl2F2N4O3S	+	386.9892	386.9906	3.8	1	0.9906
Sulfotep-ethyl	C8H20O5P2S2	+	323.03	323.03	0.1	1	0.9950
Sulfuramid	C10H6F17NO2S	-	525.9775	525.9779	0.7	1	0.9828
Sulprofos	C12H19O2PS3	+	340.0623	340.0636	3.7	1	0.9950
Tebuconazole	C16H22ClN3O	+	308.1524	308.1522	0.7	1	0.9924
Tebufenozide	C22H28N2O2	+	353.2224	353.2223	0.3	1	0.9946
Tebufenpyrad	C18H24ClN3O	+	334.1681	334.1679	0.4	1	0.9968
Tebupirimphos	C13H23N2O3PS	+	319.124	319.124	0.1	1	0.9953
Tebuthiuron	C9H16N4OS	+	229.1118	229.1119	0.5	1	0.9947
Teflubenzuron	C14H6Cl2F4N2O2	-	378.967	378.9675	1.3	1	0.9785
Tefluthrin	C17H14ClF7O2	+	419.0643	419.0635	1.9	50	0.9203
Tembotrione	C17H16ClF3O6S	+	458.0647	458.0649	0.5	10	0.9866
Temephos	C16H20O6P2S3	+	484.0236	484.0236	0.1	1	0.9953
Tepraloxydim	C17H24ClNO4	-	340.1321	340.1322	0.2	1	0.9947
Terbacil	C9H13ClN2O2	-	215.0593	215.0596	1.3	1	0.9911
Terbufos	C9H21O2PS3	+	289.0514	289.052	2	1	0.9928
Terbufos oxon sulfoxide	C9H21O4PS2	+	289.0692	289.0691	0.4	1	0.9927
Terbufos sulfone	C9H21O4PS3	+	338.0678	338.0678	0.1	1	0.9963
Terbumeton	C10H19N5O	+	226.1662	226.1664	0.7	1	0.9991
Terbuthylazine	C9H16ClN5	+	230.1167	230.1168	0.5	1	0.9976
Terbutryn	C10H19N5S	+	242.1434	242.1434	0.2	1	0.9985

LC/MS data for Pesticide Standards *(Table 1 continued)*

Compound	Formula	Polarity	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOQ (ppb)	R^2
Tetrachlorvinphos	C10H9Cl4O4P	+	381.9331	381.9331	0	1	0.9973
Tetraconazole	C13H11Cl2F4N3O	+	372.0288	372.0289	0.3	1	0.9967
Tetramethrin	C19H25NO4	+	332.1856	332.1856	0.3	1	0.9977
Thiabendazole	C10H7N3S	+	202.0433	202.0433	0.4	1	0.9967
Thiacloprid	C10H9ClN4S	+	253.0309	253.0309	0.3	1	0.9975
Thiamethoxam	C8H10ClN5O3S	+	292.0266	292.0266	0.1	1	0.9908
Thiazopyr	C16H17F5N2O2S	+	397.1004	397.1003	0.1	1	0.9972
Thidiazuron	C9H8N4OS	+	221.0492	221.0492	0.4	1	0.9922
Thiofanox	C9H18N2O2S	+	236.1427	236.1428	0.5	1	0.9923
Thiometon	C6H15O2PS3	+	264.031	264.0301	3.3	10	0.9594
Thiophanate-methyl	C12H14N4O4S2	+	343.0529	343.0531	0.4	1	0.9932
Tolclofos-methyl	C9H11Cl2O3PS	+	300.9616	300.9626	3.3	25	0.8855
Tolfenpyrad	C21H22C N3O2	+	384.1473	384.1475	0.3	1	0.9878
Topramezone	C16H17N3O5S	+	364.0962	364.0944	5	1	0.9250
Tralkoxydim	C20H27NO3	+	330.2064	330.2063	0.2	1	0.9918
Tralomethrin	C22H19Br4NO3	+	678.8437	678.8447	1.4	10	0.9880
Triadimefon	C14H16C N3O2	+	294.1004	294.1003	0.4	1	0.9973
Triadimenol	C14H18C N3O2	+	296.116	296.1161	0.3	1	0.9905
Tri-allate	C10H16Cl3NOS	+	304.0091	304.009	0.3	10	0.9673
Triazophos	C12H16N3O3PS	+	314.0723	314.0721	0.7	1	0.9984
Trichlamide	C13H16Cl3NO3	+	340.0269	340.026	2.6	1	0.9986
Trichlorfon	C4H8Cl3O4P	+	256.9299	256.9298	0.1	1	0.9983
Triclopyr	C7H4Cl3NO3	-	253.9184	253.9186	0.7	1	0.9891
Tricyclazole	C9H7N3S	+	190.0433	190.0433	0.4	1	0.9996
Tridemorph	C19H39NO	+	298.3104	298.3103	0.4	1	0.9972
Trietazine	C9H16ClN5	+	230.1167	230.1168	0.5	1	0.9976
Trifloxystrobin	C20H19F3N2O4	+	409.137	409.1367	0.8	1	0.9981
Triflumizole	C15H15C F3N3O	+	346.0929	346.0928	0.1	1	0.9957
Triflumuron	C15H10C F3N2O3	-	357.0259	357.0251	2.2	1	0.9914
Trifluralin	C13H16F3N3O4	+	353.1431	353.143	0.2	10	0.9871
Triforine	C10H14Cl6N4O2	+	449.9586	449.9587	0.1	10	0.9851
Trinexapac-ethyl	C13H16O5	+	253.1071	253.1071	0.2	1	0.9871
Triticonazole	C17H20C N3O	+	318.1368	318.1367	0.3	1	0.9943
Uniconazole	C15H18C N3O	+	292.1211	292.1211	0.2	1	0.9884
Validamycin	C20H35NO13	+	498.2181	498.2172	1.9	1	0.8371
Vamidothion	C8H18NO4PS2	+	288.0488	288.0484	1.3	1	0.9984
Vamidothion sulfone	C8H18NO6PS2	+	320.0386	320.0386	0.1	1	0.9986
Vernolate	C10H21NOS	+	204.1417	204.1417	0.1	1	0.9929
Warfarin	C19H16O4	+	309.1121	309.112	0.5	1	0.9871
Zoxamide	C14H16Cl3NO2	+	336.0319	336.0318	0.4	1	0.9975

Table 1: LC/MS data for 510 pesticide standards



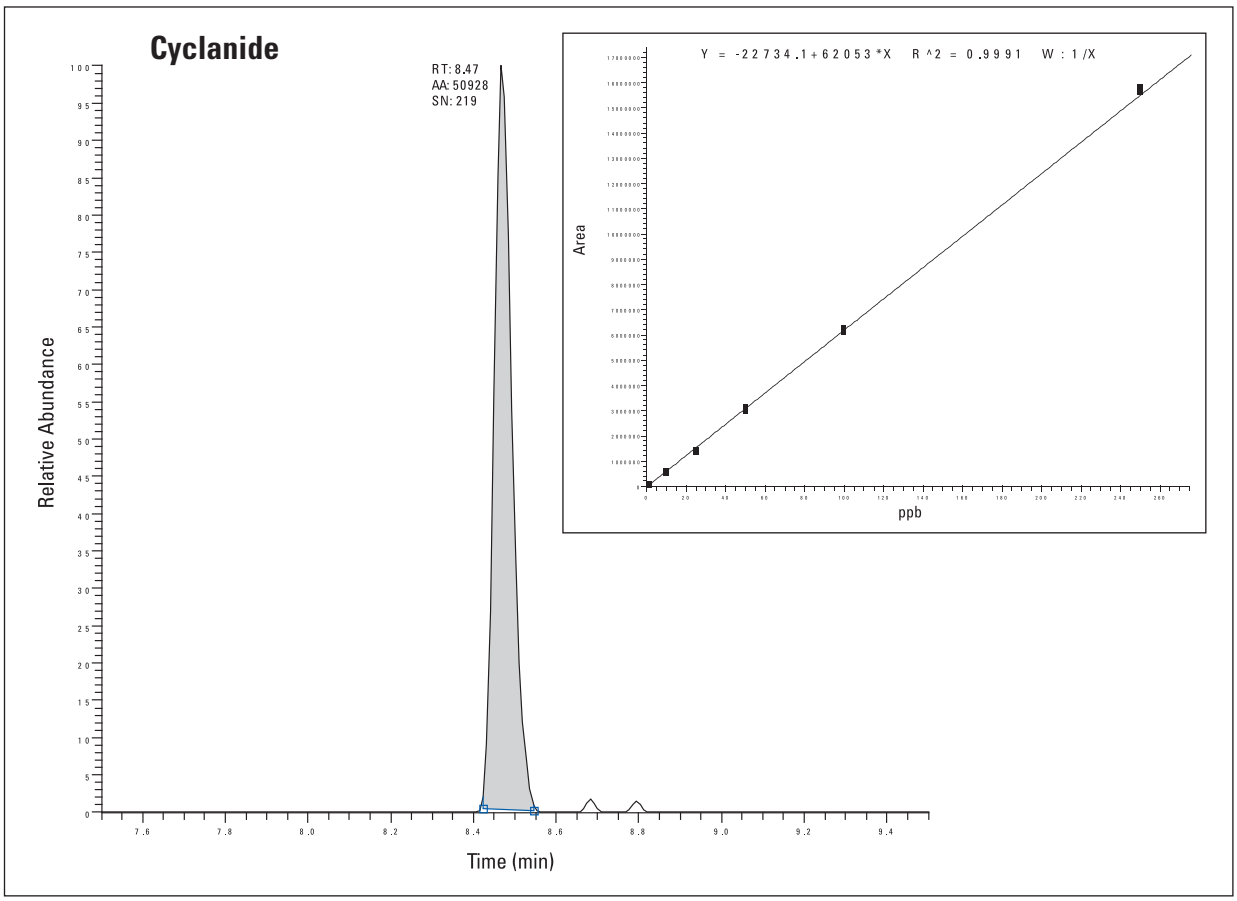
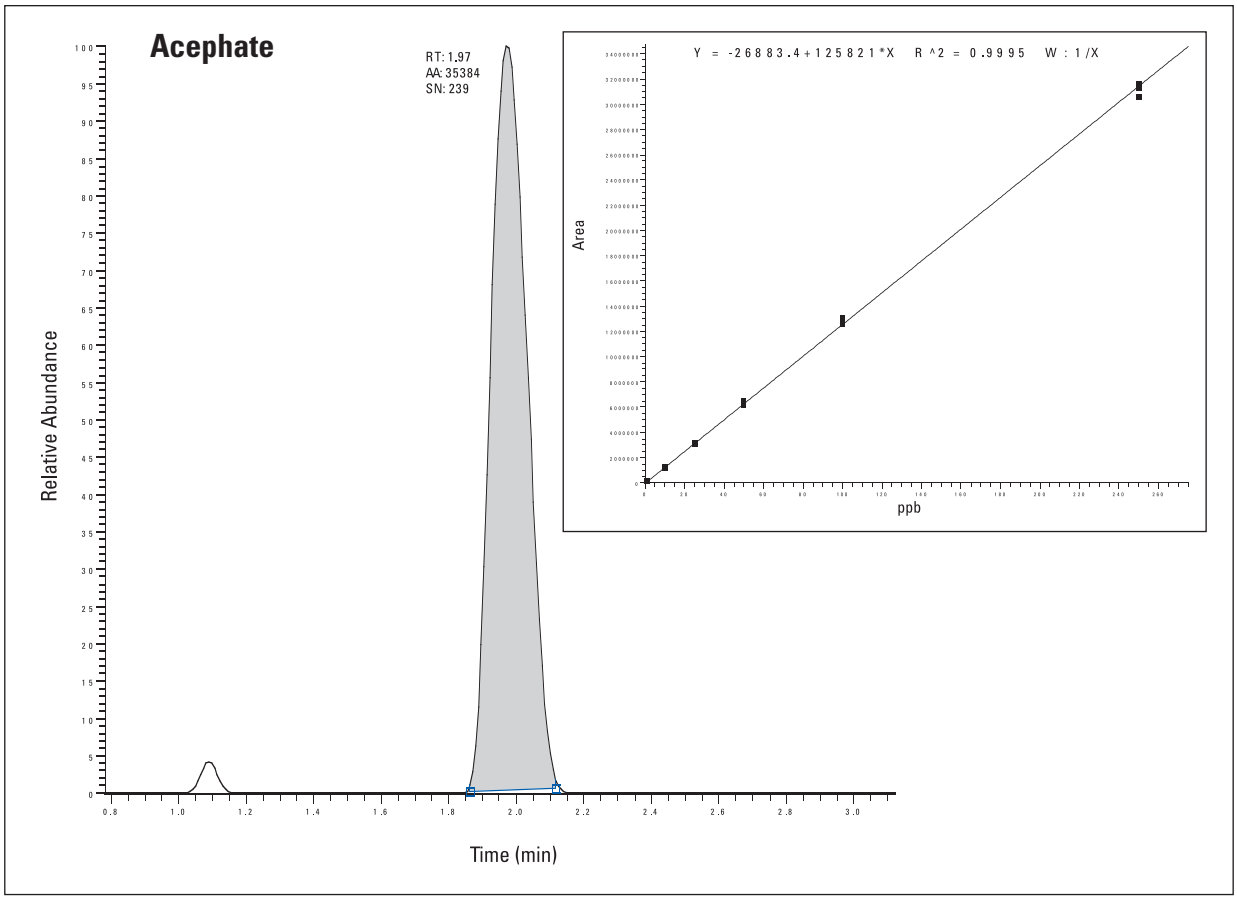


Figure 4: Extracted ion chromatograms (at 1 ppb level) and calibration curves (1-250 ppb) of eight pesticides



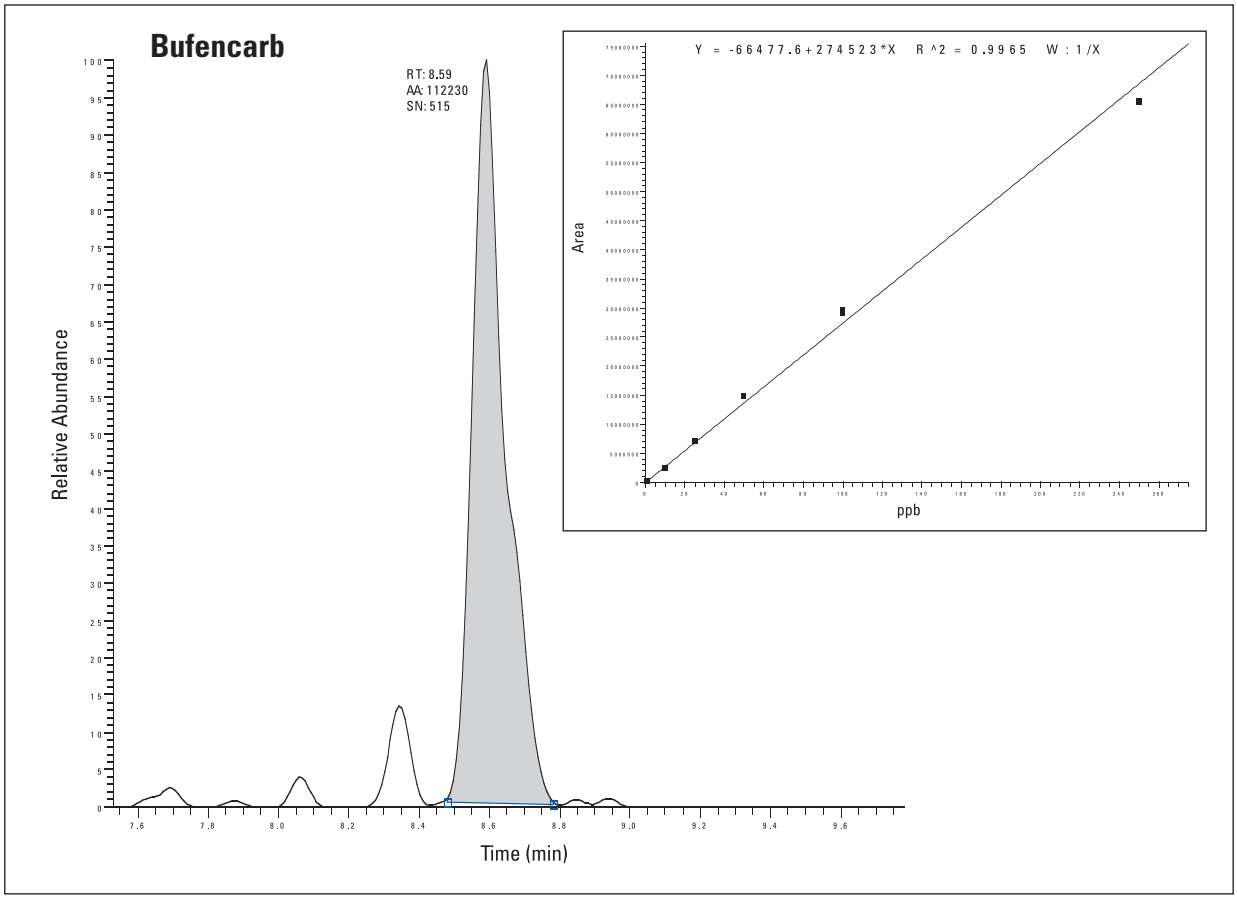
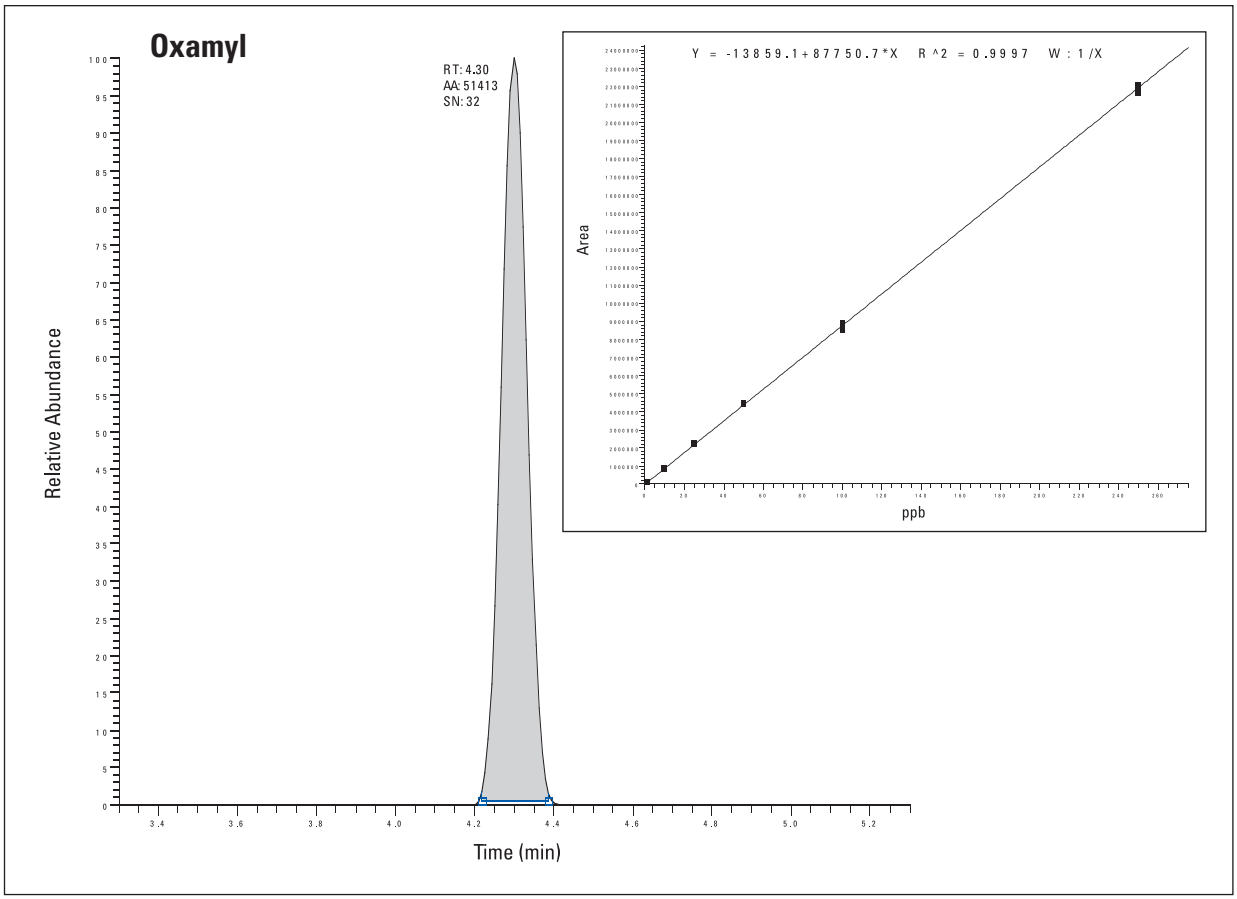


Figure 4 Continued: Extracted ion chromatograms (at 1 ppb level) and calibration curves (1-250 ppb) of eight pesticides



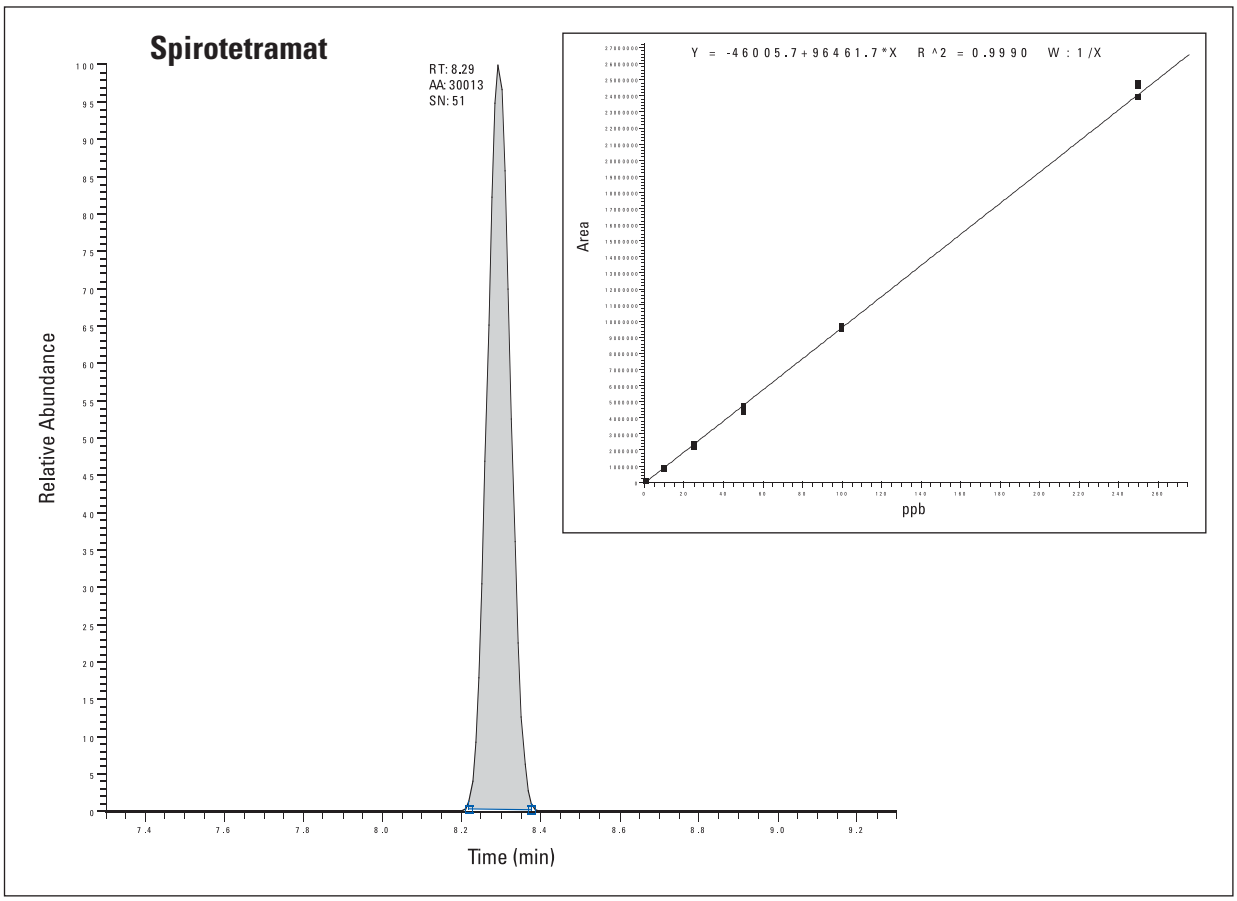
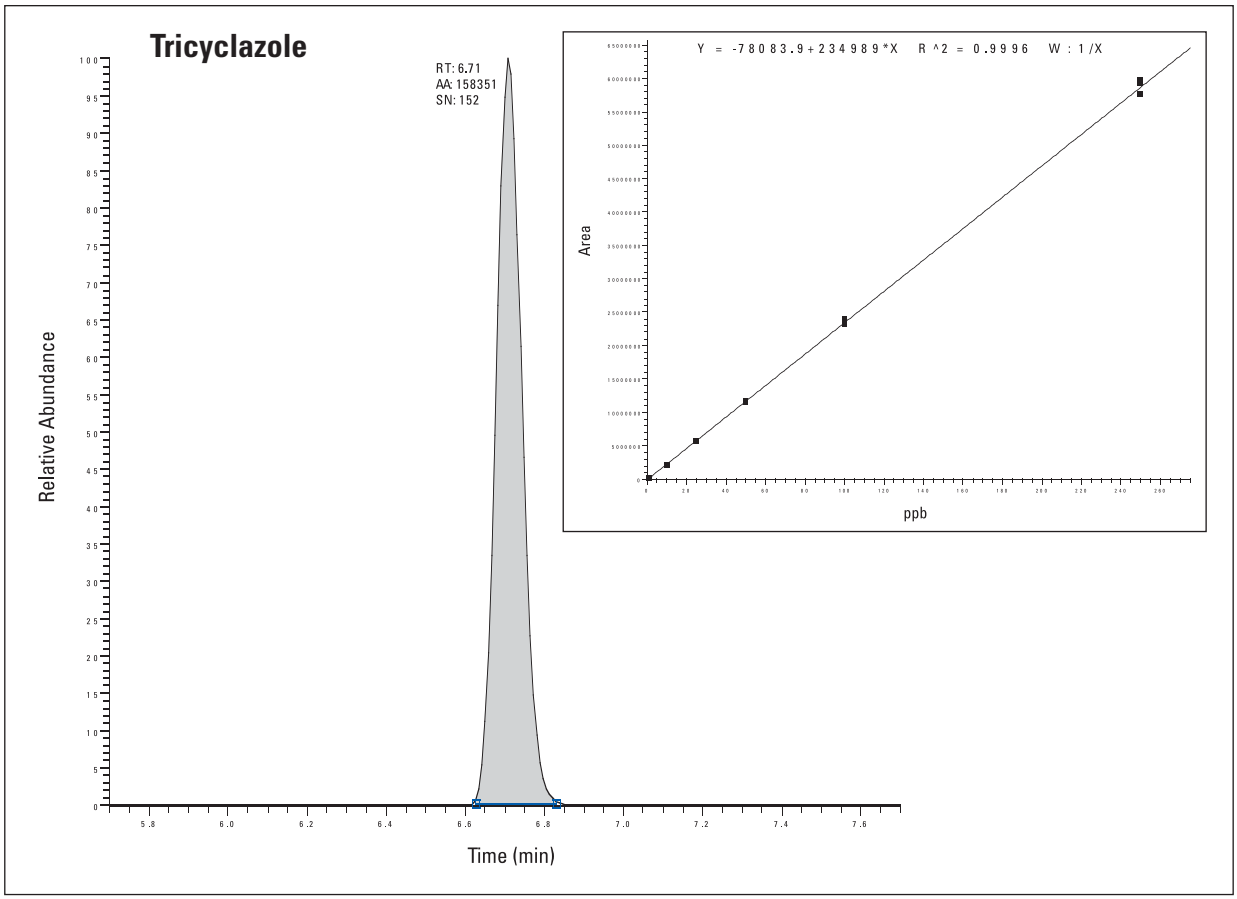


Figure 4 Continued: Extracted ion chromatograms (at 1 ppb level) and calibration curves (1-250 ppb) of eight pesticides



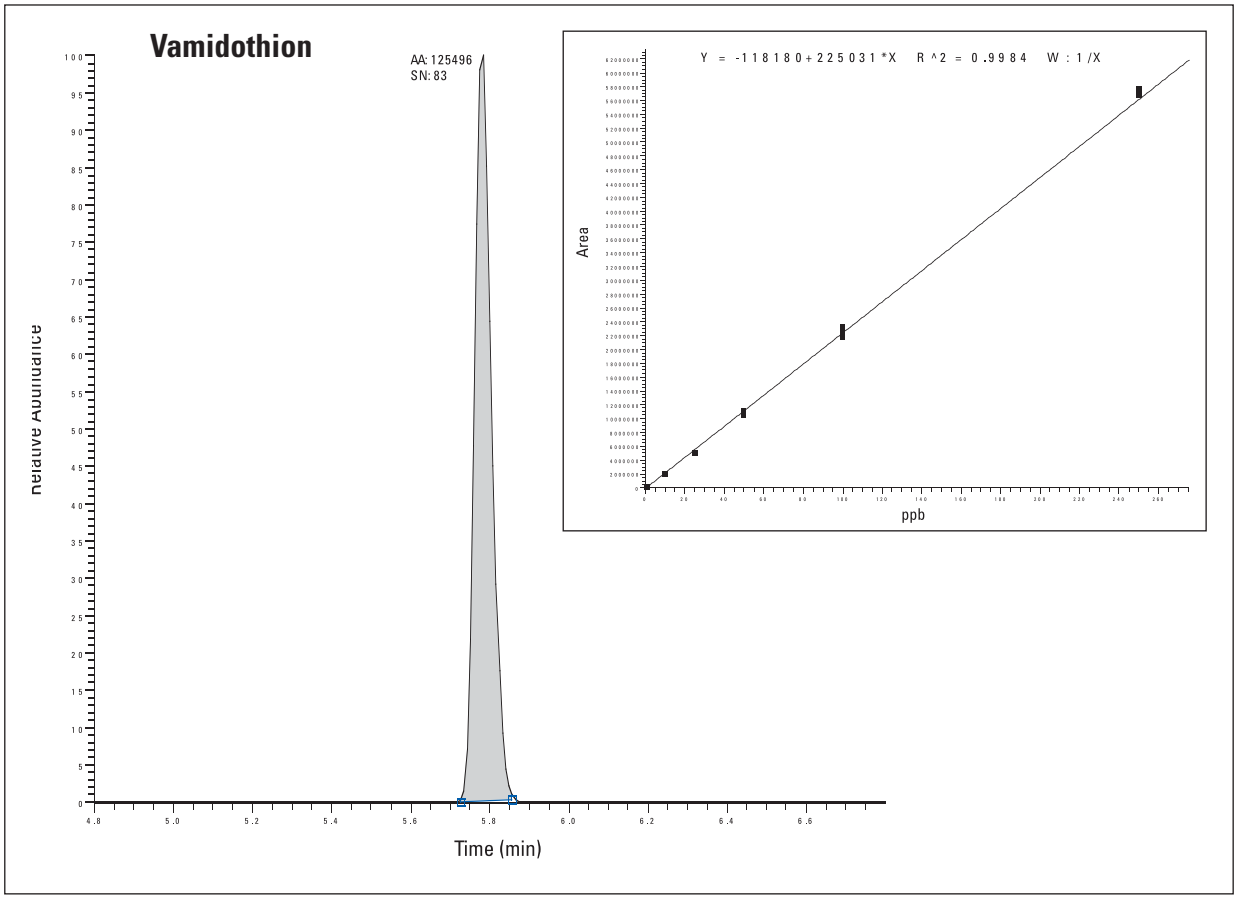


Figure 4 Continued: Extracted ion chromatograms (at 1 ppb level) and calibration curves (1-250 ppb) of eight pesticides

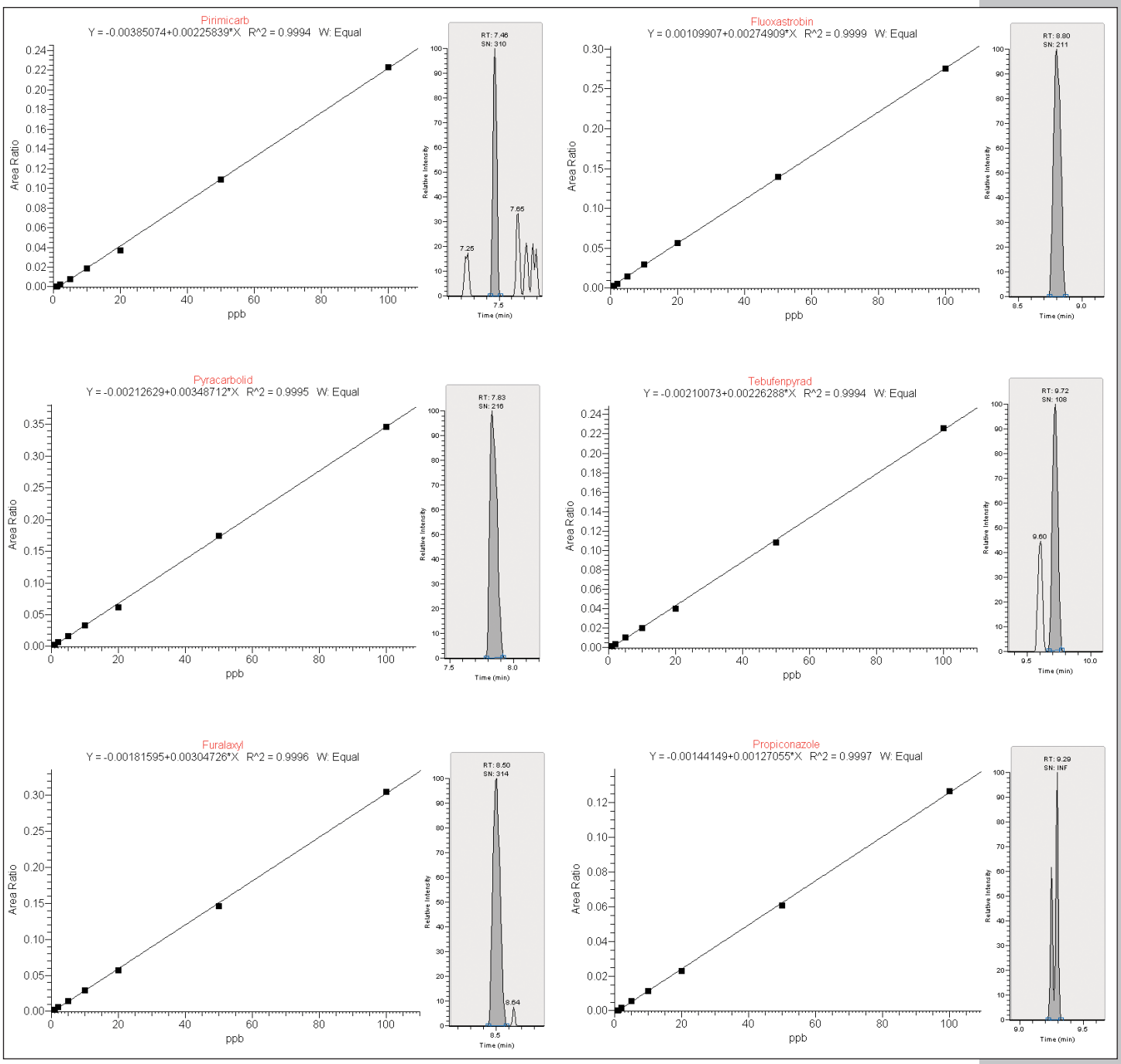


Figure 5: Extracted ion chromatograms (at 1 ppb) and calibration curves (1-250 ppb) of six pesticides extracted from spiked spinach sample

LC/MS data for representative pesticides extracted from spinach matrix *(Table 2)*

Compound	Formula	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOD (ppb)	LOQ (ppb)
Azoxystrobin	C22H17N3O5	404.1241	404.12466	1.4	0.2	0.7
Bendiocarb	C11H13NO4	224.09173	224.09169	0.2	0.2	0.7
Benthiavalicarb	C18H24FN3O3S	382.15952	382.1597	0.5	0.2	0.7
Benzoximate	C18H18ClNO5	364.09463	386.07663	0.2	0.2	0.5
Bifenazate	C17H20N2O3	301.15467	301.15457	0.3	0.3	0.9
Bupirimate	C13H24N4O3S	317.16419	317.16431	0.4	0.2	0.5
Buprofezin	C16H23N3OS	306.16346	306.16354	0.3	0.2	0.6
Butafenacil	C20H18ClF3N2	492.11437	492.11469	0.6	0.3	0.9
Carbaryl	C12H11NO2	219.1128	219.1127	0.5	0.3	0.9
Carbendazim	C9H9N3O2	192.07675	192.07684	0.5	0.2	0.7
Carbofuran	C12H15NO3	222.11247	222.11241	0.3	0.2	0.7
Carboxin	C12H13NO2S	236.07398	236.07358	1.7	0.2	0.5
Chlortoluron	C10H13ClN2O	213.07892	213.07925	1.6	0.2	0.6
Clethodim	C17H26ClNO3S	360.13947	360.13962	0.4	0.2	0.6
Clofentezine	C14H8Cl2N4	303.01988	303.01993	0.2	0.1	0.4
Cyazofamid	C13H13ClN4O2S	342.0786	342.077	4.7	0.3	0.8
Cycluron	C11H22N2O	199.18049	199.18054	0.3	0.2	0.7
Cyproconazole	C15H18ClN3O	292.12112	292.12115	0.1	0.2	0.7
Cyprodinil	C14H15N3	226.13387	226.13385	0.1	0.2	0.7
Diclobutrazol	C15H19Cl2N3O	328.09779	328.09781	0	0.2	0.5
Dicrotophos	C8H16NO5P	238.08389	238.08391	0.1	0.3	0.8
Difenoconazol	C19H17Cl2N3O3	406.07197	406.07251	1.3	0.2	0.6
Dimethoate	C5H12NO3PS2	230.0069	230.00685	0.2	0.3	0.8
Dimethomorph	C21H22ClNO4	388.13101	388.13113	0.3	0.3	0.9
Dimoxystrobin	C19H22N2O3	327.17032	327.17047	0.5	0.2	0.5
Dinotefuran	C7H14N4O3	203.11387	203.11389	0.1	0.2	0.7
Dioxacarb	C11H13NO4	203.11387	224.09169	0.2	0.2	0.7
Emamectin B1b	C49H75NO13	886.53112	886.53168	0.6	0.3	0.8
Epoxiconazole	C17H13ClFN3O	330.08039	330.08029	0.3	0.2	0.6
Etaconazole	C14H15Cl2N3O2	328.06141	328.06143	0.1	0.3	0.9
Ethiofencarb	C11H15NO2S	226.08963	226.08969	0.3	0.3	0.9
Etoxazole	C21H23F2NO2	360.17696	360.17715	0.5	0.1	0.4
Famoxadone	C22H18N2O4	392.16048	397.11591	0.1	0.2	0.7
Fenamidone	C17H17N3OS	312.11651	312.11652	0	0.2	0.6
Fenazaquin	C20H22N2O	307.18049	307.18039	0.3	0.3	0.8
Fenbuconazole	C19H17ClN4	337.12145	337.12128	0.5	0.2	0.6
Fenoxycarb	C17H19NO4	302.13868	324.12073	0.3	0.1	0.4
Fenpropimorph	C20H33NO	304.26349	304.26349	0	0.1	0.3
Fenpyroximate	C24H27N3O4	422.20743	422.20789	1.1	0.3	0.9
Fenuron	C9H12N2O	165.10224	165.10239	0.9	0.3	0.9
Flufenacet	C14H13F4N3O	364.07374	364.07401	0.7	0.2	0.6
Fluometuron	C10H11F3N2O	233.08962	233.08958	0.2	0.2	0.7
Fluoxastrobin	C21H16ClFN4O5	459.0866	459.08704	0.9	0.3	0.8
Flusiazole	C16H15F2N3Si	316.10761	316.10776	0.5	0.2	0.7
Flutolanil	C17H16F3NO2	324.12059	324.12073	0.4	0.3	0.9
Flutriafol	C16H13F2N3O	302.10995	302.10999	0.1	0.1	0.3
Forchlorfenuron	C12H10ClN3O	248.05852	248.05832	0.8	0.2	0.6
Formetanate	C11H15N3O2	239.15025	239.15018	0.3	0.2	0.5
Fuberidazole	C11H8N2O	185.07094	185.07108	0.7	0.3	0.9
Furalaxyl	C17H19NO4	302.13868	324.12073	0.3	0.1	0.4
Hexaconazole	C14H17Cl2N3O	314.08214	314.08206	0.3	0.2	0.7

Compound	Formula	Theoretical Mass (*m/z*)	Experimental Mass (*m/z*)	Mass Deviation (ppm)	LOD (ppb)	LOQ (ppb)
Hydramethylnon	C25H24F6N4	495.19779	495.19824	0.9	0.2	0.6
Imazalil	C14H14Cl2N2O	297.0556	297.05566	0.2	0.2	0.6
Iprovalicarb	C18H28N2O3	321.21727	321.21744	0.5	0.1	0.4
Isoproturon	C12H18N2O	207.14919	207.14932	0.6	0.2	0.5
Mefenacet	C16H14N2O2S	299.08487	299.08484	0.1	0.2	0.7
Mepanipyrim	C14H13N3	224.11822	224.11821	0.1	0.2	0.7
Mepronil	C17H19NO2	270.14886	270.14886	0	0.1	0.1
Metalaxyl	C15H21NO4	280.15433	280.15445	0.4	0.2	0.5
Methabenzhiazuron	C10H11N3OS	222.06956	222.06952	0.2	0.1	0.4
Methamidophos	C2H8NO2PS	142.00861	142.00865	0.3	0.2	0.5
Methiocarb	C11H15NO2S	226.08963	226.08969	0.3	0.3	0.9
Methomyl	C5H10N2O2S	163.05357	163.05357	0	0.2	0.6
Methoprotryne	C11H21N5OS	272.15396	272.15393	0.1	0.2	0.6
Methoxyfenozide	C22H28N2O3	369.21727	369.21738	0.3	0.1	0.2
Neburon	C12H16Cl2N2O	275.07125	275.07126	0	0.3	0.8
Oxadixyl	C14H18N2O4	279.13393	279.13397	0.1	0.1	0.4
Penconazole	C13H15Cl2N3	284.07158	284.07153	0.2	0.3	0.8
Pinoxaden	C23H32N2O4	401.24348	401.24393	1.1	0.1	0.1
Pirimicarb	C11H18N4O2	239.15025	239.15018	0.3	0.2	0.5
Promecarb	C12H17NO2	208.13321	208.13329	0.4	0.2	0.5
Prometon	C10H19N5O	226.16624	226.16623	0	0.2	0.5
Prometryn	C10H19N5S	242.14339	242.14348	0.4	0.2	0.5
Propamocarb	C9H20N2O2	189.15975	189.15988	0.7	0.1	0.4
Propargite	C19H26O4S	189.15975	368.18933	0.9	0.2	0.6
Propiconazole	C15H17Cl2N3O2	342.07706	342.077	0.2	0.3	0.9
Pyrimethanil	C12H13N3	200.11822	200.11826	0.2	0.2	0.6
Pyriproxyfen	C20H19NO3	322.14377	322.14392	0.5	0.2	0.6
Quinoxyfen	C15H8Cl2FNO	308.00397	308.00394	0.1	0.2	0.6
Rotenone	C23H22O6	395.14891	395.14923	0.8	0.2	0.6
Siduron	C14H20N2O	233.16484	233.16492	0.3	0.3	0.9
Simetryn	C8H15N5S	214.11209	214.11174	1.6	0.2	0.4
Spiroxamine	C18H35NO2	298.27406	298.27417	0.4	0.2	0.5
Tebuconazole	C16H22ClN3O	308.15242	308.15234	0.2	0.2	0.5
Tebufenozide	C22H28N2O2	353.22235	353.22247	0.3	0.1	0.2
Tebufenpyrad	C18H24ClN3O	334.16807	334.16821	0.4	0.2	0.7
Terbumeton	C10H19N5O	226.16624	226.16623	0	0.2	0.5
Terbutryn	C10H19N5S	242.14339	242.14348	0.4	0.2	0.5
Tetraconazole	C13H11Cl2F4N	372.02881	372.02902	0.6	0.3	0.8
Thiabendazole	C10H7N3S	202.04334	202.04344	0.5	0.2	0.6
Thiamethoxam	C8H10ClN5O3S	292.02656	292.02655	0	0.3	1
Thiobencarb	C12H16ClNOS	258.07139	280.05246	3.1	0.3	0.8
Triadimefon	C14H16ClN3O2	294.10038	294.10031	0.2	0.3	0.8
Tricyclazole	C9H7N3S	190.04334	190.04356	1.2	0.1	0.4
Trifloxystrobin	C20H19F3N2O4	409.13697	409.13745	1.2	0.2	0.6
Triflumizole	C15H15ClF3N3O	346.09285	346.09302	0.5	0.1	0.2
Triticonazole	C17H20ClN3O	318.13677	318.13687	0.3	0.3	0.8
Uniconazole	C15H18ClN3O	292.12112	292.12115	0.1	0.2	0.6
Vamidothion	C8H18NO4PS2	288.04876	288.04883	0.2	0.2	0.5
Zoxamide	C14H16Cl3NO2	336.03194	336.03189	0.1	0.3	0.9

Table 2: LC/MS data for representative pesticides extracted from spiked spinach matrix. All MS data reported below was obtained with Orbitrap MS operating in positive ion mode. LODs and LOQs were assessed using the EPA method detection limit (MDL) procedure.[9]

Conclusion

A rapid and robust U-HPLC Exactive Orbitrap MS method for multiresidue pesticide screening was developed and validated. Screening of 510 pesticides at low ppb levels was achieved within 12 minutes, and the high mass resolution and accuracy of the Exactive mass spectrometer enabled identification of all compounds. LOQs for the majority of pesticides in a standard mixture and in spiked matrix were lower than MRLs established by the EU and Japan. The Exactive LC/MS platform is ideally suited for the routine monitoring of targeted and non-targeted pesticides by regulatory laboratories.

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MZ-Analysentechnik GmbH, Barcelona-Allee 17• D-55129 Mainz

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