Application Note

Food and Beverage Testing

Analysis of Pesticides in Kale Using the Agilent 7010C Triple Quadrupole GC/MS with Agilent Bond Elut QuEChERS High Pigment dSPE with Carbon S Cleanup

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Abstract

This application note focuses on the reliable quantitation of over 100 pesticides in kale by GC/MS/MS. The workflow was demonstrated on an Agilent 8890 GC system coupled to an Agilent 7010C triple quadrupole GC/MS using a previously developed dynamic multiple reaction monitoring (dMRM) method. The kale sample preparation strategy used the QuEChERS EN 15662 method with the Agilent Bond Elut QuEChERS High Pigment dispersive SPE kit (EN like) with Carbon S cleanup.

Introduction

Food safety testing is paramount in today's regulated environment. Much of the food we eat and enjoy today is provided through complex global systems of food production, processing, and distribution. Analytical testing at every step along the supply chain is essential to ensure food safety and quality. The Agilent multiclass, multiresidue methods based on GC/MS deliver routine monitoring, high-throughput, sensitive detection levels, and rapid quantitative analysis for hundreds of pesticides in a single sample. The 7010C triple quadrupole GC/MS maintains the benefits of the multiclass, multiresidue methods.

The QuEChERS method is the industry standard for pesticide extraction and cleanup for a wide variety of food samples. As part of the QuEChERS methodology, the dispersive solid phase extraction (dSPE) cleanup is chosen based upon the matrix that is extracted. The sorbents within the selected dSPE are specified to remove other parts of the matrix while minimizing pesticide loss. Graphitized carbon black (GCB) has widely been used in sample preparation for efficient pigment removal.[1,2] Although GCB has been shown to be efficient in pigment removal, it also causes unwanted analyte loss, especially for compounds with planar structure. Agilent Carbon S sorbent is an advanced hybrid carbon material with optimized carbon content and pore structure. Compared to GCB, the improved sorbent provides equivalent or better pigment removal from plant-origin sample matrices and significantly improves sensitive analyte recoveries. As a result, Carbon S sorbent delivers a better balance between analyte recovery and matrix pigment-removal efficiency than traditional GCB sorbent.[3,4]

Experimental

Sample preparation

Organic kale was analyzed via the QuEChERS EN 15662 methodology with the High Pigment dSPE (EN like) with Carbon S (part number 5610-2074 and 5610-2076) tubes. The full procedure can be found in the Agilent application note by Westland (2022).[5]

Instrumentation

The study was performed using an Agilent 8890 GC coupled with an Agilent 7010C triple quadrupole GC/MS (Figure 1). The GC system was equipped with an Agilent 7693A automatic liquid sampler (ALS) tower and tray, a multimode inlet (MMI), an electronic pneumatic control (EPC), and an Agilent purged Ultimate union (PUU) for backflush system. Agilent MassHunter Workstation software was used for data acquisition and analysis. The GC/TQ instrument conditions are provided in Table 1.[6] The target and ISTD compound MRM parameters are listed in Appendix 1.

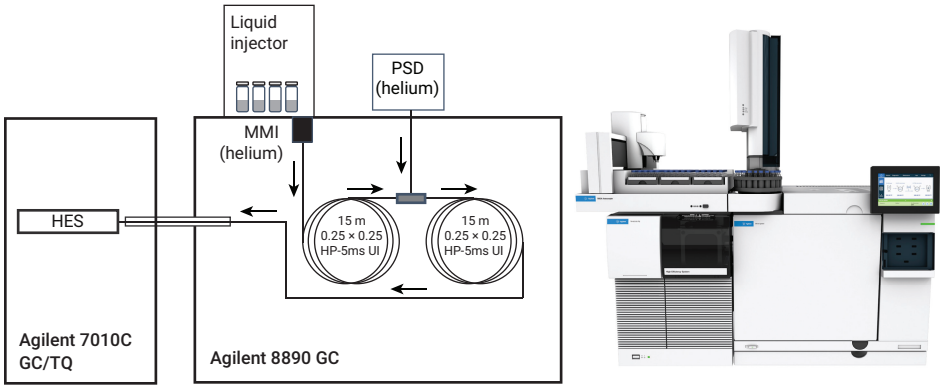

Figure 1. The Agilent 7010C triple quadrupole GC/MS (GC/TQ) coupled with an Agilent 8890 GC.

Table 1. GC/MS conditions for pesticide quantitation.

Multimode Inlet (MMI)	
Mode	Splitless
Purge Flow to Split Vent	60 mL/min at 0.75 min
Injection Volume (L1)	1.0 µL
Injection	Reversed three-layer switch (L3, L1, L2)
L1 Air Gap	0.2 µL
L2 Volume	1 µL
L2 Air Gap	0.2 µL
L3 Volume	1 µL
L3 Air Gap	0.2 µL
Inlet Temperature	280 °C
Type Carrier Gas	Helium
Inlet Liner	Agilent Ultra Inert inlet liner, splitless, dimpled, 2 mm id (p/n 5190-2297)
Oven	
Initial Oven Temperature	60 °C
Initial Oven Hold	1 min
Ramp Rate 1	40 °C/min
Final Temperature 1	170 °C
Final Hold	0 min
Ramp Rate	10 °C/min
Final Temperature 2	310 °C
Final Hold	2.25 min
Total Run Time	20 min
Postrun Time	1.5 min
Equilibration Time	0.5 min

Columns	
Column 1	Agilent J&W HP-5ms Ultra Inert, 15 m × 0.25 mm, 0.25 µm (p/n 19091S-431UI)
Control Mode	Constant flow
Flow	1.205 mL/min
Inlet Connection	MMI
Outlet Connection	PSD (PUU)
Postrun Flow (Backflushing)	–7.793 mL/min
Column 2	HP-5ms Ultra Inert, 15 m × 0.25 mm, 0.25 µm (p/n 19091S-431UI)
Control Mode	Constant flow
Flow	1.405 mL/min
Inlet Connection	PSD (PUU)
Outlet Connection	MSD
Postrun Flow (Backflushing)	8.203 mL/min
MSD	
Model	7010C
Source	HES
Tune	atunes.eihs.tune.xml
Mode	dMRM
Solvent Delay	3.75 min
EM Voltage Gain Mode	10
Quad Temperature (MS1 and MS2)	150 °C
Source Temperature	280 °C
Transfer Line Temperature	280 °C
He Quench Gas	2.25 mL/min
N_2 Collision Gas	1.5 mL/min

Results and discussion

Following matrix-matched linearity with an R^2 >0.990 over a calibration range of 0.5 to 50 parts per billion (ppb) (w/v) for all target pesticides, the pesticide recoveries were analyzed at both the pre- and postspiked values of 24 ppb. Figure 2 shows an MRM chromatogram of the 150 compounds prespiked at 24 ppb in kale.

Quantitation by matrix-matched calibration determined that 98.6% of the pesticides of the prespiked samples had recoveries between 70 and 130% at 24 ppb in kale. The quantitation accuracy and precision (n = 6) were also determined to verify the results. Prespiked kale samples resulted in 99.3% of the pesticides with RSDs <25%. Figures 3 to 7 provide the graphical quantitation data for the prespiked pesticides extracted from kale.

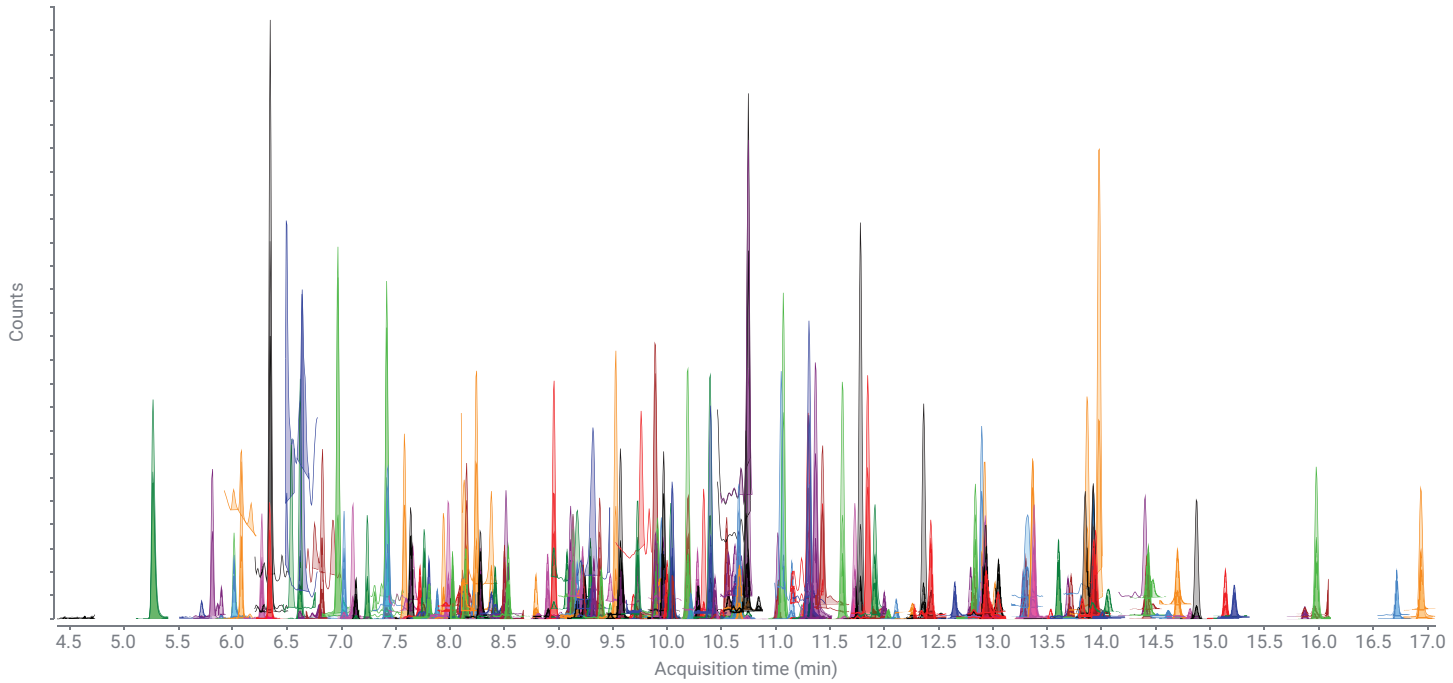

Figure 2. MRM chromatogram of 150 compounds prespiked at 24 ppb in kale.

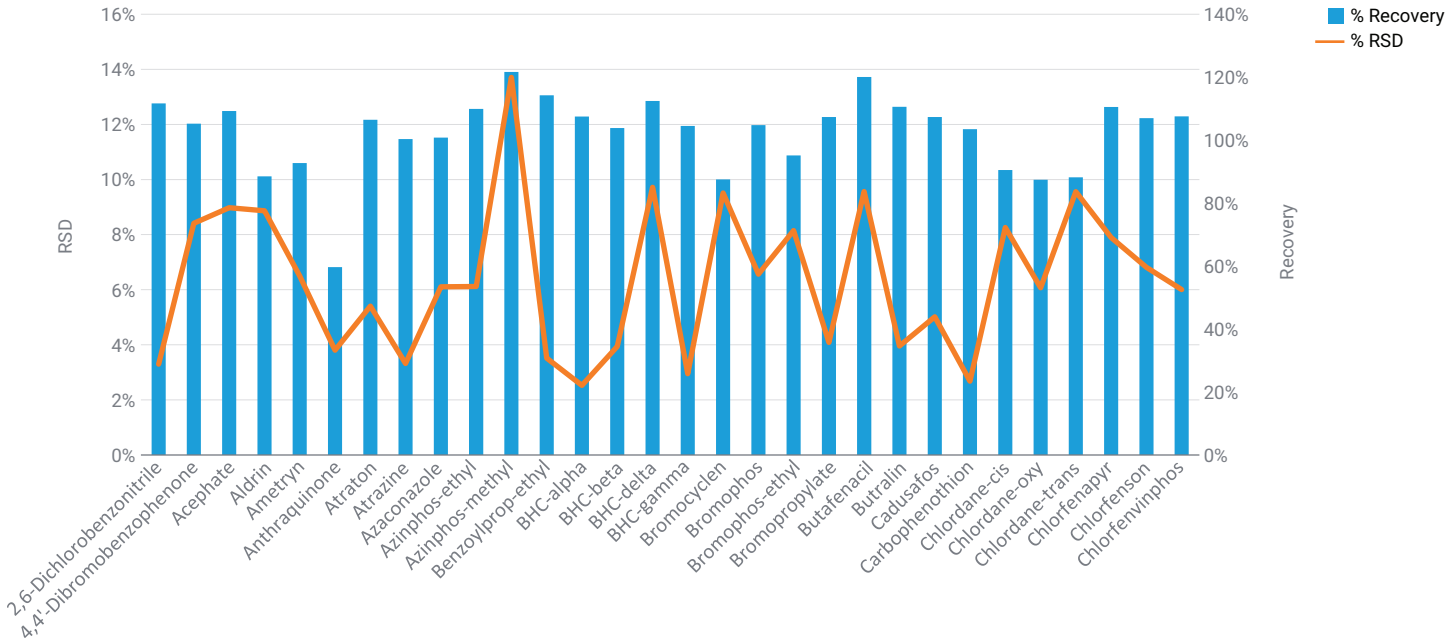

Figure 3. Recovery and RSD (%) of prespiked pesticides in kale.

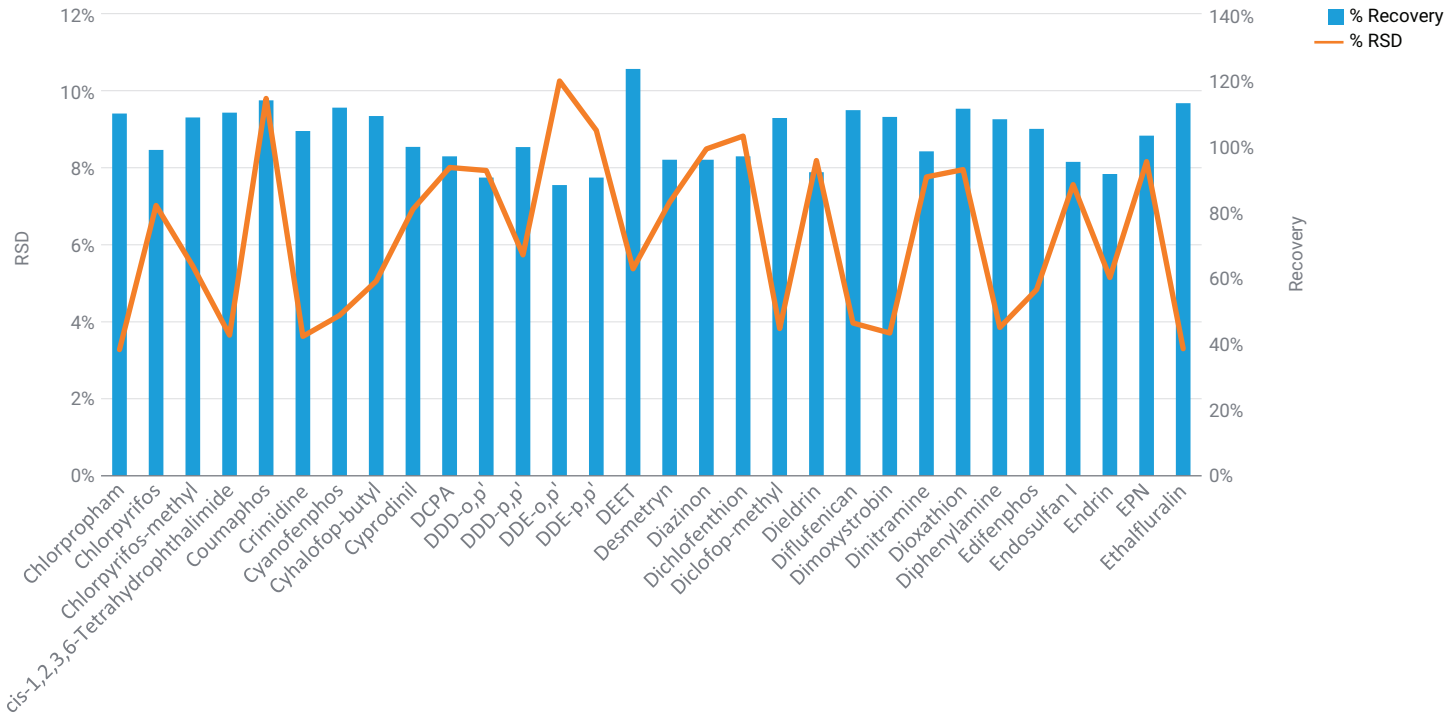

Figure 4. Recovery and RSD (%) of prespiked pesticides in kale.

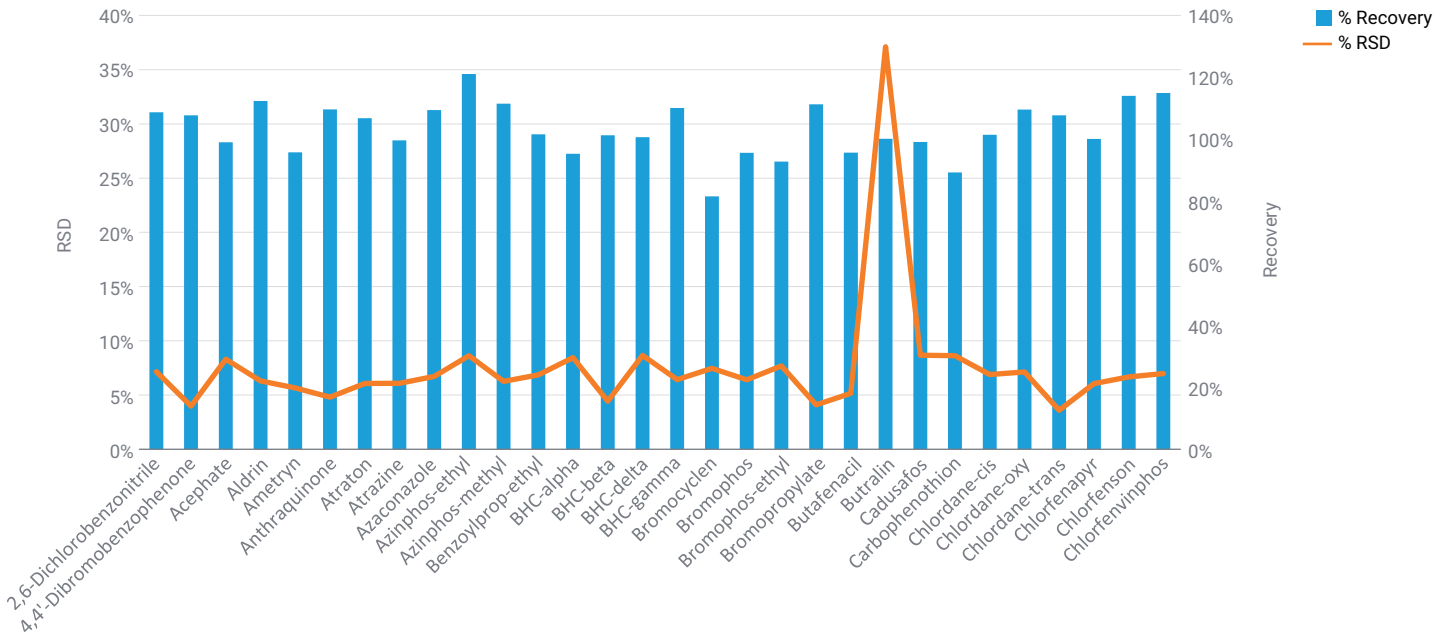

Figure 5. Recovery and RSD (%) of prespiked pesticides in kale.

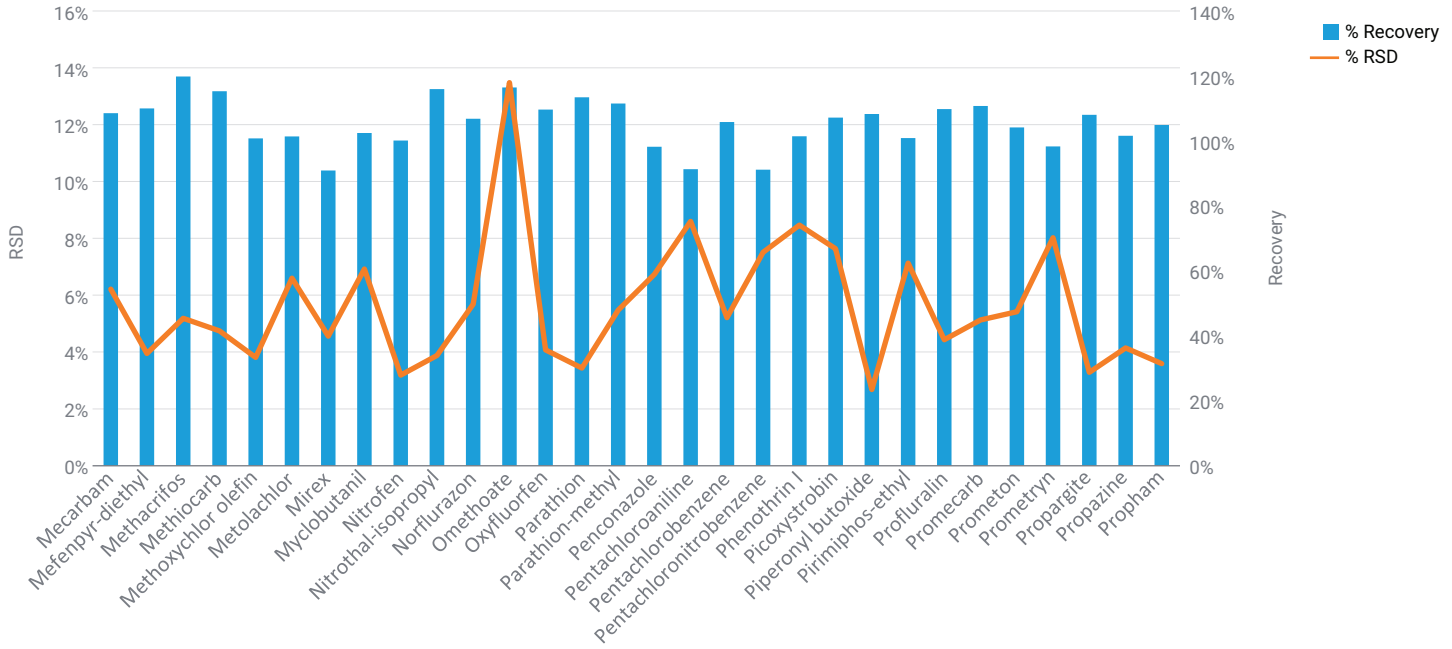

Figure 6. Recovery and RSD (%) of prespiked pesticides in kale.

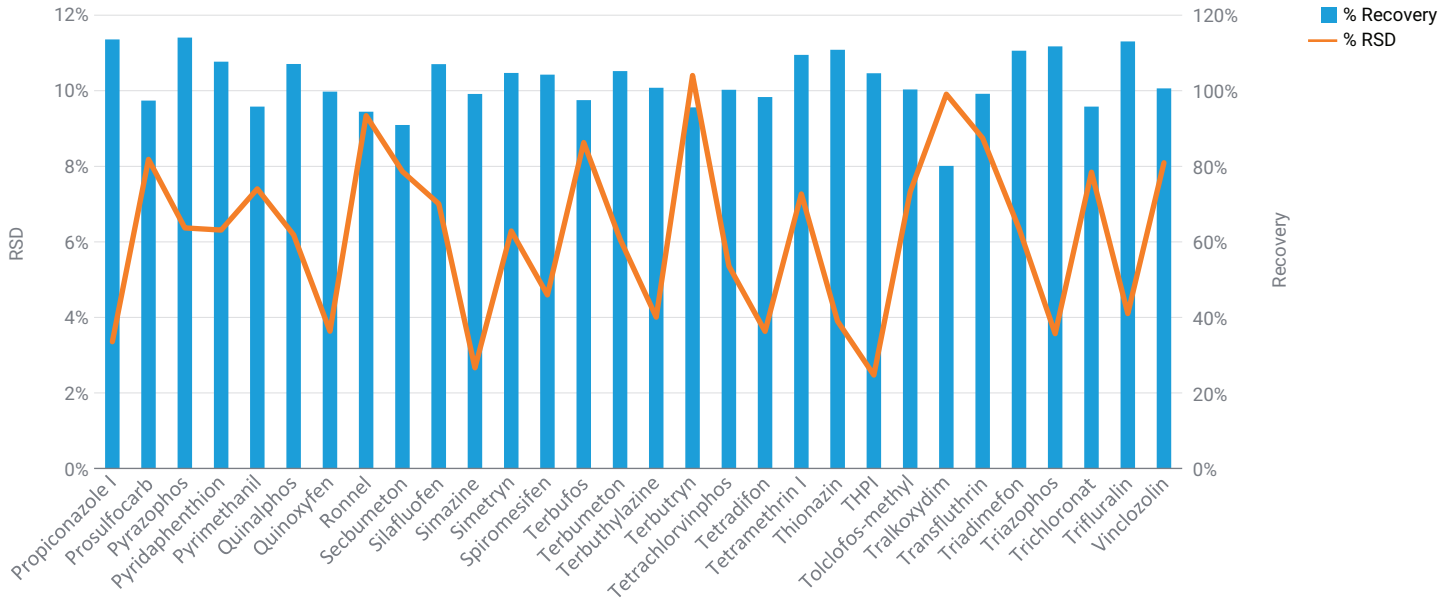

Figure 7. Recovery and RSD (%) of prespiked pesticides in kale.

Conclusion

A simple, rapid, and reliable method using extraction with the Agilent Bond Elut QuEChERS EN extraction kit, followed by cleanup with the Agilent Bond Elut QuEChERS High Pigment dispersive SPE kit (EN like) with Carbon S was shown for 150 GC/MS/MS-amenable pesticides.

References

1. González-Curbelo, M. Á. *et al.* Evolution and Applications of the QuEChERS Method. *Trends in Analytical Chemistry* **2015**, *71*, 169–185.
2. Varela-Martínez, D. A *et al.* Chapter 14: Quick, Easy, Cheap, Effective, Rugged, and Safe (QuEChERS) Extraction. *In* Handbooks in Separation Science: Liquid-Phase Extraction; Elsevier, 2020; pp 399–437.
3. Ferlin, C.; Zhao, L. Analysis of Pesticide Residues in Spinach Using AOAC Pigmented dSPE with Carbon S Cleanup and LC/MS/MS. *Agilent Technologies application note*, publication number 5994-4769EN, **2022**.
4. Yang, X.; Li, Z. Quantitative Analysis of Pesticides in Celery and Grape, *Agilent Technologies application note*, publication number 5994-4763EN, **2022**.
5. Westland, J. Analysis of Pesticides in Tomato and Kale on GC/MS/MS with Agilent Bond Elut QuEChERS EN High Pigment dSPE with Carbon S, *Agilent Technologies application note*, publication number 5994-5050EN, **2022**.
6. Andrianova, A.; Zhao, L. Five Keys to Unlock Maximum Performance in the Analysis of Over 200 Pesticides in Challenging Food Matrices by GC/MS/MS, *Agilent Technologies application note*, publication number 5994-4965EN, **2022**.

Appendix 1

GC/TQ MRM parameters of target and ISTD compounds

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
2,6-Dichlorobenzonitrile	FALSE	5.26	173.0	Wide	100.0	Wide	132.5	25
2,6-Dichlorobenzonitrile	FALSE	5.26	171.0	Wide	136.1	Wide	132.5	15
2,6-Dichlorobenzonitrile	FALSE	5.26	171.0	Wide	100.0	Wide	132.5	25
4,4'-Dibromobenzophenone	FALSE	11.91	182.9	Wide	154.9	Wide	18.6	15
4,4'-Dibromobenzophenone	FALSE	11.91	182.9	Wide	76.0	Wide	18.6	35
4,4'-Dibromobenzophenone	FALSE	11.91	156.9	Wide	76.0	Wide	18.6	15
Acephate	FALSE	5.66	136.0	Wide	94.0	Wide	80.6	15
Acephate	FALSE	5.66	94.0	Wide	64.0	Wide	80.6	10
Acephate	FALSE	5.66	78.9	Wide	47.0	Wide	80.6	10
Aldrin	FALSE	9.94	262.9	Wide	192.9	Wide	12.5	35
Aldrin	FALSE	9.94	262.9	Wide	190.9	Wide	12.5	35
Aldrin	FALSE	9.94	254.9	Wide	220.0	Wide	12.5	20
Allethrin	FALSE	10.63	123.0	Wide	81.0	Wide	7.7	10
Allethrin	FALSE	10.63	107.0	Wide	91.0	Wide	7.7	10
Allethrin	FALSE	10.63	91.0	Wide	65.0	Wide	7.7	15
alpha-BHC-d_6	TRUE	7.58	224.0	Wide	187.0	Wide	20.7	15
alpha-BHC-d_6	TRUE	7.58	224.0	Wide	150.0	Wide	20.7	15
Ametryn	FALSE	9.23	227.0	Wide	170.1	Wide	10.8	10
Ametryn	FALSE	9.23	227.0	Wide	58.1	Wide	10.8	10
Ametryn	FALSE	9.23	185.0	Wide	170.0	Wide	10.8	5

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Anilazine	FALSE	10.57	241.0	Wide	143.1	Wide	9.4	25
Anilazine	FALSE	10.57	239.1	Wide	178.1	Wide	9.4	15
Anilazine	FALSE	10.57	239.1	Wide	143.1	Wide	9.4	25
Anthraquinone	FALSE	9.92	208.0	Wide	180.2	Wide	14.2	10
Anthraquinone	FALSE	9.92	208.0	Wide	152.2	Wide	14.2	20
Anthraquinone	FALSE	9.92	180.0	Wide	152.1	Wide	14.2	10
Atraton	FALSE	7.70	211.0	Wide	169.1	Wide	18.0	5
Atraton	FALSE	7.70	211.0	Wide	58.1	Wide	18.0	10
Atraton	FALSE	7.70	169.0	Wide	154.1	Wide	18.0	5
Atrazine	FALSE	7.89	214.9	Wide	200.2	Wide	15.4	5
Atrazine	FALSE	7.89	214.9	Wide	58.1	Wide	15.4	10
Atrazine	FALSE	7.89	200.0	Wide	122.1	Wide	15.4	5
Azaconazole	FALSE	11.84	219.0	Wide	175.0	Wide	18.6	15
Azaconazole	FALSE	11.84	217.0	Wide	173.1	Wide	18.6	15
Azaconazole	FALSE	11.84	173.0	Wide	145.0	Wide	18.6	15
Azinphos-ethyl	FALSE	15.21	160.0	Wide	132.1	Wide	80.6	0
Azinphos-ethyl	FALSE	15.21	160.0	Wide	77.1	Wide	80.6	20
Azinphos-ethyl	FALSE	15.21	132.0	Wide	77.1	Wide	80.6	15
Azinphos-methyl	FALSE	14.60	160.0	Wide	132.1	Wide	39.1	5
Azinphos-methyl	FALSE	14.60	160.0	Wide	77.0	Wide	39.1	20
Azinphos-methyl	FALSE	14.60	132.1	Wide	77.0	Wide	39.1	15
Benfuracarb	FALSE	15.19	164.2	Wide	149.1	Wide	58.4	10
Benfuracarb	FALSE	15.19	164.2	Wide	103.1	Wide	58.4	30
Benfuracarb	FALSE	15.19	163.0	Wide	107.0	Wide	58.4	15
Benzoylprop-ethyl	FALSE	13.67	292.0	Wide	105.0	Wide	19.4	5
Benzoylprop-ethyl	FALSE	13.67	105.0	Wide	77.1	Wide	19.4	15
Benzoylprop-ethyl	FALSE	13.67	105.0	Wide	51.1	Wide	19.4	35
BHC-alpha	FALSE	7.64	218.9	Wide	183.0	Wide	19.7	5
BHC-alpha	FALSE	7.64	216.9	Wide	181.0	Wide	19.7	5
BHC-alpha	FALSE	7.64	180.9	Wide	145.0	Wide	19.7	15
BHC-beta	FALSE	8.03	218.9	Wide	183.1	Wide	14.2	5
BHC-beta	FALSE	8.03	216.9	Wide	181.1	Wide	14.2	5
BHC-beta	FALSE	8.03	181.0	Wide	145.0	Wide	14.2	15
BHC-delta	FALSE	8.51	219.0	Wide	183.1	Wide	21.0	5
BHC-delta	FALSE	8.51	217.0	Wide	181.1	Wide	21.0	5
BHC-delta	FALSE	8.51	181.1	Wide	145.1	Wide	21.0	15
BHC-gamma	FALSE	8.15	218.9	Wide	183.1	Wide	12.6	5
BHC-gamma	FALSE	8.15	216.9	Wide	181.0	Wide	12.6	5
BHC-gamma	FALSE	8.15	181.0	Wide	145.0	Wide	12.6	15
Binapacryl	FALSE	11.99	100.0	Wide	84.9	Wide	20.9	5
Binapacryl	FALSE	11.99	100.0	Wide	82.0	Wide	20.9	5
Binapacryl	FALSE	11.99	83.0	Wide	55.1	Wide	20.9	5
Bromocyclen	FALSE	8.80	356.8	Wide	277.7	Wide	39.5	5
Bromocyclen	FALSE	8.80	271.8	Wide	236.9	Wide	39.5	15
Bromocyclen	FALSE	8.80	236.9	Wide	118.9	Wide	39.5	30
Bromophos	FALSE	10.28	330.9	Wide	315.9	Wide	14.5	20
Bromophos	FALSE	10.28	125.0	Wide	79.0	Wide	14.5	5

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Bromophos	FALSE	10.28	125.0	Wide	47.0	Wide	14.5	15
Bromophos-ethyl	FALSE	11.02	358.7	Wide	302.8	Wide	23.4	15
Bromophos-ethyl	FALSE	11.02	302.8	Wide	284.7	Wide	23.4	15
Bromophos-ethyl	FALSE	11.02	241.9	Wide	96.9	Wide	23.4	30
Bromopropylate	FALSE	13.91	338.8	Wide	182.9	Wide	20.1	20
Bromopropylate	FALSE	13.91	185.0	Wide	157.0	Wide	20.1	15
Bromopropylate	FALSE	13.91	183.0	Wide	155.0	Wide	20.1	15
Bromoxynil	FALSE	7.41	276.8	Wide	88.0	Wide	21.4	30
Bromoxynil	FALSE	7.41	274.7	Wide	167.9	Wide	21.4	15
Bromoxynil	FALSE	7.41	274.7	Wide	88.0	Wide	21.4	30
Butafenacil	FALSE	15.96	331.0	Wide	180.0	Wide	80.5	25
Butafenacil	FALSE	15.96	331.0	Wide	123.9	Wide	80.5	45
Butafenacil	FALSE	15.96	180.0	Wide	124.0	Wide	80.5	15
Butralin	FALSE	10.22	266.0	Wide	220.2	Wide	13.6	10
Butralin	FALSE	10.22	266.0	Wide	174.2	Wide	13.6	20
Butralin	FALSE	10.22	224.1	Wide	132.1	Wide	13.6	15
Cadusafos	FALSE	7.43	158.8	Wide	131.0	Wide	22.6	5
Cadusafos	FALSE	7.43	158.8	Wide	97.0	Wide	22.6	15
Cadusafos	FALSE	7.43	157.9	Wide	96.9	Wide	22.6	15
Captafol	FALSE	13.43	183.0	Wide	79.0	Wide	22.0	10
Captafol	FALSE	13.43	150.0	Wide	79.0	Wide	22.0	5
Captafol	FALSE	13.43	150.0	Wide	71.9	Wide	22.0	5
Carbophenothion	FALSE	12.82	342.0	Wide	157.0	Wide	19.1	10
Carbophenothion	FALSE	12.82	199.0	Wide	143.0	Wide	19.1	10
Carbophenothion	FALSE	12.82	153.0	Wide	96.9	Wide	19.1	10
Chlordane-*cis*	FALSE	11.29	372.8	Wide	300.9	Wide	15.7	10
Chlordane-*cis*	FALSE	11.29	372.8	Wide	265.9	Wide	15.7	25
Chlordane-*cis*	FALSE	11.29	271.8	Wide	236.9	Wide	15.7	15
Chlordane-oxy	FALSE	10.64	184.9	Wide	121.0	Wide	7.7	15
Chlordane-oxy	FALSE	10.64	114.9	Wide	87.0	Wide	7.7	15
Chlordane-oxy	FALSE	10.64	114.9	Wide	51.1	Wide	7.7	25
Chlordane-*trans*	FALSE	11.03	374.8	Wide	265.8	Wide	23.0	15
Chlordane-*trans*	FALSE	11.03	372.8	Wide	265.8	Wide	23.0	15
Chlordane-*trans*	FALSE	11.03	271.7	Wide	236.9	Wide	23.0	15
Chlorfenapyr	FALSE	12.04	328.0	Wide	247.0	Wide	23.1	20
Chlorfenapyr	FALSE	12.04	247.1	Wide	227.1	Wide	23.1	20
Chlorfenapyr	FALSE	12.04	137.0	Wide	102.0	Wide	23.1	15
Chlorfenson	FALSE	11.37	177.0	Wide	113.0	Wide	23.7	10
Chlorfenson	FALSE	11.37	175.0	Wide	111.0	Wide	23.7	10
Chlorfenson	FALSE	11.37	111.0	Wide	75.0	Wide	23.7	15
Chlorfenvinphos	FALSE	10.66	294.9	Wide	266.9	Wide	8.1	5
Chlorfenvinphos	FALSE	10.66	266.9	Wide	159.0	Wide	8.1	20
Chlorfenvinphos	FALSE	10.66	266.9	Wide	81.0	Wide	8.1	30
Chlorpropham	FALSE	7.11	153.0	Wide	125.1	Wide	22.5	10
Chlorpropham	FALSE	7.11	153.0	Wide	90.0	Wide	22.5	25
Chlorpropham	FALSE	7.11	127.0	Wide	65.1	Wide	22.5	25
Chlorpyrifos	FALSE	9.95	313.8	Wide	257.8	Wide	12.5	15

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Chlorpyrifos	FALSE	9.95	198.9	Wide	171.0	Wide	12.5	15
Chlorpyrifos	FALSE	9.95	196.9	Wide	169.0	Wide	12.5	15
Chlorpyrifos-methyl	FALSE	9.14	285.9	Wide	93.0	Wide	11.8	25
Chlorpyrifos-methyl	FALSE	9.14	124.9	Wide	47.0	Wide	11.8	15
Chlorpyrifos-methyl	FALSE	9.14	78.9	Wide	47.0	Wide	11.8	10
cis-1,2,3,6-Tetrahydrophthalimide	FALSE	5.98	151.1	Wide	80.0	Wide	37.8	5
cis-1,2,3,6-Tetrahydrophthalimide	FALSE	5.98	79.0	Wide	77.0	Wide	37.8	15
cis-1,2,3,6-Tetrahydrophthalimide	FALSE	5.98	79.0	Wide	51.0	Wide	37.8	30
Coumaphos	FALSE	15.85	361.9	Wide	109.0	Wide	80.5	15
Coumaphos	FALSE	15.85	225.9	Wide	163.1	Wide	80.5	15
Coumaphos	FALSE	15.85	210.0	Wide	182.0	Wide	80.5	10
Crimidine	FALSE	6.25	172.9	Wide	144.1	Wide	47.5	5
Crimidine	FALSE	6.25	170.9	Wide	142.1	Wide	47.5	5
Crimidine	FALSE	6.25	142.0	Wide	106.1	Wide	47.5	10
Cyanofenphos	FALSE	12.89	185.0	Wide	157.0	Wide	16.3	5
Cyanofenphos	FALSE	12.89	169.0	Wide	141.1	Wide	16.3	5
Cyanofenphos	FALSE	12.89	169.0	Wide	77.1	Wide	16.3	25
Cyhalofop-butyl	FALSE	14.68	256.2	Wide	120.1	Wide	39.1	10
Cyhalofop-butyl	FALSE	14.68	229.2	Wide	109.1	Wide	39.1	15
Cyhalofop-butyl	FALSE	14.68	120.1	Wide	91.0	Wide	39.1	15
Cyprodinil	FALSE	10.39	226.2	Wide	225.3	Wide	13.3	10
Cyprodinil	FALSE	10.39	225.2	Wide	224.3	Wide	13.3	10
Cyprodinil	FALSE	10.39	224.2	Wide	208.2	Wide	13.3	20
DCPA	FALSE	10.06	331.8	Wide	300.9	Wide	12.4	10
DCPA	FALSE	10.06	300.9	Wide	223.0	Wide	12.4	25
DCPA	FALSE	10.06	298.9	Wide	221.0	Wide	12.4	25
DDD-o,p'	FALSE	11.78	235.0	Wide	200.1	Wide	19.5	10
DDD-o,p'	FALSE	11.78	235.0	Wide	165.1	Wide	19.5	25
DDD-o,p'	FALSE	11.78	199.1	Wide	164.1	Wide	19.5	20
DDD-p,p'	FALSE	12.36	237.0	Wide	200.1	Wide	31.1	15
DDD-p,p'	FALSE	12.36	237.0	Wide	165.1	Wide	31.1	25
DDD-p,p'	FALSE	12.36	165.1	Wide	115.0	Wide	31.1	35
DDE-o,p'	FALSE	11.08	317.8	Wide	248.0	Wide	19.3	15
DDE-o,p'	FALSE	11.08	248.0	Wide	176.2	Wide	19.3	30
DDE-o,p'	FALSE	11.08	246.0	Wide	176.2	Wide	19.3	30
DDE-p,p'	FALSE	11.61	317.8	Wide	246.0	Wide	33.9	15
DDE-p,p'	FALSE	11.61	315.8	Wide	246.0	Wide	33.9	15
DDE-p,p'	FALSE	11.61	246.1	Wide	176.2	Wide	33.9	30
DEET	FALSE	6.63	119.1	Wide	91.0	Wide	43.6	10
DEET	FALSE	6.63	119.1	Wide	65.1	Wide	43.6	20
DEET	FALSE	6.63	91.0	Wide	65.1	Wide	43.6	10
Desmedipham	FALSE	7.59	135.0	Wide	79.0	Wide	20.7	15
Desmedipham	FALSE	7.59	135.0	Wide	52.0	Wide	20.7	25
Desmedipham	FALSE	7.59	109.0	Wide	80.0	Wide	20.7	15
Desmetryn	FALSE	8.89	213.0	Wide	171.2	Wide	30.4	5
Desmetryn	FALSE	8.89	213.0	Wide	58.1	Wide	30.4	10
Desmetryn	FALSE	8.89	171.0	Wide	156.0	Wide	30.4	5

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Diazinon	FALSE	8.29	199.1	Wide	93.0	Wide	13.0	15
Diazinon	FALSE	8.29	137.1	Wide	84.0	Wide	13.0	10
Diazinon	FALSE	8.29	137.1	Wide	54.0	Wide	13.0	20
Dichlofenthion	FALSE	8.97	279.0	Wide	223.0	Wide	19.4	15
Dichlofenthion	FALSE	8.97	279.0	Wide	204.9	Wide	19.4	30
Dichlofenthion	FALSE	8.97	223.0	Wide	204.9	Wide	19.4	15
Dichlofluanid	FALSE	9.76	167.1	Wide	124.0	Wide	19.6	10
Dichlofluanid	FALSE	9.76	123.0	Wide	77.0	Wide	19.6	20
Dichlofluanid	FALSE	9.76	123.0	Wide	51.0	Wide	19.6	40
Diclofop-methyl	FALSE	13.26	339.9	Wide	252.9	Wide	25.5	10
Diclofop-methyl	FALSE	13.26	280.8	Wide	119.9	Wide	25.5	10
Diclofop-methyl	FALSE	13.26	253.0	Wide	162.1	Wide	25.5	15
Dicofol, p, p'-	FALSE	14.07	183.9	Wide	169.3	Wide	39.3	5
Dicofol, p, p'-	FALSE	14.07	183.9	Wide	155.0	Wide	39.3	30
Dicofol, p, p'-	FALSE	14.07	183.9	Wide	141.2	Wide	39.3	20
Dieldrin	FALSE	11.72	277.0	Wide	241.0	Wide	20.5	5
Dieldrin	FALSE	11.72	262.9	Wide	193.0	Wide	20.5	35
Dieldrin	FALSE	11.72	262.9	Wide	191.0	Wide	20.5	35
Diflufenican	FALSE	13.29	393.9	Wide	265.9	Wide	21.2	10
Diflufenican	FALSE	13.29	266.0	Wide	246.1	Wide	21.2	15
Diflufenican	FALSE	13.29	266.0	Wide	238.1	Wide	21.2	15
Dimoxystrobin	FALSE	13.85	205.0	Wide	116.0	Wide	17.4	10
Dimoxystrobin	FALSE	13.85	116.0	Wide	89.0	Wide	17.4	15
Dimoxystrobin	FALSE	13.85	116.0	Wide	63.0	Wide	17.4	30
Dinitramine	FALSE	8.40	260.7	Wide	241.0	Wide	15.0	10
Dinitramine	FALSE	8.40	260.7	Wide	195.0	Wide	15.0	20
Dinitramine	FALSE	8.40	216.0	Wide	196.0	Wide	15.0	10
Dinobuton	FALSE	10.72	211.0	Wide	163.0	Wide	9.9	5
Dinobuton	FALSE	10.72	211.0	Wide	117.0	Wide	9.9	15
Dinobuton	FALSE	10.72	211.0	Wide	89.0	Wide	9.9	30
Dinocap I	FALSE	13.31	265.9	Wide	167.2	Wide	18.8	18
Dinocap I	FALSE	13.31	69.0	Wide	41.1	Wide	18.8	10
Dinocap I	FALSE	13.31	69.0	Wide	39.1	Wide	18.8	25
Dioxathion	FALSE	15.94	271.0	Wide	96.9	Wide	58.3	30
Dioxathion	FALSE	15.94	152.9	Wide	96.9	Wide	58.3	10
Dioxathion	FALSE	15.94	124.9	Wide	96.9	Wide	58.3	5
Diphenylamine	FALSE	6.97	169.0	Wide	168.2	Wide	28.2	15
Diphenylamine	FALSE	6.97	168.0	Wide	167.2	Wide	28.2	15
Diphenylamine	FALSE	6.97	167.0	Wide	166.2	Wide	28.2	20
DMST	FALSE	8.03	106.0	Wide	79.0	Wide	14.2	5
DMST	FALSE	8.03	106.0	Wide	77.0	Wide	14.2	15
DMST	FALSE	8.03	78.9	Wide	77.0	Wide	14.2	10
Edifenphos	FALSE	12.92	201.0	Wide	109.0	Wide	15.6	10
Edifenphos	FALSE	12.92	172.9	Wide	109.0	Wide	15.6	5
Edifenphos	FALSE	12.92	108.9	Wide	65.1	Wide	15.6	15
Endosulfan I (alpha isomer)	FALSE	11.26	194.9	Wide	160.0	Wide	16.8	5
Endosulfan I (alpha isomer)	FALSE	11.26	194.9	Wide	159.0	Wide	16.8	5

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Endosulfan I (alpha isomer)	FALSE	11.26	194.9	Wide	125.0	Wide	16.8	20
Endosulfan II (beta isomer)	FALSE	12.27	206.9	Wide	172.0	Wide	30.6	15
Endosulfan II (beta isomer)	FALSE	12.27	194.9	Wide	158.9	Wide	30.6	10
Endosulfan II (beta isomer)	FALSE	12.27	194.9	Wide	124.9	Wide	30.6	25
Endrin	FALSE	12.12	316.7	Wide	280.8	Wide	27.6	5
Endrin	FALSE	12.12	262.8	Wide	193.0	Wide	27.6	35
Endrin	FALSE	12.12	244.8	Wide	173.0	Wide	27.6	30
EPN	FALSE	13.94	185.0	Wide	157.1	Wide	23.1	5
EPN	FALSE	13.94	169.0	Wide	141.1	Wide	23.1	5
EPN	FALSE	13.94	169.0	Wide	77.1	Wide	23.1	25
Esbiothrin	FALSE	10.60	123.1	Wide	41.0	Wide	8.0	30
Esbiothrin	FALSE	10.60	91.0	Wide	65.0	Wide	8.0	15
Esbiothrin	FALSE	10.60	91.0	Wide	39.1	Wide	8.0	35
Ethalfluralin	FALSE	7.14	315.9	Wide	275.9	Wide	20.7	10
Ethalfluralin	FALSE	7.14	275.9	Wide	248.1	Wide	20.7	10
Ethalfluralin	FALSE	7.14	275.9	Wide	202.1	Wide	20.7	15
Ethion	FALSE	12.42	230.9	Wide	175.0	Wide	30.8	10
Ethion	FALSE	12.42	152.9	Wide	96.9	Wide	30.8	10
Ethion	FALSE	12.42	124.9	Wide	96.9	Wide	30.8	0
Ethoprophos	FALSE	7.02	157.9	Wide	114.0	Wide	25.6	5
Ethoprophos	FALSE	7.02	157.9	Wide	97.0	Wide	25.6	15
Ethoprophos	FALSE	7.02	138.9	Wide	97.0	Wide	25.6	5
Etrimfos	FALSE	8.54	292.1	Wide	181.1	Wide	25.9	5
Etrimfos	FALSE	8.54	181.1	Wide	153.1	Wide	25.9	10
Etrimfos	FALSE	8.54	181.1	Wide	56.1	Wide	25.9	25
Famphur	FALSE	12.79	218.0	Wide	109.0	Wide	27.7	15
Famphur	FALSE	12.79	218.0	Wide	79.0	Wide	27.7	30
Famphur	FALSE	12.79	124.9	Wide	47.0	Wide	27.7	15
Fenamiphos	FALSE	11.31	302.9	Wide	287.9	Wide	18.1	10
Fenamiphos	FALSE	11.31	217.0	Wide	202.1	Wide	18.1	10
Fenamiphos	FALSE	11.31	154.0	Wide	139.0	Wide	18.1	10
Fenitrothion	FALSE	9.59	277.0	Wide	260.1	Wide	22.8	5
Fenitrothion	FALSE	9.59	125.1	Wide	79.0	Wide	22.8	5
Fenitrothion	FALSE	9.59	125.1	Wide	47.0	Wide	22.8	15
Fenpropathrin	FALSE	14.04	207.9	Wide	181.0	Wide	33.3	5
Fenpropathrin	FALSE	14.04	181.1	Wide	152.1	Wide	33.3	25
Fenpropathrin	FALSE	14.04	125.0	Wide	55.1	Wide	33.3	10
Fenson	FALSE	10.19	267.9	Wide	141.1	Wide	13.1	5
Fenson	FALSE	10.19	267.9	Wide	77.1	Wide	13.1	20
Fenson	FALSE	10.19	141.0	Wide	77.1	Wide	13.1	5
Fensulfothion	FALSE	12.25	291.8	Wide	156.0	Wide	30.2	15
Fensulfothion	FALSE	12.25	156.0	Wide	141.0	Wide	30.2	10
Fensulfothion	FALSE	12.25	140.0	Wide	125.0	Wide	30.2	10
Fipronil	FALSE	10.64	366.8	Wide	212.8	Wide	8.1	25
Fipronil	FALSE	10.64	350.8	Wide	254.8	Wide	8.1	15
Fipronil	FALSE	10.64	254.9	Wide	228.0	Wide	8.1	15
Flubenzimine	FALSE	11.52	186.0	Wide	69.0	Wide	31.8	25

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Flubenzimine	FALSE	11.52	135.0	Wide	77.1	Wide	31.8	20
Flubenzimine	FALSE	11.52	135.0	Wide	51.1	Wide	31.8	40
Flucythrinate I	FALSE	16.69	198.9	Wide	157.0	Wide	99.1	10
Flucythrinate I	FALSE	16.69	198.9	Wide	107.0	Wide	99.1	25
Flucythrinate I	FALSE	16.69	156.9	Wide	107.1	Wide	99.1	15
Flufenacet	FALSE	9.96	151.0	Wide	136.1	Wide	12.0	10
Flufenacet	FALSE	9.96	151.0	Wide	95.0	Wide	12.0	30
Flufenacet	FALSE	9.96	123.0	Wide	95.0	Wide	12.0	20
Flutriafol	FALSE	11.30	219.1	Wide	123.1	Wide	18.1	15
Flutriafol	FALSE	11.30	123.1	Wide	95.0	Wide	18.1	15
Flutriafol	FALSE	11.30	123.1	Wide	75.1	Wide	18.1	25
Fonofos	FALSE	8.25	246.1	Wide	137.0	Wide	12.9	5
Fonofos	FALSE	8.25	137.0	Wide	109.0	Wide	12.9	5
Fonofos	FALSE	8.25	109.0	Wide	80.9	Wide	12.9	5
Fosthiazate I	FALSE	10.27	199.0	Wide	102.0	Wide	14.5	5
Fosthiazate I	FALSE	10.27	195.0	Wide	103.0	Wide	14.5	5
Fosthiazate I	FALSE	10.27	195.0	Wide	60.0	Wide	14.5	20
Fuberidazole	FALSE	9.16	184.0	Wide	156.2	Wide	11.3	10
Fuberidazole	FALSE	9.16	184.0	Wide	155.1	Wide	11.3	30
Fuberidazole	FALSE	9.16	183.0	Wide	155.1	Wide	11.3	10
Furathiocarb	FALSE	14.41	163.1	Wide	135.1	Wide	40.8	5
Furathiocarb	FALSE	14.41	163.1	Wide	107.1	Wide	40.8	15
Furathiocarb	FALSE	14.41	135.1	Wide	107.1	Wide	40.8	5
Heptachlor	FALSE	9.34	273.7	Wide	238.9	Wide	13.0	15
Heptachlor	FALSE	9.34	273.7	Wide	236.9	Wide	13.0	15
Heptachlor	FALSE	9.34	271.7	Wide	236.9	Wide	13.0	15
Heptachlor endo-epoxide	FALSE	10.67	216.9	Wide	182.0	Wide	9.4	20
Heptachlor endo-epoxide	FALSE	10.67	183.0	Wide	119.0	Wide	9.4	30
Heptachlor endo-epoxide	FALSE	10.67	135.0	Wide	99.0	Wide	9.4	15
Heptachlor exo-epoxide	FALSE	10.61	354.8	Wide	264.9	Wide	8.0	15
Heptachlor exo-epoxide	FALSE	10.61	352.8	Wide	262.9	Wide	8.0	15
Heptachlor exo-epoxide	FALSE	10.61	262.9	Wide	193.0	Wide	8.0	35
Heptenophos	FALSE	6.61	124.0	Wide	89.0	Wide	43.6	10
Heptenophos	FALSE	6.61	124.0	Wide	63.0	Wide	43.6	35
Heptenophos	FALSE	6.61	108.9	Wide	78.9	Wide	43.6	5
Hexachlorobenzene	FALSE	7.78	283.8	Wide	248.8	Wide	15.4	15
Hexachlorobenzene	FALSE	7.78	283.8	Wide	213.9	Wide	15.4	30
Hexachlorobenzene	FALSE	7.78	281.8	Wide	211.9	Wide	15.4	30
Ioxynil	FALSE	9.68	370.8	Wide	117.0	Wide	22.9	25
Ioxynil	FALSE	9.68	117.1	Wide	89.0	Wide	22.9	10
Ioxynil	FALSE	9.68	117.1	Wide	62.0	Wide	22.9	15
Iprodione	FALSE	13.69	313.8	Wide	55.9	Wide	19.1	20
Iprodione	FALSE	13.69	243.9	Wide	187.0	Wide	19.1	5
Iprodione	FALSE	13.69	187.0	Wide	124.0	Wide	19.1	25
Isazofos	FALSE	8.52	256.9	Wide	162.0	Wide	21.0	5
Isazofos	FALSE	8.52	161.0	Wide	146.0	Wide	21.0	5
Isazofos	FALSE	8.52	161.0	Wide	119.1	Wide	21.0	5

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Isodrin	FALSE	10.45	195.0	Wide	123.0	Wide	12.1	30
Isodrin	FALSE	10.45	193.0	Wide	157.0	Wide	12.1	20
Isodrin	FALSE	10.45	193.0	Wide	123.0	Wide	12.1	30
Isofenphos	FALSE	10.66	212.9	Wide	185.1	Wide	8.1	5
Isofenphos	FALSE	10.66	212.9	Wide	121.1	Wide	8.1	10
Isofenphos	FALSE	10.66	185.0	Wide	121.1	Wide	8.1	5
Isofenphos-methyl	FALSE	10.39	199.0	Wide	121.0	Wide	13.3	15
Isofenphos-methyl	FALSE	10.39	121.0	Wide	65.0	Wide	13.3	20
Isofenphos-methyl	FALSE	10.39	121.0	Wide	39.1	Wide	13.3	40
Isoprocarb I	FALSE	6.34	136.0	Wide	121.1	Wide	45.8	10
Isoprocarb I	FALSE	6.34	121.0	Wide	103.1	Wide	45.8	10
Isoprocarb I	FALSE	6.34	121.0	Wide	77.1	Wide	45.8	20
Isopropalin	FALSE	10.34	280.1	Wide	238.1	Wide	14.1	10
Isopropalin	FALSE	10.34	280.1	Wide	180.1	Wide	14.1	15
Isopropalin	FALSE	10.34	280.1	Wide	165.1	Wide	14.1	20
Malaoxon	FALSE	9.07	126.9	Wide	99.0	Wide	15.7	5
Malaoxon	FALSE	9.07	126.9	Wide	55.0	Wide	15.7	5
Malaoxon	FALSE	9.07	98.9	Wide	71.0	Wide	15.7	5
Malathion	FALSE	9.73	172.9	Wide	99.0	Wide	22.0	15
Malathion	FALSE	9.73	157.8	Wide	125.0	Wide	22.0	5
Malathion	FALSE	9.73	126.9	Wide	99.0	Wide	22.0	5
Mecarbam	FALSE	10.66	158.9	Wide	131.0	Wide	8.1	5
Mecarbam	FALSE	10.66	130.9	Wide	86.0	Wide	8.1	10
Mecarbam	FALSE	10.66	130.9	Wide	74.0	Wide	8.1	5
Mefenpyr-diethyl	FALSE	13.59	299.0	Wide	252.9	Wide	22.3	10
Mefenpyr-diethyl	FALSE	13.59	253.0	Wide	190.0	Wide	22.3	20
Mefenpyr-diethyl	FALSE	13.59	253.0	Wide	189.0	Wide	22.3	30
Methacrifos	FALSE	6.06	207.9	Wide	180.1	Wide	43.8	5
Methacrifos	FALSE	6.06	124.9	Wide	79.0	Wide	43.8	5
Methacrifos	FALSE	6.06	124.9	Wide	47.1	Wide	43.8	10
Methamidophos	FALSE	4.58	141.0	Wide	95.0	Wide	99.2	5
Methamidophos	FALSE	4.58	141.0	Wide	80.0	Wide	99.2	20
Methamidophos	FALSE	4.58	141.0	Wide	64.0	Wide	99.2	25
Methiocarb	FALSE	9.58	168.0	Wide	153.1	Wide	21.4	10
Methiocarb	FALSE	9.58	168.0	Wide	109.1	Wide	21.4	15
Methiocarb	FALSE	9.58	153.0	Wide	109.1	Wide	21.4	5
Methoxychlor olefin	FALSE	12.83	308.0	Wide	238.0	Wide	18.6	20
Methoxychlor olefin	FALSE	12.83	238.0	Wide	223.1	Wide	18.6	15
Methoxychlor olefin	FALSE	12.83	238.0	Wide	195.1	Wide	18.6	20
Metolachlor	FALSE	9.89	240.0	Wide	162.2	Wide	16.6	10
Metolachlor	FALSE	9.89	238.0	Wide	162.2	Wide	16.6	10
Metolachlor	FALSE	9.89	162.2	Wide	133.2	Wide	16.6	15
Mirex	FALSE	14.87	271.8	Wide	236.8	Wide	68.0	20
Mirex	FALSE	14.87	236.9	Wide	142.9	Wide	68.0	30
Mirex	FALSE	14.87	236.9	Wide	118.9	Wide	68.0	30
Myclobutanil	FALSE	11.72	179.0	Wide	125.1	Wide	20.5	10
Myclobutanil	FALSE	11.72	179.0	Wide	90.0	Wide	20.5	30

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Myclobutanil	FALSE	11.72	150.0	Wide	123.0	Wide	20.5	15
Nitralin	FALSE	13.52	315.9	Wide	274.0	Wide	22.4	5
Nitralin	FALSE	13.52	299.7	Wide	257.9	Wide	22.4	5
Nitralin	FALSE	13.52	274.1	Wide	169.0	Wide	22.4	10
Nitrofen	FALSE	12.00	282.9	Wide	253.0	Wide	21.4	10
Nitrofen	FALSE	12.00	282.9	Wide	202.0	Wide	21.4	10
Nitrofen	FALSE	12.00	202.0	Wide	139.1	Wide	21.4	20
Nitrothal-isopropyl	FALSE	10.03	236.0	Wide	194.1	Wide	12.3	10
Nitrothal-isopropyl	FALSE	10.03	194.0	Wide	148.1	Wide	12.3	10
Nitrothal-isopropyl	FALSE	10.03	194.0	Wide	120.1	Wide	12.3	20
Norflurazon	FALSE	12.93	172.8	Wide	145.0	Wide	18.0	5
Norflurazon	FALSE	12.93	145.0	Wide	95.0	Wide	18.0	20
Norflurazon	FALSE	12.93	145.0	Wide	75.0	Wide	18.0	30
Omethoate	FALSE	6.75	156.0	Wide	110.0	Wide	43.6	10
Omethoate	FALSE	6.75	156.0	Wide	79.0	Wide	43.6	25
Omethoate	FALSE	6.75	110.0	Wide	79.0	Wide	43.6	15
Oxyfluorfen	FALSE	11.71	299.9	Wide	222.8	Wide	21.1	15
Oxyfluorfen	FALSE	11.71	252.0	Wide	196.0	Wide	21.1	20
Oxyfluorfen	FALSE	11.71	252.0	Wide	146.0	Wide	21.1	30
Paraoxon	FALSE	9.32	148.9	Wide	119.0	Wide	12.1	5
Paraoxon	FALSE	9.32	108.9	Wide	91.0	Wide	12.1	5
Paraoxon	FALSE	9.32	108.9	Wide	81.0	Wide	12.1	10
Paraoxon-methyl	FALSE	8.42	229.9	Wide	136.1	Wide	15.7	5
Paraoxon-methyl	FALSE	8.42	229.9	Wide	106.1	Wide	15.7	15
Paraoxon-methyl	FALSE	8.42	108.9	Wide	79.0	Wide	15.7	5
Parathion	FALSE	9.97	291.0	Wide	109.0	Wide	12.2	15
Parathion	FALSE	9.97	139.0	Wide	109.0	Wide	12.2	5
Parathion	FALSE	9.97	109.0	Wide	81.0	Wide	12.2	15
Parathion-d_{10}	TRUE	9.90	301.0	Wide	115.0	Wide	15.9	15
Parathion-d_{10}	TRUE	9.90	301.0	Wide	83.0	Wide	15.9	35
Parathion-methyl	FALSE	9.14	262.9	Wide	109.0	Wide	11.8	10
Parathion-methyl	FALSE	9.14	125.0	Wide	79.0	Wide	11.8	5
Parathion-methyl	FALSE	9.14	125.0	Wide	47.0	Wide	11.8	10
Penconazole	FALSE	10.54	248.0	Wide	192.1	Wide	10.4	15
Penconazole	FALSE	10.54	248.0	Wide	157.1	Wide	10.4	25
Penconazole	FALSE	10.54	159.0	Wide	89.0	Wide	10.4	35
Pentachloroaniline	FALSE	8.91	191.9	Wide	82.9	Wide	23.9	25
Pentachloroaniline	FALSE	8.91	158.0	Wide	123.0	Wide	23.9	15
Pentachloroaniline	FALSE	8.91	132.1	Wide	114.5	Wide	23.9	5
Pentachlorobenzene	FALSE	6.36	251.9	Wide	217.0	Wide	46.3	20
Pentachlorobenzene	FALSE	6.36	249.9	Wide	215.0	Wide	46.3	20
Pentachlorobenzene	FALSE	6.36	248.0	Wide	213.0	Wide	46.3	20
Pentachloronitrobenzene	FALSE	8.23	248.8	Wide	213.8	Wide	12.7	15
Pentachloronitrobenzene	FALSE	8.23	176.9	Wide	141.9	Wide	12.7	15
Pentachloronitrobenzene	FALSE	8.23	141.9	Wide	106.9	Wide	12.7	30
Phenothrin I	FALSE	14.29	183.0	Wide	168.0	Wide	71.4	10
Phenothrin I	FALSE	14.29	183.0	Wide	155.1	Wide	71.4	5

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Phenothrin I	FALSE	14.29	122.9	Wide	81.1	Wide	71.4	5
Picoxystrobin	FALSE	11.29	145.0	Wide	117.1	Wide	15.7	10
Picoxystrobin	FALSE	11.29	145.0	Wide	115.1	Wide	15.7	15
Picoxystrobin	FALSE	11.29	145.0	Wide	102.1	Wide	15.7	25
Piperonyl butoxide	FALSE	13.36	176.1	Wide	131.1	Wide	21.4	15
Piperonyl butoxide	FALSE	13.36	176.1	Wide	117.1	Wide	21.4	20
Piperonyl butoxide	FALSE	13.36	176.1	Wide	103.1	Wide	21.4	25
Pirimiphos-ethyl	FALSE	10.28	318.1	Wide	182.0	Wide	14.5	10
Pirimiphos-ethyl	FALSE	10.28	318.1	Wide	166.1	Wide	14.5	10
Pirimiphos-ethyl	FALSE	10.28	152.1	Wide	84.0	Wide	14.5	10
Profluralin	FALSE	8.11	346.9	Wide	330.1	Wide	13.8	5
Profluralin	FALSE	8.11	318.1	Wide	199.1	Wide	13.8	15
Profluralin	FALSE	8.11	318.1	Wide	55.1	Wide	13.8	15
Promecarb	FALSE	7.42	150.1	Wide	135.2	Wide	21.4	10
Promecarb	FALSE	7.42	135.1	Wide	115.1	Wide	21.4	15
Promecarb	FALSE	7.42	135.1	Wide	91.0	Wide	21.4	15
Prometon	FALSE	7.78	224.9	Wide	58.1	Wide	15.4	15
Prometon	FALSE	7.78	210.0	Wide	168.1	Wide	15.4	5
Prometon	FALSE	7.78	183.0	Wide	168.1	Wide	15.4	5
Prometryn	FALSE	9.28	241.0	Wide	184.2	Wide	11.6	10
Prometryn	FALSE	9.28	226.0	Wide	184.2	Wide	11.6	10
Prometryn	FALSE	9.28	199.0	Wide	184.1	Wide	11.6	5
Propargite	FALSE	13.32	149.9	Wide	135.1	Wide	18.8	5
Propargite	FALSE	13.32	135.0	Wide	107.1	Wide	18.8	10
Propargite	FALSE	13.32	135.0	Wide	77.1	Wide	18.8	30
Propazine	FALSE	7.95	229.1	Wide	214.2	Wide	14.9	5
Propazine	FALSE	7.95	229.1	Wide	58.1	Wide	14.9	10
Propazine	FALSE	7.95	214.2	Wide	172.2	Wide	14.9	10
Propham	FALSE	5.78	178.9	Wide	93.0	Wide	47.0	15
Propham	FALSE	5.78	136.9	Wide	93.0	Wide	47.0	10
Propham	FALSE	5.78	119.0	Wide	91.0	Wide	47.0	10
Propiconazole I	FALSE	12.93	172.9	Wide	145.0	Wide	18.0	15
Propiconazole I	FALSE	12.93	172.9	Wide	109.0	Wide	18.0	30
Propiconazole I	FALSE	12.93	172.9	Wide	74.0	Wide	18.0	45
Prosulfocarb	FALSE	9.37	251.0	Wide	128.2	Wide	14.3	5
Prosulfocarb	FALSE	9.37	128.0	Wide	86.1	Wide	14.3	0
Prosulfocarb	FALSE	9.37	91.0	Wide	65.0	Wide	14.3	15
Pyrazophos	FALSE	15.12	232.0	Wide	204.1	Wide	58.4	10
Pyrazophos	FALSE	15.12	221.0	Wide	193.1	Wide	58.4	10
Pyrazophos	FALSE	15.12	221.0	Wide	149.0	Wide	58.4	15
Pyridaphenthion	FALSE	13.80	340.0	Wide	199.0	Wide	17.5	5
Pyridaphenthion	FALSE	13.80	204.0	Wide	203.1	Wide	17.5	5
Pyridaphenthion	FALSE	13.80	188.0	Wide	82.0	Wide	17.5	10
Pyrimethanil	FALSE	8.28	198.0	Wide	183.1	Wide	13.0	15
Pyrimethanil	FALSE	8.28	198.0	Wide	158.1	Wide	13.0	20
Pyrimethanil	FALSE	8.28	198.0	Wide	118.1	Wide	13.0	35
Quinalphos	FALSE	10.73	157.0	Wide	129.1	Wide	11.6	15

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
Quinalphos	FALSE	10.73	146.0	Wide	118.0	Wide	11.6	10
Quinalphos	FALSE	10.73	146.0	Wide	91.0	Wide	11.6	30
Quinoxyfen	FALSE	12.92	306.8	Wide	237.0	Wide	15.6	20
Quinoxyfen	FALSE	12.92	271.9	Wide	237.1	Wide	15.6	10
Quinoxyfen	FALSE	12.92	237.0	Wide	208.1	Wide	15.6	30
Ronnel	FALSE	9.39	286.9	Wide	272.0	Wide	15.0	15
Ronnel	FALSE	9.39	285.0	Wide	269.9	Wide	15.0	15
Ronnel	FALSE	9.39	125.0	Wide	47.1	Wide	15.0	15
Secbumeton	FALSE	8.39	196.0	Wide	122.1	Wide	14.0	10
Secbumeton	FALSE	8.39	196.0	Wide	85.0	Wide	14.0	10
Secbumeton	FALSE	8.39	169.0	Wide	154.1	Wide	14.0	5
Silafluofen	FALSE	16.92	286.0	Wide	258.1	Wide	99.1	10
Silafluofen	FALSE	16.92	179.2	Wide	151.1	Wide	99.1	10
Silafluofen	FALSE	16.92	179.2	Wide	91.1	Wide	99.1	20
Simazine	FALSE	7.81	201.1	Wide	173.1	Wide	15.3	5
Simazine	FALSE	7.81	173.0	Wide	172.1	Wide	15.3	5
Simazine	FALSE	7.81	173.0	Wide	138.2	Wide	15.3	5
Simetryn	FALSE	9.16	213.0	Wide	185.1	Wide	11.3	5
Simetryn	FALSE	9.16	213.0	Wide	170.1	Wide	11.3	10
Simetryn	FALSE	9.16	169.9	Wide	155.0	Wide	11.3	5
Spiromesifen	FALSE	13.71	273.0	Wide	255.1	Wide	18.4	5
Spiromesifen	FALSE	13.71	272.0	Wide	254.2	Wide	18.4	5
Spiromesifen	FALSE	13.71	272.0	Wide	209.2	Wide	18.4	10
Terbufos	FALSE	8.16	230.9	Wide	175.0	Wide	12.7	10
Terbufos	FALSE	8.16	230.9	Wide	129.0	Wide	12.7	20
Terbufos	FALSE	8.16	152.9	Wide	97.0	Wide	12.7	5
Terbumeton	FALSE	7.96	225.1	Wide	169.2	Wide	14.6	0
Terbumeton	FALSE	7.96	169.0	Wide	154.1	Wide	14.6	5
Terbumeton	FALSE	7.96	169.0	Wide	141.1	Wide	14.6	5
Terbuthylazine	FALSE	8.12	228.9	Wide	173.1	Wide	13.3	5
Terbuthylazine	FALSE	8.12	172.9	Wide	172.0	Wide	13.3	5
Terbuthylazine	FALSE	8.12	172.9	Wide	138.1	Wide	13.3	5
Terbutryn	FALSE	9.51	241.1	Wide	170.2	Wide	19.3	15
Terbutryn	FALSE	9.51	185.0	Wide	170.1	Wide	19.3	5
Terbutryn	FALSE	9.51	185.0	Wide	111.1	Wide	19.3	15
Tetrachlorvinphos	FALSE	11.13	329.0	Wide	108.9	Wide	18.3	25
Tetrachlorvinphos	FALSE	11.13	109.0	Wide	78.9	Wide	18.3	5
Tetrachlorvinphos	FALSE	11.13	78.9	Wide	47.0	Wide	18.3	10
Tetradifon	FALSE	14.40	226.9	Wide	199.0	Wide	39.9	15
Tetradifon	FALSE	14.40	158.9	Wide	131.0	Wide	39.9	10
Tetradifon	FALSE	14.40	158.9	Wide	111.0	Wide	39.9	20
Tetramethrin I	FALSE	13.79	164.0	Wide	107.1	Wide	17.5	10
Tetramethrin I	FALSE	13.79	164.0	Wide	77.1	Wide	17.5	25
Tetramethrin I	FALSE	13.79	123.0	Wide	81.1	Wide	17.5	10
Thionazin	FALSE	6.82	175.0	Wide	79.0	Wide	39.5	10
Thionazin	FALSE	6.82	143.0	Wide	79.0	Wide	39.5	10
Thionazin	FALSE	6.82	107.1	Wide	79.0	Wide	39.5	15

Compound Name	ISTD	RT (min)	Precursor Ion	MS1 Resolution	Product Ion	MS2 Resolution	Dwell	CE (eV)
THPI	FALSE	6.01	151.0	Wide	122.0	Wide	38.8	10
THPI	FALSE	6.01	151.0	Wide	79.0	Wide	38.8	10
Tolclofos-methyl	FALSE	9.23	267.0	Wide	252.0	Wide	10.8	15
Tolclofos-methyl	FALSE	9.23	267.0	Wide	93.0	Wide	10.8	30
Tolclofos-methyl	FALSE	9.23	125.0	Wide	79.0	Wide	10.8	5
Tolylfluanid	FALSE	10.63	238.0	Wide	137.0	Wide	7.7	15
Tolylfluanid	FALSE	10.63	137.0	Wide	91.1	Wide	7.7	20
Tolylfluanid	FALSE	10.63	137.0	Wide	65.0	Wide	7.7	35
Tralkoxydim	FALSE	14.75	137.0	Wide	109.0	Wide	46.3	5
Tralkoxydim	FALSE	14.75	137.0	Wide	57.0	Wide	46.3	10
Tralkoxydim	FALSE	14.75	109.0	Wide	57.0	Wide	46.3	5
Transfluthrin	FALSE	9.12	165.1	Wide	91.1	Wide	12.6	10
Transfluthrin	FALSE	9.12	163.1	Wide	143.1	Wide	12.6	20
Transfluthrin	FALSE	9.12	163.1	Wide	91.1	Wide	12.6	10
Triadimefon	FALSE	10.00	208.0	Wide	181.1	Wide	12.2	5
Triadimefon	FALSE	10.00	208.0	Wide	111.0	Wide	12.2	20
Triadimefon	FALSE	10.00	128.0	Wide	65.0	Wide	12.2	20
Triazophos	FALSE	12.64	161.2	Wide	134.2	Wide	39.4	5
Triazophos	FALSE	12.64	161.2	Wide	106.1	Wide	39.4	10
Triazophos	FALSE	12.64	161.2	Wide	91.0	Wide	39.4	15
Trichloronat	FALSE	10.20	298.8	Wide	270.9	Wide	13.1	10
Trichloronat	FALSE	10.20	296.8	Wide	268.9	Wide	13.1	10
Trichloronat	FALSE	10.20	268.9	Wide	223.0	Wide	13.1	20
Trifluralin	FALSE	7.25	306.1	Wide	264.0	Wide	20.0	5
Trifluralin	FALSE	7.25	264.0	Wide	206.0	Wide	20.0	5
Trifluralin	FALSE	7.25	264.0	Wide	160.1	Wide	20.0	15
Triphenyl phosphate	TRUE	13.35	326.0	Wide	325.0	Wide	19.6	5
Triphenyl phosphate	TRUE	13.35	232.9	Wide	215.1	Wide	19.6	10
Triphenyl phosphate	TRUE	13.35	214.9	Wide	168.1	Wide	19.6	15
Vinclozolin	FALSE	9.11	212.0	Wide	172.1	Wide	14.2	15
Vinclozolin	FALSE	9.11	197.9	Wide	145.0	Wide	14.2	15
Vinclozolin	FALSE	9.11	187.0	Wide	124.0	Wide	14.2	20

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