QuEChERS-Based LC/MS/MS Method for Multiresidue Pesticide Analysis in Fruits and Vegetables*

UCT Part Numbers

EC4MSSA50CT-MP 4 g anhydrous $MgSO_4$, 1.0 g Sodium Acetate	**ECMS12CPSA415CT** 1.2 g anhydrous $MgSO_4$, 400 mg PSA

Introduction:

A high-throughput, QuEChERS analytical method (LC-MS/MS) is described for the part per trillion (ppt) determination of 191 pesticides in orange, peach, spinach and ginseng. Pesticide classes include carbamates, polar organophosphates, phenylureas, anilides, benzoyl phenylureas, conazoles, macrocyclic lactone, neonicotinoids, strobilurines, and triazines. This method was validated by the U.S. Food and Drug Administration (FDA), National Research Centre for Grapes (NRCG), India, and Ontario Ministry of the Environment (MOE) laboratories.

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Analytes Covered in this Method			
Analyte	**CASRN**	**Analyte**	**CASRN**
Acephate	30560-19-1	Imazalil	35554-44-0
Acetamiprid	135410-20-7	Imidacloprid	138261-41-3
Acibenzolar-S-methyl	135158-54-2	Indoxacarb	173584-44-6
Alanycarb	83130-01-2	Ipconazole	125225-28-7
Aldicarb	116-06-3	Iprovalicarb	140923-17-7
Aldicarb sulfone	1646-88-4	Isoprocarb	2631-40-5
Aldicarb sulfoxide	1646-87-3	Isoproturon	34123-59-6
Ametryn	834-12-8	Isoxaflutole	141112-29-0
Aminocarb	2032-59-9	Ivermectin	70288-86-7
Amitraz	33089-61-1	Kresoxim-methyl	143390-89-0
Avermectin B_{1a}	65195-55-3	Linuron	330-55-2
Avermectin B_{1b}	65195-56-4	Lufenuron	103055-07-8
Azoxystrobin	131860-33-8	Mefenacet	73250-68-7
Benalaxyl	71626-11-4	Mepanipyrim	110235-47-7
Bendiocarb	22781-23-3	Mepronil	55814-41-0
Benfuracarb	82560-54-1	Mesotrione	104206-82-8
Benzoximate	29104-30-1	Metalaxyl	57837-19-1
Bifenazate	149877-41-8	Metconazole.1	125116-23-6
Bitertanol	55179-31-2	Methabenzhiazuron	18691-97-9
Boscalid	188425-85-6	Methamidophos	10265-92-6
Bromuconazole 46	116255-48-2	Methiocarb	2032-65-7
Bromuconazole 47	116255-48-2	Methomyl	16752-77-5
Bupirimate	41483-43-6	Methoprotryne	841-06-5
Buprofezin	953030-84-7	Methoxyfenozide	161050-58-4
Butafenacil	134605-64-4	Metobromuron	3060-89-7
Butocarboxin	34681-10-2	Metribuzin	21087-64-9
Butoxycarboxin	34681-23-7	Mevinphos-E	813-78-5
Carbaryl	63-25-2	Mevinphos-Z	7786-34-7
Carbendazim	10605-21-7	Mexacarbate	315-18-4
Carbetamide	16118-49-3	Monocrotophos	6923-22-4
Carbofuran	1563-66-2	Monolinuron	1746-81-2
Carbofuran, 3OH-	16655-82-6	Moxidectin	113507-06-5
Carboxin	5234-68-4	Myclobutanil	88671-89-0
Carfentrazone-ethyl	128639-02-1	Neburon	555-37-3
Chlorfluazuron	71422-67-8	Nitenpyram	150824-47-8
Chlorotoluron	15545-48-9	Novaluron	116714-46-6
Chloroxuron	1982-47-4	Nuarimol	63284-71-9
Clethodim	99129-21-2	Omethoate	1113-02-6
Clofentezine	74115-24-5	Oxadixyl	77732-09-3

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Analytes Covered in this Method			
Analyte	**CASRN**	**Analyte**	**CASRN**
Clothianidin	210880-92-5	Oxamyl	23135-22-0
Cyazofamid	120116-88-3	Paclobutrazol	76738-62-0
Cycluron	2163-69-1	Penconazole	66246-88-6
Cymoxanil	57966-95-7	Phenmedipham	13684-63-4
Cyproconazole A	94361-06-5	Picoxystrobin	117428-22-5
Cyproconazole B	94361-07-6	Piperonyl butoxide	51-03-6
Cyprodinil	121552-61-2	Pirimicarb	23103-98-2
Desmedipham	13684-56-5	Prochloraz	67747-09-5
Diclobutrazol	75736-33-3	Promecarb	2631-37-0
Dicrotophos	141-66-2	Prometon	1610-18-0
Diethofencarb	87130-20-9	Prometryn	7287-19-6
Difenoconazole	119446-68-3	Propamocarb	24579-73-5
Diflubenzuron	35367-38-5	Propargite	2312-35-8
Dimethoate	60-51-5	Propham	122-42-9
Dimethomorph A	110488-70-5	Propiconazole	60207-90-1
Dimethomorph B	2274-67-1	Propoxur	114-26-1
Dimoxystrobin	149961-52-4	Pymetrozine	123312-89-0
Diniconazole	83657-24-3	Pyracarbolid	24691-76-7
Dioxacarb	6988-21-2	Pyraclostrobin	175013-18-0
Diuron	330-54-1	Pyridaben	96489-71-3
Doramectin	117704-25-3	Pyrimethanil	53112-28-0
Emamectin B_{1a}	155569-91-8	Pyriproxyfen	95737-68-1
Epoxiconazole	133855-98-8	Quinoxyfen	124495-18-7
Eprinomectin B_{1a}	123997-26-2	Rotenone	83-79-4
Etaconazole	60207-93-4	Secbumeton	372137-35-4
Ethiofencarb	29973-13-5	Siduron	26259-45-0
Ethiprole	181587-01-9	Simetryne	1014-70-6
Ethofumesate	26225-79-6	Spinosyn A	168316-95-8
Etoxazole	153233-91-1	Spirodiclofen	148477-71-8
Famoxadone	131807-57-3	Spiromefesin	283594-90-1
Fenamidone	161326-34-7	Spiroxamine	118134-30-8
Fenarimol	60168-88-9	Sulfentrazone	122836-35-5
Fenazaquin	120928-09-8	Tebuconazole	107534-96-3
Fenbuconazole	114369-43-6	Tebufenozide	112410-23-8
Fenhexamid	126833-17-8	Tebufenpyrad	119168-77-3
Fenoxycarb	79127-80-3	Tebuthiuron	34014-18-1
Fenpropimorph	67564-91-4	Teflubenzuron	83121-18-0
Fenpyroximate	134098-61-6	Terbumeton	33693-04-8
Fenuron	134098-61-6	Terbutryne	886-50-0

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Analytes Covered in this Method			
Analyte	**CASRN**	**Analyte**	**CASRN**
Fludioxinil	131341-86-1	Tetraconazole	112281-77-3
Flufenacet	142459-58-3	Thiabendazole	148-79-8
Flufenoxuron	101463-69-8	Thiacloprid	111988-49-9
Fluometuron	2164-17-2	Thiamethoxam	153719-23-4
Fluoxastrobin	361377-29-9	Thidiazuron	51707-55-2
Fluquinconazole	136426-54-5	Thiobencarb	28249-77-6
Flusilazole	85509-19-9	Thiofanox	39196-18-4
Flutolanil	66332-96-5	Thiophanate-methyl	23564-05-8
Flutriafol	76674-21-0	Triadimefon	43121-43-3
Forchlorfenuron	68157-60-8	Triadimenol	55219-65-3
Formetanate HCl	22259-30-9	Tricyclazole	41814-78-2
Fuberidazole	3878-19-1	Trifloxystrobin	141517-21-7
Furalaxyl	57646-30-7	Triflumizole	99387-89-0
Furathiocarb	65907-30-4	Triflumuron	64628-44-0
Hexaconazole	79983-71-4	Triticonazole	131983-72-7
Hexythiazox	78587-05-0	Vamidothion	2275-23-2
Hydramethylnon	67485-29-4	Zoxamide	156052-68-5

Deuterium Isotope Internal Standards	
D10-Diazinon	D6-diuron
D6-Dichlorvos	D6-Linuron
D6-Dimethoate	D6-Malathion

CDN-Isotopes (Montreal, QC, Canada)

Analytical Stock Solutions:

Prepare separate stock solutions of analytical standards, including the isotope labeled internal standards (ILIS) for individual compounds.

- weigh 10-75 mg each and dissolve in 10 or 25mL of acetonitrile, methanol, or methanol/water (50:50 v/v) in volumetric flasks
- prepare intermediate solutions in 100mL volumetric flasks by mixing stock solutions
- Prepare five levels of matrix-matched calibration standards from intermediate solutions by using sample matrix extract and matrix buffer (20 mM ammonium formate) in concentrations of 1, 5, 10, 50, and 100 ppb
- Add the ILIS solution prior to sample preparation and use as an internal standard in the quantitative analysis

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Procedure:

1. Sample Preparation--orange, peach, spinach

a) Weigh 10 ± 0.1 g of cryoground sample into 50 mL centrifuge tube
b) Add 10 mL of 1% acetic acid in acetonitrile and contents of **EC4MSSA50CT-MP** pouch
c) Shake by hand then add 200 µL of surrogate solution and a steel ball
d) Place on a Geno/Grinder shaker (or equivalent) for 1 min @ 1000 strokes/minute
e) When shaking is complete centrifuge @ 4500 rpm for 5 min
f) Transfer 9 mL of supernatant to a 15 mL centrifuge tube containing **ECMS12CPSA415CT**
g) Shake on Geno/Grinder for 1 min @ 500 strokes/min
h) Centrifuge @ 4500 rpm for 5 min
i) Transfer 2.0 mL of supernatant to injection vials for analysis. Filter cloudy extracts using 0.2 nylon or PTFE membrane filter directly into the LC autosampler vials

2. Calibration Standards-- orange, peach, spinach

a) Prepare matrix-matched calibration standards by mixing 300 µL of 0.0167, 0.033, 0.067, 0.167, and 0.333 ppm standard solutions. Use 200 µL of matrix blank extracts and 500 µL of 20 mM ammonium formate sample buffer
b) Add 500 µL of sample buffer just prior to sample analysis
c) Filter cloudy extracts using 0.2 nylon or PTFE membrane filter directly into the LC autosampler vials
d) Filtered samples should be clear and can be stored in a freezer until analysis

1a. Sample Preparation--ginseng

a) Prepare ginseng samples by using 1.0 ± 0.05 g of ginseng
b) Add 10 mL of HPLC-grade water and a steel ball bearing
c) Shake on a GenoGrinder at 1000 strokes/min for 1 minute
d) Add 10 mL of 1% acetic acid in acetonitrile, 200 µL of surrogate solution and contents of **EC4MSSA50CT-MP** pouch
e) Shake by hand
f) Place on a Geno/Grinder shaker (or equivalent) for 1 min @ 1000 strokes/minute
g) When shaking is complete centrifuge @ 4500 rpm for 5 min
h) Transfer 9 mL of supernatant to a 15 mL centrifuge tube containing **ECMS12CPSA415CT**
i) Shake on Geno/Grinder for 1 min @ 500 strokes/min
j) Centrifuge @ 4500 rpm for 5 min
k) Transfer 2.0 mL of supernatant to injection vials for analysis. Filter cloudy extracts using 0.2 nylon or PTFE membrane filter directly into the LC autosampler vials

2a. Calibration Standards--ginseng

a) Prepare matrix-matched calibration standards by adding 100 µL of 0.033, 0.067, 0.167, 0.333,0.8, 1.6 ppm standard solutions to 400 µL of ginseng blank extracts
b) Add 500 µL of sample matrix buffer just prior to analysis to achieve matrixmatched calibration standards of 1.67, 3.33, 6.67, 16.7, 33.3, 80, and 160 ppb, respectively
c) Filter using 0.2 m Nylon or PTFE membrane filters
d) Filtered samples should be clear and can be stored in a freezer until analysis

3. Sample Analysis

a) HPLC analysis with Shimadzu Prominence/20 series (Columbia, MD) or equivalent interfaced to an ABSciex (Forest City, CA) 4000QTrapmass spectrometer through an ESI interface (IonSpray)
b) Acquire MRM data in positive ion mode
c) Identify target pesticides using two specific MRM transitions for each pesticide to achieve an identification point (IP) of 4
d) Quantify using either external standard calibration (NRCG) or internal standard calibration (FDA and MOE) with $^{2}H_{10}$-diazinon as IS
e) Use N_2 of 99% purity from a nitrogen generator (Parker Balston, Haverhill, MA) in the ESI source and the collision cell
f) Restek LC column (Bellefonte, PA; Ultra Aqueous, C-18, 100 x 2.1 mm, 3 µm) and guard column (Ultra Aqueous, C-18 cartridges, 10 x 2.1 mm in guard cartridge holder) or equivalent
g) Curtain, collision, nebulizer, auxiliary gases, and source temperature of the ESI source were set at 15, 6, 35, and 45 psi and 450° C, respectively
h) Ion spray voltage: 5200
i) Declustering potential (DP), collision energy (CE), and collision cell exit potential (CXP) are optimized by direct infusion. The two most intense ion pairs of each analyte are chosen for the analysis. Values of DP, CE, and CXP and the two specific, most intense MRM pairs are listed in Table 3. Principal component analysis (PCA) is carried out using Infometrix Pirouette 4 (Bothell, WA)
j) Table 2 lists mobile phases, column temperatures, injection volume, flow rate, and LC gradient parameters

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HPLC Gradient Elution Parameters	
Mobile Phase	**A:** 5 mM ammonium formate, 0.1% formic acid in water **B:** 5 mM ammonium formate, 0.1% formic acid in MeOH
Column Temperature	35°C
Flow Rate	0.3 mL/min
Total Run Time	14.0 min
Gradient Program	10% B at 0 min, hold for 1 min 5% B at 0 min 20% B at 0 min to 98%
Injection Volume	20 µL

DP: declustering potential, V; CE: collision energy, V; CXP: collision cell exit potential

Pesticide	Formula	Mol Wt	MRM Transitions #1 & #2	DP	CE	CXP
Carbofuran, 3OH-	$C_{12}H_{15}NO_4$	237	238→163 / 181	66	21	16
Acephate	$C_4H_{10}NO_3PS$	183	184→143 / 49	61	13	4
Acetamiprid	$C_{10}H_{11}N_3ClN_4$	223	223→126 / 99	61	29	12
Acibenzolar-S-methyl	$C_8H_6N_2OS_2$	210	211→136 / 140	46	39	9
Alanycarb	$C_{17}H_{25}N_3O_4S_2$	400	400→238 / 91	35	14	4
Aldicarb sulfoxide	$C_7H_{14}N_2O_3S$	206	207→132 / 89	30	10	8
Aldicarb	$C_7H_{14}N_2O_2S$	190	208→116 / 89	36	11	10
Aldicarb sulfone	$C_7H_{14}N_2O_4S$	222	223→86 / 148	52	21	5
Ametryn	$C_9H_{17}N_5S$	227	209→152 / 137	71	21	8
Aminocarb	$C_{11}H_{16}N_2O_2$	208	209→152 / 137	71	21	8
Amitraz	$C_{19}H_{23}N_3$	293	294→163 / 107	46	21	4
Avermectin B_{1a}	$C_{48}H_{72}O_{14}$	873	895→751 / 449	176	61	20
Avermectin B_{1b}	$C_{48}H_{70}O_{14}$	859	890→567 / 305	76	23	18
Azoxystrobin	$C_{22}H_{17}N_3O_5$	403	404→372 / 344	51	19	4
Benalaxyl	$C_{20}H_{23}NO_3$	325	326→148 / 294	71	31	8
Bendiocarb	$C_{11}H_{13}NO_4$	223	224→109 / 167	61	27	20
Benfuracarb	$C_{20}H_{30}N_2O_5S$	411	411→195 / 252	50	30	4
Benzoximate	$C_{18}H_{18}ClNO_5$	364	364→199 / 105	51	13	14
Bifenazate	$C_{17}H_{20}N_2O_3$	300	301→170 / 198	61	29	10
Bitertanol	$C_{20}H_{23}N_3O_2$	337	338→70 / 269	51	31	12
Boscalid	$C_{18}H_{12}Cl_2N_2O$	343	343→307 / 140	91	27	4
Bromuconazole 46	$C_{13}H_{12}BrCl_2N_3O$	377	378→159 / 70	61	37	14
Bromuconazole 47	$C_{13}H_{12}BrCl_2N_3O$	377	378→159 / 70	61	37	14
Bupirimate	$C_{13}H_{24}N_4O_3S$	316	317→166 / 108	86	33	12

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DP: declustering potential, V; CE: collision energy, V; CXP: collision cell exit potential						
Pesticide	**Formula**	**Mol Wt**	**MRM Transitions #1 & #2**	**DP**	**CE**	**CXP**
Buprofezin	$C_{16}H_{23}N_3OS$	305	306→201 / 116	46	17	4
Butafenacil	$C_{20}H_{18}ClF_3N_2O_6$	475	492→331 / 349	61	35	20
Butocarboxin	$C_7H_{14}N_2O_2S$	190	213→75 / 116	50	20	5
Butoxycarboxin	$C_7H_{14}N_2O_4S$	222	223→106 / 166	45	15	8
Carbaryl	$C_{12}H_{11}NO_2$	201	202→145 / 127	56	15	10
Carbendazim	$C_9H_9N_3O_2$	191	192→160 / 132	80	24	10
Carbetamide	$C_{12}H_{16}N_2O_3$	236	237→192 / 118	56	13	12
Carbofuran	$C_{12}H_{15}NO_3$	221	222→123 / 165	66	31	22
Carboxin	$C_{12}H_{13}NO_2S$	235	484→452 / 285	66	23	14
Carfentrazone-ethyl	$C_{13}H_{10}Cl_2F_3N_3O_3$	412	412→346 / 366	81	31	4
Chlorfluazuron	$C_{20}H_9Cl_3F_5N_3O_3$	541	540→158 / 383	91	27	4
Chlorotoluron	$C_{10}H_{13}ClN_2O$	213	213→72 / 46	61	31	4
Chloroxuron	$C_{15}H_{15}ClNO_2$	291	291→72 / 218	65	30	4
Clethodim	$C_{17}H_{26}ClNO_3S$	360	360→164 / 268	61	29	10
Clofentezine	$C_{14}H_8Cl_2N_4$	303	303→138 / 102	61	23	8
Clothianidin	$C_6H_8ClN_5O_2S$	250	250→169 / 132	51	17	4
Cyazofamid	$C_{13}H_{13}ClN_4O_2S$	325	325→108 / 261	61	21	10
Cycluron	$C_{11}H_{22}N_2O$	198	199→89 / 72	50	21	4
Cymoxanil	$C_7H_{10}N_4O_3$	198	199→128 / 111	60	13	4
Cyproconazole A	$C_{15}H_{18}ClN_3O$	292	292→70 / 125	66	39	12
Cyproconazole B	$C_{15}H_{18}ClN_3O$	292	292→70 / 125	66	39	12
Cyprodinil	$C_{14}H_{15}N_3$	225	226→93 / 77	101	51	16
Desmedipham	$C_{16}H_{16}N_2O_4$	300	318→182 / 136	41	19	12
Diclobutrazol	$C_{15}H_{19}Cl_2N_3O$	328	328→70 / 158	81	49	12
Dicrotophos	$C_8H_{16}NO_5P$	237	238→112 / 193	66	19	8
Diethofencarb	$C_{14}H_{21}NO_4$	267	268→226 / 124	61	15	14
Difenoconazole	$C_{19}H_{17}Cl_2N_3O_3$	406	406→251 / 253	81	37	16
Diflubenzuron	$C_{14}H_9Cl_2FN_2O_2$	311	311→158 / 141	71	23	10
Dimethoate	$C_5H_{12}NO_3PS_2$	229	230→199 / 125	50	14	15
Dimethomorph A	$C_{21}H_{22}ClNO_4$	388	388→301 / 165	66	25	4
Dimethomorph B	$C_{21}H_{22}ClNO_4$	388	388→301 / 165	66	25	4
Dimoxystrobin	$C_{19}H_{22}N_2O_3$	326	327→205 / 116	40	15	4
Diniconazole	$C_{15}H_{17}Cl_2N_3O$	326	326→70 / 158	86	51	12
Dioxacarb	$C_{11}H_{13}NO_4$	223	224→167 / 123	51	13	10
Diuron	$C_9H_{10}Cl_2N_2O$	233	233→72 / 72	56	33	4
Doramectin	$C_{50}H_{74}O_{14}$	899	921→777 / 449	71	65	15
Fenpyroximate	$C_{24}H_{27}N_3O_4$	422	422→366 / 135	56	23	4
Emamectin B_{1a}	$C_{49}H_{75}NO_{13}$	886	886→158 / 82	111	51	10
Epoxiconazole	$C_{17}H_{13}ClFN_3O$	330	330→121 / 101	66	29	10
Eprinomectin B_{1a}	$C_{50}H_{75}NO_{14}$	914	914→186 / 154	76	27	12
Etaconazole	$C_{14}H_{15}Cl_2N_3O_2$	328	328→159 / 205	46	37	10

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DP: declustering potential, V; CE: collision energy, V; CXP: collision cell exit potential						
Pesticide	**Formula**	**Mol Wt**	**MRM Transitions #1 & #2**	**DP**	**CE**	**CXP**
Ethiofencarb	$C_{11}H_{15}NO_2S$	225	226→106 / 164	41	21	4
Ethiprole	$C_{13}H_9Cl_2F_3N_4OS$	397	397→350 / 255	81	29	24
Ethofumesate	$C_{13}H_{18}O_5S$	286	287→121 / 259	81	23	8
Etoxazole	$C_{21}H_{23}F_2NO_2$	359	360→141 / 57	76	45	4
Famoxadone	$C_{22}H_{18}N_2O_4$	374	392→331 / 238	31	15	4
Fenamidone	$C_{17}H_{17}N_3OS$	311	312→92 / 236	66	39	16
Fenarimol	$C_{17}N_{12}Cl_2N_2O$	331	331→268 / 81	61	31	4
Fenazaquin	$C_{20}H_{22}N_2O$	306	307→161 / 147	71	25	12
Fenbuconazole	$C_{19}H_{17}ClN_4$	337	337→124 / 70	81	41	8
Fenhexamid	$C_{14}H_{17}Cl_2NO_2$	302	302→97 / 55	66	35	18
Fenoxycarb	$C_{17}H_{19}NO_4$	301	302→88 / 116	66	31	6
Fenpropimorph	$C_{20}H_{33}NO$	303	304→147 / 117	66	39	4
Fenuron	$C_9H_{12}N_2O$	164	165v72 / 46	56	25	4
Fludioxinil	$C_{12}H_6F_2N_2O_2$	248	266→229 / 227	41	23	14
Flufenacet	$C_{14}H_{13}F_4N_3O_2S$	363	364→152 / 194	51	29	10
Flufenoxuron	$C_{21}H_{11}ClF_6N_2O_3$	489	489→158 / 141	86	29	10
Fluometuron	$C_{10}H_{11}F_3N_2O$	232	233→72 / 46	71	37	12
Fluoxastrobin	$C_{21}H_{16}ClFN_4O_5$	459	459→427 / 188	55	28	4
Fluquinconazole	$C_{16}H_8Cl_2FN_5O$	376	376→307 / 349	71	33	4
Flusilazole	$C_{16}H_{15}F_2N_3Si$	315	316→247 / 165	81	27	16
Flutolanil	$C_{17}H_{16}F_3NO_2$	323	324→262 / 242	76	27	16
Flutriafol	$C_{16}H_{13}F_2N_3O$	301	302→70 / 123	66	37	12
Forchlorfenuron	$C_{12}H_{10}ClN_3O$	248	248→129 / 93	52	25	4
Formetanate HCl	$C_{11}H_{15}N_3O_2$	221	222→165 / 120	60	21	12
Fuberidazole	$C_{11}H_8N_2O$	184	185→157 / 65	81	33	14
Furalaxyl	$C_{17}H_{19}NO_4$	301	302→95 / 242	56	41	18
Furathiocarb	$C_{18}H_{26}N_2O_5S$	382	383→195 / 252	76	27	12
Hexaconazole	$C_{14}H_{17}Cl_2N_3O$	314	314→70 / 159	56	41	12
Hexaflumuron	$C_{16}H_8Cl_2F_6N_2O_3$	461	461→158 / 141	56	25	4
Hexythiazox	$C_17H_{21}ClN_2O_2S$	353	353→228 / 168	61	23	14
Hydramethylnon	$C_{25}H_{24}F6N_4$	494	495→323 / 151	146	45	20
Imazalil	$C_{14}H_{14}Cl_2N_2O$	297	297→159 / 201	66	33	14
Imidacloprid	$C_9H_{10}ClN_5O_2$	256	256→209 / 175	61	23	12
Indoxacarb	$C_{22}H_{17}ClF_3N_3O_7$	528	528→203 / 218	86	55	12
Ipconazole	$C_{18}H_{24}ClN_3O$	334	334→70 / 125	76	55	12
Iprovalicarb	$C_{18}H_{28}N_2O_3$	320	321→119 / 203	66	29	8
Isoprocarb	$C_{11}H_{15}NO_2$	193	194→95 / 137	61	23	16
Isoproturon	$C_{12}H_{18}N_2O$	206	207→72 / 46	66	29	4
Isoxaflutole	$C_{15}H_{12}F_2NO_4S$	359	377→251 / 360	36	41	16
Ivermectin	$C_{48}H_{74}O_{14}$	875	897→754 / 610	65	65	8
Kresoxim-methyl	$C_{18}H_{19}NO_4$	313	314→116 / 206	51	21	4

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DP: declustering potential, V; CE: collision energy, V; CXP: collision cell exit potential						
Pesticide	**Formula**	**Mol Wt**	**MRM Transitions #1 & #2**	**DP**	**CE**	**CXP**
Linuron	$C_9H_{10}Cl_2N_2O_2$	249	249→160 / 182	61	23	4
Lufenuron	$C_9H_{10}Cl_2N_2O_2$	511	511→158 / 141	61	27	4
Mefenacet	$C_{16}H_{14}N_2O_2S$	298	299→148 / 120	56	21	10
Mepanipyrim	$C_{14}H_{13}N_3$	223	224→106 / 77	86	37	8
Mepronil	$C_{17}H_{19}NO_2$	269	270→119 / 228	76	33	8
Mesotrione	$C_{14}H_{13}NO_7S$	339	357→228 / 288	60	31	9
Metalaxyl	$C_{15}H_{21}NO_4$	279	280→220 / 192	61	21	14
Metconazole.1	$C_{17}H_{22}ClN_3O$	319	320→70 / 125	81	51	12
Methabenzhiazuron	$C_{10}H_{11}N_3OS$	221	222→165 / 150	51	21	4
Methamidophos	$C_2H_8NO_2PS$	141	142→94 / 125	55	20	4
Methiocarb	$C_{11}H_{15}NO_2S$	225	226→169 / 121	61	13	12
Methomyl	$C_5H_{10}N_2O_2S$	162	163→88 / 106	35	12	5
Methoprotryne	$C_{11}H_{21}N_5OS$	271	272→240 / 198	50	27	4
Methoxyfenozide	$C_{22}H_{28}N_2O_3$	368	369→149 / 313	56	25	10
Metobromuron	$C_9H_{11}BrN_2O_2$	259	259→170 / 148	56	23	4
Metribuzin	$C_8H_{14}N_4OS$	214	215→84 / 187	71	29	4
Mevinphos-Z	$C_7H_{13}O_6P$	224	225→127 / 193	55	20	8
Mevinphos-E	$C_7H_{13}O_6P$	224	225→127 / 193	55	20	8
Mexacarbate	$C_{12}H_{18}N_2O_2$	222	223→166 / 151	66	23	12
Monocrotophos	$C_7H_{14}NO_5P$	223	224→127 / 98	51	23	12
Monolinuron	$C_9H_{11}ClN_2O_2$	215	215→126 / 99	51	23	4
Moxidectin	$C_{37}H_{53}NO_8$	640	662→549 / 467	90	45	16
Myclobutanil	$C_{15}H_{17}ClN_4$	289	289→70 / 125	71	37	12
Neburon	$C_{12}H_{16}Cl_2N_2O$	275	275→88 / 114	56	23	4
Nitenpyram	$C_{11}H_{15}ClN_4O_2$	271	271→225 / 126	51	17	14
Novaluron	$C_{17}H_9ClF_8N_2O4$	493	493→158 / 141	71	27	4
Nuarimol	$C_{17}H_{12}ClFN_2O$	315	315→252 / 81	81	31	16
Omethoate	$C_5H_{12}NO_4PS$	213	214→124 / 182	46	29	4
Oxadixyl	$C_{14}H_{18}N_2O_4$	278	279→219 / 132	61	17	14
Oxamyl	$C_7H_{13}N_3O_3S$	219	237→72 / 90	36	25	4
Paclobutrazol	$C_{15}H_{20}ClN_3O$	294	294→70 / 125	66	49	12
Penconazole	$C_{13}H_{15}Cl_2N_3$	284	284→159 / 70	71	39	10
Phenmedipham	$C_{16}H_{16}N_2O_4$	300	301→136 / 168	50	26	4
Picoxystrobin	$C_{18}H_{16}F_3NO_4$	367	368→145 / 205	56	27	4
Piperonyl butoxide	$C_{19}H_{30}O_5$	338	356→177 / 119	51	19	10
Pirimicarb	$C_{11}H_{18}N_4O_2$	238	239→72 / 182	66	35	12
Prochloraz	$C_{15}H_{16}Cl_3N_3O_2$	377	376→308 / 70	46	17	10
Promecarb	$C_{12}H_{17}NO_2$	207	208→109 / 151	36	23	8
Prometon	$C_{10}H_{19}N_5O$	225	226→142 / 86	76	33	10
Prometryn	$C_{10}H_{19}N_5S$	241	242→200 / 158	71	19	4
Propamocarb	$C_9H_{20}N_2O_2$	188	189→102 / 144	61	25	8

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Pesticide	**Formula**	**Mol Wt**	**MRM Transitions #1 & #2**	**DP**	**CE**	**CXP**
Propargite	$C_{19}H_{26}O_4S$	350	368→231 / 175	46	15	14
Propham	$C_{10}H_{13}NO_2$	179	180→138 / 120	36	13	10
Propiconazole	$C_{15}H_{17}Cl_2N_3O_2$	342	342→159 / 69	61	39	10
Propoxur	$C_{11}H_{15}NO_3$	209	210→111 / 168	39	19	6
Pymetrozine	$C_{10}H_{11}H_5O$	217	218→105 / 78	71	27	4
Pyracarbolid	$C_{13}H_{15}NO_2$	217	218→125 / 97	61	27	8
Pyraclostrobin	$C_{19}H_{18}ClN_3O_4$	388	388→194 / 163	31	19	4
Pyridaben	$C_{19}H_{25}ClN_2OS$	365	365→147 / 309	46	31	4
Pyrimethanil	$C_{12}H_{13}N_3$	199	200→107 / 82	71	33	4
Pyriproxyfen	$C_{20}H_{19}NO_3$	321	322→96 / 185	46	21	4
Quinoxyfen	$C_{15}H_8Cl_2FNO$	308	308→162 / 197	81	65	10
Rotenone	$C_{23}H_{22}O_6$	394	395→213 / 192	91	33	14
Secbumeton	$C_{10}H_{15}N_5O$	225	226→170 / 100	50	35	4
Siduron	$C_{14}H_{20}N_2O$	232	233→137 / 94	66	21	4
Simetryne	$C_8H_{15}N_5S$	213	214→124 / 144	51	27	4
Spinosyn A	$C_{41}H_{65}NO_{10}$	732	748→142 / 98	86	45	8
Spirodiclofen	$C_{21}H_{24}Cl_2O_4$	411	411→313 / 71	71	17	8
Spiromefesin	$C_{23}H_{30}O_4$	370	371→273 / 255	71	19	8
Spiroxamine	$C_{18}H_{35}NO_2$	297	298→144 / 100	76	29	12
Sulfentrazone	$C_{11}H_{10}Cl_2F_2N_4O_3S$	387	387→307 / 146	81	27	4
Tebuconazole	$C_{16}H_{22}ClN_3O$	308	308→70 / 125	81	49	12
Tebufenozide	$C_{22}H_{28}N_2O_2$	352	353→133 / 297	51	25	10
Tebufenpyrad	$C_{18}H_{24}ClN_3O$	334	334→117 / 145	71	47	4
Tebuthiuron	$C_9H_{16}N_4OS$	228	229→172 / 116	46	21	4
Teflubenzuron	$C_{14}H_6Cl_2F_4N_2O_2$	381	381→141 / 158	66	53	4
Terbumeton	$C_{10}H_{19}N_5O$	225	226→170 / 100	76	27	12
Terbutryne	$C_{10}H_{19}N_5S$	241	242→186 / 68	71	27	12
Tetraconazole	$C_{13}H_{11}Cl_2F_4N_3O$	372	372→159 / 70	76	45	10
Thiabendazole	$C_{10}H_7N_3S$	201	202→175 / 131	85	35	12
Thiacloprid	$C_{10}H_9ClN_4S$	253	253→126 / 99	71	31	10
Thiamethoxam	$C_8H_{10}ClN_5O_3S$	292	292→211 / 181	61	19	12
Thidiazuron	$C_9H_8N_4OS$	220	221→102 / 127	66	21	4
Thiobencarb	$C_{12}H_{16}ClNOS$	258	258→125 / 89	56	27	8
Thiofanox	$C_9H_{18}N_2O_2S$	218	219→76 / 57	36	20	8
Thiophanate-methyl	$C_{12}H_{14}N_4O_4S_2$	342	343→151 / 311	61	29	14
Triadimefon	$C_{14}H_{16}ClN_3O_2$	294	294→197 / 225	66	23	14
Triadimenol	$C_{14}H_{18}ClN_3O_2$	296	296→70 / 227	46	31	12
Tricyclazole	$C_9H_7N_3S$	189	190→163 / 136	81	33	10
Trifloxystrobin	$C_{20}H_{19}F_3N_2O_4$	408	409→186 / 206	31	23	4
Triflumizole	$C_{15}H_{15}ClF_3N_3O$	346	346→278 / 73	51	15	8
Triflumuron	$C_{15}H_{10}ClF_3N_2O_3$	359	359→156 / 139	51	23	4
Triticonazole	$C_{17}H_{20}ClN_3O$	318	318→70 / 125	66	45	12
Vamidothion	$C_8H_{18}NO_4PS_2$	287	288→146 / 118	61	19	10
Zoxamide	$C_{14}H_{16}Cl_3NO_2$	337	336→187 / 159	45	35	15
D10-Diazinon	$C_{12}D_{10}H_{11}N_2O_3PS$	314	315→170	50	29	4
D6-Dimethoate	$C_5D_6H_6NO_3PS_2$	235	236→131	50	30	4
D6-diuron	$C_9D_6H_4Cl_2N_2O$	239	239→78	90	30	4
D6-Linuron	$C_9D_6H_4Cl_2N_2O_2$	255	255→166	90	30	4
D6-Dichlorvos	$C_4D_6H_1Cl_2O_4P$	227	227→115	70	27	4
D6-Malathion	$C_{10}D_6H_{13}O_6PS_2$	330	337→291	55	12	4

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References:

[1] *Summarized with permission from Wong, Jon, Hao, Chunyan, Zhang, Kai, et al., J. Agric. Food Chem. 2010, 58, 5897–5903 5897, DOI:10.1021/jf903849n

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