



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

UCT Products:

EC4MSSA50CT-MP (4 g anhydrous MgSO₄, 1.0 g Sodium Acetate)

ECMS12CPSA415CT (1.2 g anhydrous MgSO₄, 400 mg PSA)

July 18, 2011

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.

Analytes Covered in this Method

Table 1

| 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 | lprovalicarb | 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 | Methabenzthiazuron | 18691-97-9 |

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|------------------------------|-------------|--------------------|-------------|
| 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 |
| 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 |
| Epoconazole | 133855-98-8 | Quinoxifen | 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 |

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|-----------------|-------------|--------------------|-------------|
| 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 |
| 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

Procedures

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 μ L 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
- a) Add 10 mL of HPLC-grade water and a steel ball bearing
- b) Shake on a GenoGrinder at 1000 strokes/min for 1 minute
- c) Add 10 mL of 1% acetic acid in acetonitrile, 200 µL of surrogate solution and contents of **EC4MSSA50CT-MP** pouch
- d) Shake by hand
- e) Place on a Geno/Grinder shaker (or equivalent) for 1 min @ 1000 strokes/minute
- f) When shaking is complete centrifuge @ 4500 rpm for 5 min
- g) Transfer 9 mL of supernatant to a 15 mL centrifuge tube containing **ECMS12CPSA415CT**
- h) Shake on Geno/Grinder for 1 min @ 500 strokes/min
- i) Centrifuge @ 4500 rpm for 5 min
- j) 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 matrix-matched 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) 4000QTrap mass 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 $^2\text{H}_{10}$ -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

Table 2

| HPLC Gradient Elution Parameters | |
|---|---|
| Mobil 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 |

Table 3

| 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 ₄ H ₁₀ NO ₃ PS | 183 | 184→143 / 49 | 61 | 13 | 4 |
| Acetamiprid | C ₁₀ H ₁₁ N ₃ CIN ₄ | 223 | 223→126 / 99 | 61 | 29 | 12 |
| Acibenzolar-S-methyl | C ₈ H ₆ N ₂ OS ₂ | 210 | 211→136 / 140 | 46 | 39 | 9 |
| Alanycarb | C ₁₇ H ₂₅ N ₃ O ₄ S ₂ | 400 | 400→238 / 91 | 35 | 14 | 4 |
| Aldicarb sulfoxide | C ₇ H ₁₄ N ₂ O ₃ S | 206 | 207→132 / 89 | 30 | 10 | 8 |
| Aldicarb | C ₇ H ₁₄ N ₂ O ₂ S | 190 | 208→116 / 89 | 36 | 11 | 10 |
| Aldicarb sulfone | C ₇ H ₁₄ N ₂ O ₄ S | 222 | 223→86 / 148 | 52 | 21 | 5 |
| Ametryn | C ₉ H ₁₇ N ₅ S | 227 | 209→152 / 137 | 71 | 21 | 8 |
| Aminocarb | C ₁₁ H ₁₆ N ₂ O ₂ | 208 | 209→152 / 137 | 71 | 21 | 8 |
| Amitraz | C ₁₉ H ₂₃ N ₃ | 293 | 294→163 / 107 | 46 | 21 | 4 |
| Avermectin B1a | C ₄₈ H ₇₂ O ₁₄ | 873 | 895→751 / 449 | 176 | 61 | 20 |
| Avermectin B1b | C ₄₈ H ₇₀ O ₁₄ | 859 | 890→567 / 305 | 76 | 23 | 18 |
| Azoxystrobin | C ₂₂ H ₁₇ N ₃ O 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 ₂ O ₅ S | 411 | 411→195 / 252 | 50 | 30 | 4 |
| Benzoximate | C ₁₈ H ₁₈ CINO ₅ | 364 | 364→199 / 105 | 51 | 13 | 14 |
| Bifenazate | C ₁₇ H ₂₀ N ₂ O ₃ | 300 | 301→170 / 198 | 61 | 29 | 10 |
| Bitertanol | C ₂₀ H ₂₃ N ₃ O ₂ | 337 | 338→70 / 269 | 51 | 31 | 12 |
| Boscalid | C ₁₈ H ₁₂ Cl ₂ N ₂ O | 343 | 343→307 / 140 | 91 | 27 | 4 |
| Bromuconazole 46 | C ₁₃ H ₁₂ BrC ₁₂ N ₃ O | 377 | 378→159 / 70 | 61 | 37 | 14 |
| Bromuconazole 47 | C ₁₃ H ₁₂ BrC ₁₂ N ₃ O | 377 | 378→159 / 70 | 61 | 37 | 14 |
| Bupirimate | C ₁₃ H ₂₄ N ₄ O ₃ S | 316 | 317→166 / 108 | 86 | 33 | 12 |
| Buprofezin | C ₁₆ H ₂₃ N ₃ OS | 305 | 306→201 / 116 | 46 | 17 | 4 |
| Butafenacil | C ₂₀ H ₁₈ ClF ₃ N ₂ O ₆ | 475 | 492→331 / 349 | 61 | 35 | 20 |
| Butocarboxin | C ₇ H ₁₄ N ₂ O ₂ S | 190 | 213→75 / 116 | 50 | 20 | 5 |
| Butoxycarboxin | C ₇ H ₁₄ N ₂ O ₄ S | 222 | 223→106 / 166 | 45 | 15 | 8 |
| Carbaryl | C ₁₂ H ₁₁ NO ₂ | 201 | 202→145 / 127 | 56 | 15 | 10 |
| Carbendazim | C ₉ H ₉ N ₃ O ₂ | 191 | 192→160 / 132 | 80 | 24 | 10 |
| Carbetamide | C ₁₂ H ₁₆ N ₂ O 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 ₂ S | 235 | 484→452 / 285 | 66 | 23 | 14 |
| Carfentrazone-ethyl | C ₁₃ H ₁₀ Cl ₂ F ₃ N ₃ O ₃ | 412 | 412→346 / 366 | 81 | 31 | 4 |
| Chlorfluazuron | C ₂₀ H ₉ Cl ₃ F ₅ N ₃ O ₃ | 541 | 540→158 / 383 | 91 | 27 | 4 |
| Chlorotoluron | C ₁₀ H ₁₃ CIN ₂ O | 213 | 213→72 / 46 | 61 | 31 | 4 |
| Chloroxuron | C ₁₅ H ₁₅ CINO ₂ | 291 | 291→72 / 218 | 65 | 30 | 4 |
| Clethodim | C ₁₇ H ₂₆ CINO ₃ S | 360 | 360→164 / 268 | 61 | 29 | 10 |
| Clofentezine | C ₁₄ H ₈ Cl ₂ N ₄ | 303 | 303→138 / 102 | 61 | 23 | 8 |
| Clothianidin | C ₆ H ₈ CIN ₅ O ₂ S | 250 | 250→169 / 132 | 51 | 17 | 4 |
| Cyazofamid | C ₁₃ H ₁₃ CIN ₄ O ₂ S | 325 | 325→108 / 261 | 61 | 21 | 10 |
| Cycluron | C ₁₁ H ₂₂ N ₂ O | 198 | 199→89 / 72 | 50 | 21 | 4 |
| Cymoxanil | C ₇ H ₁₀ N ₄ O ₃ | 198 | 199→128 / 111 | 60 | 13 | 4 |
| Cyproconazole A | C ₁₅ H ₁₈ CIN ₃ O | 292 | 292→70 / 125 | 66 | 39 | 12 |
| Cyproconazole B | C ₁₅ H ₁₈ CIN ₃ O | 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 ₂ O ₄ | 300 | 318→182 / 136 | 41 | 19 | 12 |
| Diclobutrazol | C ₁₅ H ₁₉ Cl ₂ N ₃ O | 328 | 328→70 / 158 | 81 | 49 | 12 |
| Dicrotophos | C ₈ H ₁₆ NO ₅ P | 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 ₂ N ₃ O ₃ | 406 | 406→251 / 253 | 81 | 37 | 16 |
| Diflubenzuron | C ₁₄ H ₉ Cl ₂ FN ₂ O ₂ | 311 | 311→158 / 141 | 71 | 23 | 10 |
| Dimethoate | C ₅ H ₁₂ NO ₃ PS ₂ | 229 | 230→199 / 125 | 50 | 14 | 15 |

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|------------------------------------|---|-----|---------------|-----|----|----|
| 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 ₂ O ₃ | 326 | 327→205 / 116 | 40 | 15 | 4 |
| Diniconazole | C ₁₅ H ₁₇ Cl ₂ N ₃ O | 326 | 326→70 / 158 | 86 | 51 | 12 |
| Dioxacarb | C ₁₁ H ₁₃ NO ₄ | 223 | 224→167 / 123 | 51 | 13 | 10 |
| Diuron | C ₉ H ₁₀ Cl ₂ N ₂ O | 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 ₃ O 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 ₃ O | 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 ₂ N ₃ O ₂ | 328 | 328→159 / 205 | 46 | 37 | 10 |
| Ethiofencarb | C ₁₁ H ₁₅ NO ₂ S | 225 | 226→106 / 164 | 41 | 21 | 4 |
| Ethiprole | C ₁₃ H ₉ Cl ₂ F ₃ N ₄ OS | 397 | 397→350 / 255 | 81 | 29 | 24 |
| Ethofumesate | C ₁₃ H ₁₈ O ₅ S | 286 | 287→121 / 259 | 81 | 23 | 8 |
| Etoxazole | C ₂₁ H ₂₃ F ₂ NO ₂ | 359 | 360→141 / 57 | 76 | 45 | 4 |
| Famoxadone | C ₂₂ H ₁₈ N ₂ O ₄ | 374 | 392→331 / 238 | 31 | 15 | 4 |
| Fenamidone | C ₁₇ H ₁₇ N ₃ OS | 311 | 312→92 / 236 | 66 | 39 | 16 |
| Fenarimol | C ₁₇ N ₁₂ Cl ₂ N ₂ O | 331 | 331→268 / 81 | 61 | 31 | 4 |
| Fenazaquin | C ₂₀ H ₂₂ N ₂ O | 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 ₂ NO 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 ₉ H ₁₂ N ₂ O | 164 | 165→72 / 46 | 56 | 25 | 4 |
| Fludioxinil | C ₁₂ H ₆ F ₂ N ₂ O ₂ | 248 | 266→229 / 227 | 41 | 23 | 14 |
| Flufenacet | C ₁₄ H ₁₃ F ₄ N ₃ O ₂ S | 363 | 364→152 / 194 | 51 | 29 | 10 |
| Flufenoxuron | C ₂₁ H ₁₁ ClF ₆ N ₂ O ₃ | 489 | 489→158 / 141 | 86 | 29 | 10 |
| Fuometuron | C ₁₀ H ₁₁ F ₃ N ₂ O | 232 | 233→72 / 46 | 71 | 37 | 12 |
| Fluoxastrobin | C ₂₁ H ₁₆ ClFN ₄ O ₅ | 459 | 459→427 / 188 | 55 | 28 | 4 |
| Fluquinconazole | C ₁₆ H ₈ Cl ₂ FN ₅ O | 376 | 376→307 / 349 | 71 | 33 | 4 |
| Flusilazole | C ₁₆ H ₁₅ F ₂ N ₃ Si | 315 | 316→247 / 165 | 81 | 27 | 16 |
| Flutolanil | C ₁₇ H ₁₆ F ₃ NO ₂ | 323 | 324→262 / 242 | 76 | 27 | 16 |
| Flutriafol | C ₁₆ H ₁₃ F ₂ N ₃ O | 301 | 302→70 / 123 | 66 | 37 | 12 |
| Forchlorfenuron | C ₁₂ H ₁₀ ClN ₃ O | 248 | 248→129 / 93. | 52 | 25 | 4 |
| Formetanate HCl | C ₁₁ H ₁₅ N ₃ O ₂ | 221 | 222→165 / 120 | 60 | 21 | 12 |
| Fuberidazole | C ₁₁ H ₈ N ₂ O | 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 ₂ O ₅ S | 382 | 383→195 / 252 | 76 | 27 | 12 |
| Hexaconazole | C ₁₄ H ₁₇ Cl ₂ N ₃ O | 314 | 314→70 / 159 | 56 | 41 | 12 |
| Hexaflumuron | C ₁₆ H ₈ Cl ₂ F ₆ N ₂ O ₃ | 461 | 461→158 / 141 | 56 | 25 | 4 |
| Hexythiazox | C ₁₇ H ₂₁ ClN ₂ O ₂ S | 353 | 353→228 / 168 | 61 | 23 | 14 |
| Hydramethylnon | C ₂₅ H ₂₄ F ₆ N ₄ | 494 | 495→323 / 151 | 146 | 45 | 20 |
| Imazalil | C ₁₄ H ₁₄ Cl ₂ N ₂ O | 297 | 297→159 / 201 | 66 | 33 | 14 |
| Imidacloprid | C ₉ H ₁₀ ClN ₅ O ₂ | 256 | 256→209 / 175 | 61 | 23 | 12 |
| Indoxacarb | C ₂₂ H ₁₇ ClF ₃ N ₃ O ₇ | 528 | 528→203 / 218 | 86 | 55 | 12 |
| Ipconazole | C ₁₈ H ₂₄ ClN ₃ O | 334 | 334→70 / 125 | 76 | 55 | 12 |
| Iprovalicarb | C ₁₈ H ₂₈ N ₂ O ₃ | 320 | 321→119 / 203 | 66 | 29 | 8 |
| Isoprocab | C ₁₁ H ₁₅ NO ₂ | 193 | 194→95 / 137 | 61 | 23 | 16 |
| Isoproturon | C ₁₂ H ₁₈ N ₂ O | 206 | 207→72 / 46 | 66 | 29 | 4 |
| Isoxaflutole | C ₁₅ H ₁₂ F ₂ NO ₄ S | 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 |
| Linuron | C ₉ H ₁₀ Cl ₂ N ₂ O ₂ | 249 | 249→160 / 182 | 61 | 23 | 4 |
| Lufenuron | C ₉ H ₁₀ Cl ₂ N ₂ O ₂ | 511 | 511→158 / 141 | 61 | 27 | 4 |
| Mefenacet | C ₁₆ H ₁₄ N ₂ O ₂ S | 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 ₇ S | 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 ₃ O | 319 | 320→70 / 125 | 81 | 51 | 12 |
| Methabenzthiazuron | C ₁₀ H ₁₁ N ₃ OS | 221 | 222→165 / 150 | 51 | 21 | 4 |
| Methamidophos | C ₂ H ₈ NO ₂ PS | 141 | 142→94 / 125 | 55 | 20 | 4 |

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| Methiocarb | C ₁₁ H ₁₅ NO ₂ S | 225 | 226→169 / 121 | 61 | 13 | 12 |
| Methomyl | C ₅ H ₁₀ N ₂ O ₂ S | 162 | 163→88 / 106 | 35 | 12 | 5 |
| Methoprotryne | C ₁₁ H ₂₁ N ₅ OS | 271 | 272→240 / 198 | 50 | 27 | 4 |
| Methoxyfenozide | C ₂₂ H ₂₈ N ₂ O ₃ | 368 | 369→149 / 313 | 56 | 25 | 10 |
| Metobromuron | C ₉ H ₁₁ BrN ₂ O ₂ | 259 | 259→170 / 148 | 56 | 23 | 4 |
| Metribuzin | C ₈ H ₁₄ N ₄ OS | 214 | 215→84 / 187 | 71 | 29 | 4 |
| Mevinphos-Z | C ₇ H ₁₃ O ₆ P | 224 | 225→127 / 193 | 55 | 20 | 8 |
| Mevinphos-E | C ₇ H ₁₃ O ₆ P | 224 | 225→127 / 193 | 55 | 20 | 8 |
| Mexacarbate | C ₁₂ H ₁₈ N ₂ O ₂ | 222 | 223→166 / 151 | 66 | 23 | 12 |
| Monocrotophos | C ₇ H ₁₄ NO ₅ P | 223 | 224→127 / 98 | 51 | 23 | 12 |
| Monolinuron | C ₉ H ₁₁ CIN ₂ O 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 CIN ₄ | 289 | 289→70 / 125 | 71 | 37 | 12 |
| Neburon | C ₁₂ H ₁₆ Cl ₂ N ₂ O | 275 | 275→88 / 114 | 56 | 23 | 4 |
| Nitenpyram | C ₁₁ H ₁₅ CIN ₄ O ₂ | 271 | 271→225 / 126 | 51 | 17 | 14 |
| Novaluron | C ₁₇ H ₉ ClF ₈ N ₂ O ₄ | 493 | 493→158 / 141 | 71 | 27 | 4 |
| Nuarimol | C ₁₇ H ₁₂ ClFN ₂ O | 315 | 315→252 / 81 | 81 | 31 | 16 |
| Omethoate | C ₅ H ₁₂ NO ₄ PS | 213 | 214→124 / 182 | 46 | 29 | 4 |
| Oxadixyl | C ₁₄ H ₁₈ N ₂ O ₄ | 278 | 279→219 / 132 | 61 | 17 | 14 |
| Oxamyl | C ₇ H ₁₃ N ₃ O ₃ S | 219 | 237→72 / 90 | 36 | 25 | 4 |
| Paclobutrazol | C ₁₅ H ₂₀ CIN ₃ O | 294 | 294→70 / 125 | 66 | 49 | 12 |
| Penconazole | C ₁₃ H ₁₅ Cl ₂ N ₃ | 284 | 284→159 / 70 | 71 | 39 | 10 |
| Phenmedipham | C ₁₆ H ₁₆ N ₂ O ₄ | 300 | 301→136 / 168 | 50 | 26 | 4 |
| Picoxystrobin | C ₁₈ H ₁₆ F ₃ NO 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 ₄ O ₂ | 238 | 239→72 / 182 | 66 | 35 | 12 |
| Prochloraz | C ₁₅ H ₁₆ Cl ₃ N ₃ O 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 ₅ O | 225 | 226→142 / 86 | 76 | 33 | 10 |
| Prometryn | C ₁₀ H ₁₉ N ₅ S | 241 | 242→200 / 158 | 71 | 19 | 4 |
| Propamocarb | C ₉ H ₂₀ N ₂ O ₂ | 188 | 189→102 / 144 | 61 | 25 | 8 |
| Propargite | C ₁₉ H ₂₆ O ₄ S | 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 ₂ N ₃ O 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 ₅ O | 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 CIN ₃ O ₄ | 388 | 388→194 / 163 | 31 | 19 | 4 |
| Pyridaben | C ₁₉ H ₂₅ CIN ₂ OS | 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 |
| Quinoxifen | C ₁₅ H ₈ Cl ₂ FNO | 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 ₅ O | 225 | 226→170 / 100 | 50 | 35 | 4 |
| Siduron | C ₁₄ H ₂₀ N ₂ O | 232 | 233→137 / 94 | 66 | 21 | 4 |
| Simetryne | C ₈ H ₁₅ N ₅ S | 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 ₂ O 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 ₂ F ₂ N ₄ O ₃ S | 387 | 387→307 / 146 | 81 | 27 | 4 |
| Tebuconazole | C ₁₆ H ₂₂ CIN ₃ O | 308 | 308→70 / 125 | 81 | 49 | 12 |
| Tebufenozide | C ₂₂ H ₂₈ N ₂ O ₂ | 352 | 353→133 / 297 | 51 | 25 | 10 |
| Tebufenpyrad | C ₁₈ H ₂₄ CIN ₃ O | 334 | 334→117 / 145 | 71 | 47 | 4 |
| Tebuthiuron | C ₉ H ₁₆ N ₄ OS | 228 | 229→172 / 116 | 46 | 21 | 4 |
| Teflubenzuron | C ₁₄ H ₆ Cl ₂ F ₄ N ₂ O ₂ | 381 | 381→141 / 158 | 66 | 53 | 4 |
| Terbumeton | C ₁₀ H ₁₉ N ₅ O | 225 | 226→170 / 100 | 76 | 27 | 12 |
| Terbutryne | C ₁₀ H ₁₉ N ₅ S | 241 | 242→186 / 68 | 71 | 27 | 12 |
| Tetraconazole | C ₁₃ H ₁₁ Cl ₂ F ₄ N ₃ O | 372 | 372→159 / 70 | 76 | 45 | 10 |
| Thiabendazole | C ₁₀ H ₇ N ₃ S | 201 | 202→175 / 131 | 85 | 35 | 12 |
| Thiacloprid | C ₁₀ H ₉ CIN ₄ S | 253 | 253→126 / 99 | 71 | 31 | 10 |
| Thiamethoxam | C ₈ H ₁₀ CIN ₅ O ₃ S | 292 | 292→211 / 181 | 61 | 19 | 12 |
| Thidiazuron | C ₉ H ₈ N ₄ OS | 220 | 221→102 / 127 | 66 | 21 | 4 |

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| Thiobencarb | C ₁₂ H ₁₆ CINOS | 258 | 258→125 / 89 | 56 | 27 | 8 |
| Thiofanox | C ₉ H ₁₈ N ₂ O ₂ S | 218 | 219→76 / 57 | 36 | 20 | 8 |
| Thiophanate-methyl | C ₁₂ H ₁₄ N ₄ O ₄ S ₂ | 342 | 343→151 / 311 | 61 | 29 | 14 |
| Triadimefon | C ₁₄ H ₁₆ CIN ₃ O ₂ | 294 | 294→197 / 225 | 66 | 23 | 14 |
| Triadimenol | C ₁₄ H ₁₈ CIN ₃ O ₂ | 296 | 296→70 / 227 | 46 | 31 | 12 |
| Tricyclazole | C ₉ H ₇ N ₃ S | 189 | 190→163 / 136 | 81 | 33 | 10 |
| Trifloxystrobin | C ₂₀ H ₁₉ F ₃ N ₂ O ₄ | 408 | 409→186 / 206 | 31 | 23 | 4 |
| Triflumizole | C ₁₅ H ₁₅ ClF ₃ N ₃ O | 346 | 346→278 / 73 | 51 | 15 | 8 |
| Triflumuron | C ₁₅ H ₁₀ ClF ₃ N ₂ O ₃ | 359 | 359→156 / 139 | 51 | 23 | 4 |
| Triticonazole | C ₁₇ H ₂₀ CIN ₃ O | 318 | 318→70 / 125 | 66 | 45 | 12 |
| Vamidothion | C ₈ H ₁₈ NO ₄ PS ₂ | 287 | 288→146 / 118 | 61 | 19 | 10 |
| Zoxamide | C ₁₄ H ₁₆ Cl ₃ NO ₂ | 337 | 336→187 / 159 | 45 | 35 | 15 |
| D10-Diazinon | C ₁₂ D ₁₀ H ₁₁ N ₂ O ₃ PS | 314 | 315→170 | 50 | 29 | 4 |
| D6-Dimethoate | C ₅ D ₆ H ₆ NO ₃ PS ₂ | 235 | 236→131 | 50 | 30 | 4 |
| D6-diuron | C ₉ D ₆ H ₄ Cl ₂ N ₂ O | 239 | 239→78 | 90 | 30 | 4 |
| D6-Linuron | C ₉ D ₆ H ₄ Cl ₂ N ₂ O ₂ | 255 | 255→166 | 90 | 30 | 4 |
| D6-Dichlorvos | C ₄ D ₆ H ₁ Cl ₂ O ₄ P | 227 | 227→115 | 70 | 27 | 4 |
| D6-Malathion | C ₁₀ D ₆ H ₁₃ O ₆ PS ₂ | 330 | 337→291 | 55 | 12 | 4 |

*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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