

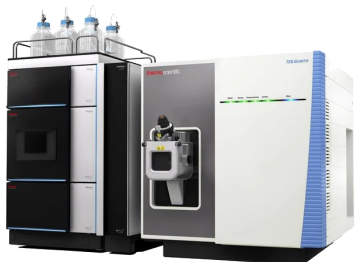
การวิเคราะห์สาร Pesticide ตกค้างจำนวน 437 ชนิดในการฉีดเพียงครั้งเดียว ด้วยเทคนิค LC-MS/MS

ผู้จัดทำ : พงศกร โพรธวาร

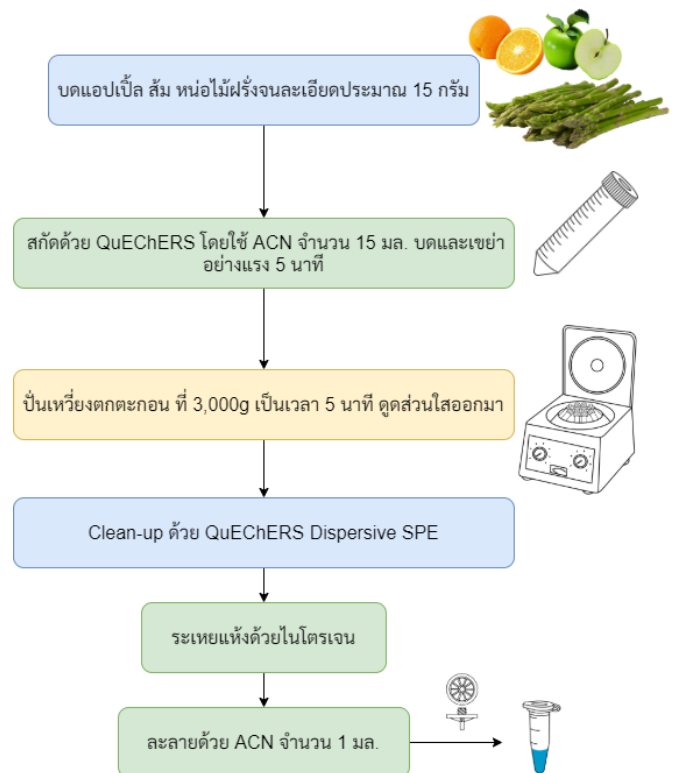
ในปัจจุบันนี้มาตรฐานเรื่องความปลอดภัยทางอาหารได้มีข้อกำหนดที่เข้มข้นขึ้นเรื่อยๆ การค้าขายสินค้าเกษตรระหว่างประเทศมีเกณฑ์การทดสอบที่ยากยิ่งขึ้น ในปี 2006 ได้มีการประกาศปริมาณสารตกค้างสูงสุดที่ยอมรับได้ (Maximum Residue Levels—MRLs) ประกอบด้วยวัตถุเคมีทางการเกษตรในอาหาร หนึ่งในนั้นคือสารเคมีกำจัดศัตรูพืช (Pesticide) จำนวนกว่า 400 ชนิด และตั้งค่า MRLs สำหรับสารเคมีกำจัดศัตรูพืชบางชนิดที่ยังไม่ได้กำหนดค่าชัดเจน เป็น 10 ไมโครกรัมต่อกิโลกรัม และทาง EU ก็ได้เห็นชอบกับกฎเกณฑ์ดังกล่าว โดยได้ออกข้อกำหนด (EC) No. 396/2005 ออกมาเช่นเดียวกัน นอกจากนี้ยังได้ตรวจสอบสารกำจัดศัตรูพืชจำนวนกว่า 1,000 ชนิด ในตลาดภายใต้ข้อกำหนด EU Directive 91/414/EEC และในปี 2009 จึงได้ข้อกำหนด MRLs ใหม่จำนวนกว่า 700 ชนิดในปัจจุบัน

เทคนิค LC-MS/MS เป็นเทคนิคมาตรฐานที่นิยมใช้ในการตรวจวิเคราะห์สารเคมีกำจัดศัตรูพืช ด้วยความจำเพาะและความไวที่พัฒนาสูงขึ้นมา ทำให้การวิเคราะห์และการยืนยันทั้งเชิงคุณภาพและปริมาณ ทำได้อย่างดีเยี่ยม มีความน่าเชื่อถือสูง

ในแอปพลิเคชันนี้ ผู้เขียนได้นำเสนอวิธีการสกัดและการวิเคราะห์สารเคมีกำจัดศัตรูพืช จำนวนกว่า 400 ชนิด ด้วยเทคนิคการสกัดแบบ QuEChERS ร่วมกับการใช้เครื่อง Vanquish Flex uHPLC (Thermo Scientific) ต่อพ่วงกับเครื่องวัดมวลสารแมสสเปคโตรมิเตอร์ TSQ Quantis LC-MS/MS (Thermo Scientific) ภายใต้การประมวลผลด้วยโปรแกรมอันชาญฉลาดอย่าง TraceFinder



การเตรียมตัวอย่าง



การตั้งค่าเครื่องมือ

UHPC: Vanquish Flex (Thermo Scientific)

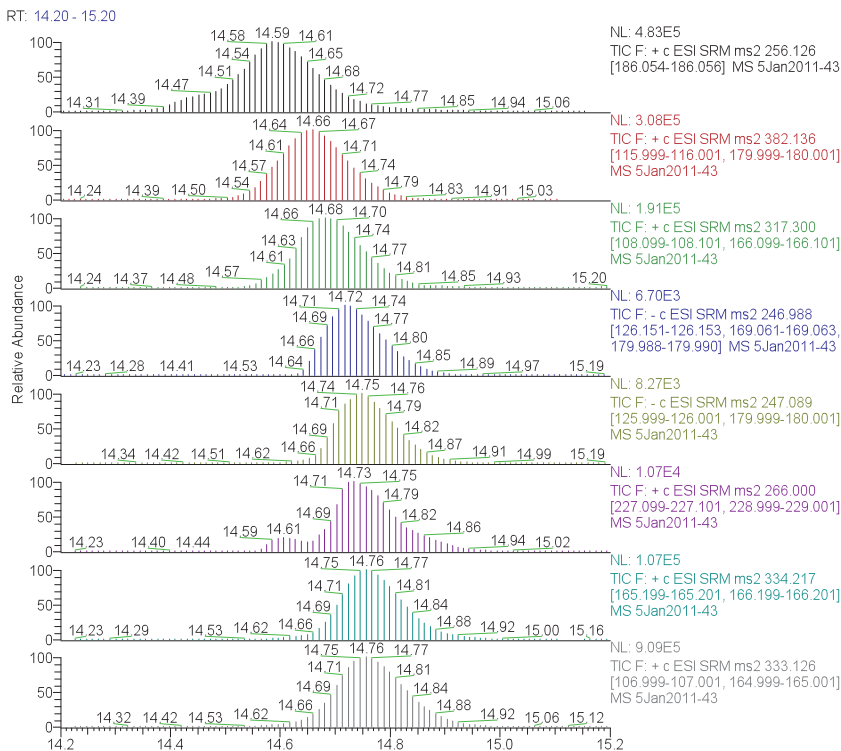
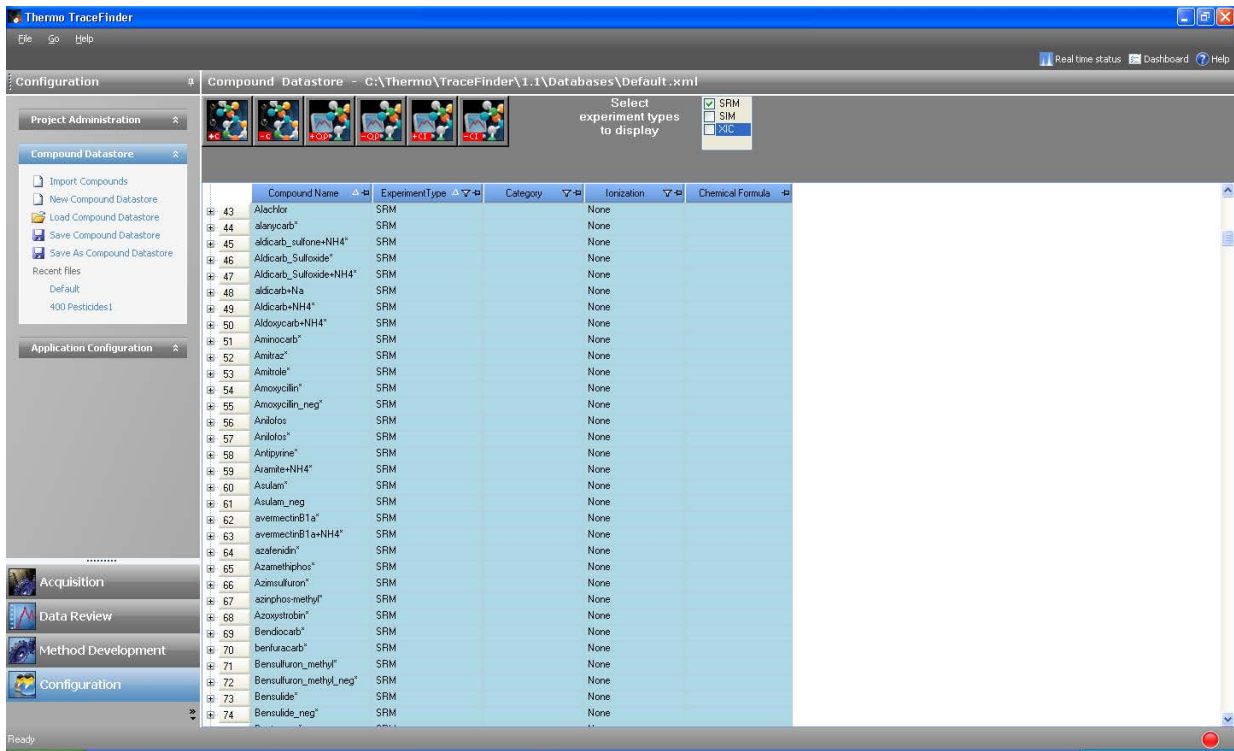
Autosampler : HTC-PAL (CTC Analytic)

Column:	Thermo Scientific Hypersil GOLD aQ 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		
Mobile Phase B:	Methanol with 0.1% formic acid and 4 mM ammonium formate		
Flow Rate:	300 µL/min		
Column Temperature:	40 °C		
Sample Injection Volume:	10 µL		
Gradient:	Gradient Time (min)	%A	%B
	0.00	98	2
	0.25	70	30
	35.00	0	100
	40.00	0	100
	40.01	98	2
	45.00	98	2

Mass Spectrometer : TSQ Quantis LC-MS/MS

Sheath Gas : 55, Aux Gas : 15, Spray Voltage : 3.5kV

Cap Temp: 280 °C, Heater Temp: 295 °C



โปรแกรม TraceFinder

การทำ Method Development, การวิเคราะห์ และการประมวลผล ทำด้วยโปรแกรม TraceFinder ตัวโปรแกรมสามารถออกแบบการฉีดตัวอย่าง การทำ QC ได้อย่างอิสระ พร้อมระบบ Intelligent Sequencing ที่สามารถควบคุมการสร้างโปรแกรมการฉีดสารได้อย่างมีประสิทธิภาพมากกว่าโปรแกรมทั่วไป นอกจากนี้ยังมีตาราง MS/MS ที่เป็นฐานข้อมูลฝังมากับโปรแกรมช่วยให้ผู้ใช้งานประหยัดเวลา

ตัวอย่างแมสสเปกตรัมของสาร 8 ชนิด แสดงให้เห็นถึงประสิทธิภาพในการสลับการสแกนประจวบและลบ

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Acephate	184.08	143.05	10	95.20	25			2.11	+
Acetamidiprid	223.10	126.10	22	90.20	36			3.87	+
Acibenzolar-S-methyl	211.09	136.00	32	140.00	24			13.17	+
Acifluorfen	360.00	316.00	10					15.26	-
Acrinathrin+NH ₄	559.00	208.00	16	181.00	33	317.00	12	27.78	+
Akton	374.80	304.90	20	97.10	40			22.05	+
Alachlor	270.10	162.00	19					15.86	+
Aldicarb sulfone+NH ₄	240.12	86.20	22	148.05	12			2.38	+
Aldicarb sulfoxide	207.00	132.00	10	89.00	16			2.3	+
Aldicarb sulfoxide +NH ₄	224.20	89.00	19	131.70	15			2.3	+
Aldicarb+NH ₄	208.10	116.10	10	89.20	17			4.97	+
Allethrin	303.16	135.05	13	123.11	18	91.16	33	23.14	+
Allidochlor	174.09	98.23	12	41.44	23	39.44	45	5.24	+
Ametryn	228.20	185.90	19	96.00	26			8.94	+
Amicarbazone	242.18	143.10	12	85.20	32			6.21	+
Aminocarb	209.12	137.10	25	152.10	15			2.2	+
Amitraz	294.08	122.19	33					2.77	+
Ancymidol	257.11	135.05	26	81.21	26	77.20	45	7.44	+
Anilofos	368.00	199.00	16	171.00	23	125.00	34	18.96	+
Aramite+NH ₄	352.00	191.00	12	255.00	10			23.2	+
Aspon	378.90	210.90	21	115.10	33			25.28	+
Asulam	231.00	156.00	12	92.00	25			2.29	+
Atrazine	216.00	174.00	16					9.32	+
Avermectin B1a +NH ₄	890.45	305.28	22	307.00	29	567.41	11	27.65	+
Avermectin B1a+Na	895.39	751.50	45	183.08	50			27.65	+
Avermectin B1b +NH ₄	876.45	291.00	30	553.40	15	145.00	35	26.77	+
Azaconazole	300.00	158.93	27	230.92	17	122.99	51	11.07	+
Azafenidrin	338.11	264.03	30	302.10	17	298.98	20	10.94	+
Azamethiphos	324.98	182.91	17	112.04	36	138.96	23	6.41	+
Azinphos-ethyl	345.96	132.10	16	160.10	7			16.14	+
Azinphos-methyl	317.93	260.98	8	125.03	19			11.9	+
Azoxystrobin	404.12	372.14	14	329.11	32			13.86	+
Bendiocarb	224.16	167.06	10	109.10	20			6.94	+
Benodanil	324.01	241.98	25	261.96	18	132.03	19	14.84	+
Benoxacor	260.03	148.69	17	133.98	13			11.31	+
Bensulide	398.00	314.00	12	158.00	25	218.00	18	18.34	+
Bentazone	239.07	132.00	28	197.00	22			6.51	-
Benthiavalicarb	382.14	180.00	33	116.00	23			14.65	+
Benzoximate	364.35	199.20	11	105.20	33			20.06	+
Bifenazate	301.23	170.00	20	152.00	40			16.02	+
Bifenoxy	342.00	310.00	15					18.99	+
Bifenthrin+NH ₄	440.00	181.00	14	166.00	42			29.35	+
Bispyribac-sodium	453.14	296.96	19					13.92	+
Bitertanol	338.08	269.00	10	99.00	16			20.15	+
Boscalid	343.24	307.00	19	271.00	34			14.21	+
Brodifacoum	522.88	335.00	23	178.20	35			28.91	+
Bromadiolone	525.07	249.96	37	263.27	40	218.93	50	23.67	-
Bromoxynil	276.07	81.00	36	79.00	36			8.86	+
Bromuconazole1	377.92	158.92	28	160.88	28	123.02	35	15.16	+
Bromuconazole2	377.92	158.92	28	160.88	28	123.02	35	17.83	+
Bufencarb	222.11	95.20	34	77.20	43			17.19	+
Bupirimate	317.30	166.10	25	108.10	27			14.68	+
Buprofezin	306.21	201.00	12	116.00	18			20.78	+
Butachlor	312.20	238.00	11					22.92	+
Butafenacil+NH ₄	492.31	331.00	26	180.00	46			16.26	+
Butocarboxin	208.10	109.20	15	91.40	39			13.82	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Butoxycarboxin	223.11	106.10	10	86.20	20			2.35	+
Butoxycarboxin+NH ₄	240.11	86.20	18	106.10	25			2.36	+
Butralin	296.14	240.03	14	222.03	22	208.00	28	24.95	+
Butylate	218.20	156.00	11					21.14	+
Cadusafos	270.97	158.90	16	97.00	36			20.21	+
Carbaryl	202.08	145.00	12	127.00	30			8.13	+
Carbendazim	192.10	160.06	20	132.10	33			2.75	+
Carbetamide	237.12	192.05	10	118.10	15			5.83	+
Carbofuran	222.14	165.06	14	123.10	25			6.91	+
Carbofuran-3-hydroxy	238.08	220.08	9	181.08	11			3.64	+
Carboxin	235.95	142.97	17	86.98	24			7.6	+
Carfentrazone-ethyl	412.19	384.00	15	366.20	19			17.94	+
Carpropamid	334.00	139.00	22	196.00	14	103.00	38	18.84	+
Chlorantraniliprole	482.13	450.89	21	283.81	19			11.79	+
Chlorbromuron	292.91	203.88	20	181.95	19	124.94	33	13.73	+
Chlordimeform	197.02	117.20	29	89.00	50			3.15	+
Chlorfenvinphos	358.81	155.20	14	99.10	33			19.16	+
Chlorfluazuron	541.90	385.00	25					26.79	+
Chlorfluazuron	539.70	383.00	20					26.79	+
Chloroxuron	291.11	72.20	20	46.20	19			15.97	+
Chlorpropham	214.00	172.00	12	154.00	19			9.96	+
Chlorpyrifos	350.00	198.00	18	97.00	35			23.81	+
Chlortoluron	213.08	140.00	22	168.00	20			9.18	+
Clethodim	360.19	164.00	20	268.00	14			21.38	+
Clofentezine	303.07	138.00	18	102.00	36			20.42	+
Clothianidin	250.12	169.06	14	132.10	18			3.38	+
Coumaphos	363.02	226.90	25					19.38	+
Coumaphos oxon	347.02	290.92	18	210.92	28	318.93	14	12.72	+
Crotoxyphos	332.07	126.99	23	99.04	27			14.36	+
Dumyluron	303.00	185.00	14	125.00	34	119.00	22	15.44	+
Cyanazine	241.10	214.00	17					6.18	+
Cyazofamid	325.22	108.00	15	261.00	10			17.23	+
Dycloate	216.00	154.00	12	134.00	14	83.00	18	19.81	+
Cyclohexamide	299.18	264.16	14	246.12	19	159.16	30	5.5	+
Cycluron	199.11	89.10	16	72.20	24			10.42	+
Cyflufenamid	413.00	295.00	16	241.00	25	203.00	42	20.34	+
Cyfluthrin	434.10	191.00	17					26.68	+
Cyhalothrin+NH ₄	467.00	225.00	18	450.00	10			26.79	+
Cymoxanil	199.06	128.10	10	111.10	20			4.07	+
Cyphenothrin	393.08	315.89	23	376.00	10			20.84	+
Cyproconazole	292.13	125.00	32					15.58	+
Cyromazine	167.09	85.17	19	68.23	28	81.21	26	1.97	+
Daimuron	269.00	151.00	14	91.00	45	119.00	25	14.55	+
DEF	315.02	169.00	17	259.09	13			26.36	+
Deltamethrin	506.10	281.00	11					26.9	+
Demeton S-methyl	231.01	89.16	10	61.26	32			7.06	+
Demeton-O	259.00	89.10	11	61.21	29			11.72	+
Demeton-S	259.00	89.25	12	61.20	47			11.72	+
Desmedipham+NH ₄	318.16	182.00	15	136.00	28			11.72	+
Desmetyrn	214.11	172.07	18	82.21	30	57.34	33	6.63	+
Di-allate	269.99	86.15	17	109.04	30	143.03	20	20.67	+
Diamidafos (Nellite)	201.10	107.20	28					3.96	+
Diazinon	305.03	169.10	25	153.13	23			18.51	+
Diazinon Oxon	289.00	233.00	20					16.12	+
Dichlorfenthion	314.98	258.82	16					26.36	+
Dichlormid	208.04	81.26	13	98.18	13	41.47	20	6.85	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Dichlorvos	221.00	109.00	18	145.00	14	127.00	10	6.72	+
Dichlorvos+NH ₄	238.00	109.00	24	221.00	18	127.00	24	6.72	+
Diclobutrazol	328.14	159.00	35	70.20	25			16.24	+
Dicrotophos	238.10	193.10	10	112.10	14			3.04	+
Diethofencarb	268.21	226.00	13	180.10	18			12.43	+
Difenacoum	445.13	179.00	30	256.97	21	177.83	59	26.63	+
Difenoconazole	406.17	251.00	25	111.00	55			21.12	+
Difenoxuron	287.09	123.04	22	72.22	26	95.15	30	11.19	+
Dimepiperate	264.12	146.08	11	119.13	17	91.15	35	20.36	+
Dimethametryn	256.13	186.05	22					14.59	+
Dimethenamid	276.00	243.97	14	168.02	23	111.15	33	12.76	+
Dimethoate	230.11	199.10	12	125.10	23			3.68	+
Dimethomorph	388.14	301.00	22	165.00	34			15.25	+
Dimethylvinphos1	331.00	127.04	13	99.06	26			14.47	+
Dimethylvinphos2	331.00	127.04	13	99.06	26			15.55	+
Dimetilan	241.10	72.20	21					4	+
Dimoxystrobin	327.13	205.00	12	116.00	25			17.73	+
Diniconazole	326.17	148.20	27	70.20	35			18.7	+
Dinotefuran	203.02	129.00	10	114.00	15			2.31	+
Dioxacarb	224.08	167.06	10	123.10	18			6.94	+
Dioxathion	473.99	271.09	10	153.04	28			22.8	+
Diphenamid	240.12	134.13	21	167.09	24	165.09	48	11.18	+
Diphenylamine	170.09	114.09	17	100.13	22	69.21	26	7.91	+
Dipropetryn	256.15	214.06	19	144.06	29	172.03	21	14.46	+
Disulfoton	274.94	89.27	5	61.28	34			19.59	+
Ditalimfos	300.10	145.30	22	144.20	21			14.47	+
Dithiopyr	402.10	354.00	20	272.30	32			21.84	+
Diuron	233.11	72.00	20	46.30	35			8.81	+
DNOC	199.14	117.10	28	89.00	53			3.15	+
Dodemorph	282.23	116.16	20	98.22	25	69.29	31	11.66	+
Doramectin	916.40	331.40	35	593.50	25			28.79	+
Edifenphos	310.98	283.00	12	109.11	35			18.62	+
Eamectin	886.70	158.00	33	302.00	20			24.99	+
Eamectin B1b	872.40	158.20	33	302.30	20			24.02	+
Epoxiconazole	330.20	121.00	21	123.00	20			16.84	+
Eprinomectin B1a	936.53	490.22	52	352.13	57			27.15	+
EPTC	190.07	128.20	13	86.20	14			16.67	+
Esprocarb	266.20	91.00	24	71.10	17			22.34	+
Etaconazole	328.19	159.00	32	123.00	58			16.62	+
Ethaboxam	321.00	183.10	24	200.10	28			8.89	+
Ethalfuralin	334.22	166.20	21	165.20	20			14.76	+
Ethidimuron	265.09	208.20	16	114.20	20			3.32	+
Ethiofencarb	226.09	107.00	16					13.16	+
Ethiolate	162.10	132.16	23	147.16	15	117.14	30	22.92	+
Ethion	384.92	142.97	29	97.09	49			23.56	+
Ethion monoxon	368.85	199.20	13	142.90	27			17.7	+
Ethirimol	210.20	140.10	23	98.10	28			4.82	+
Ethofumesate	286.96	258.90	11	120.90	20			12.86	+
Ethoprophos	243.07	97.10	30	131.10	40			15.93	+
Ethoxyquin	218.00	174.00	34	160.00	34			8.81	+
Ethoxyquin	218.00	174.00	34	160.00	34			8.81	+
Etobenzanid	340.13	179.10	20	121.00	33			19.13	+
Etofenprox	394.15	177.07	14	107.11	38	135.03	28	28.5	+
Etoxazole	360.21	177.10	22					19.06	+
Etrimfos	293.10	265.00	17					17.81	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Famoxadone+NH ₄	392.11	331.22	8	238.03	18			20.08	+
Famphur	325.96	217.03	21	280.98	13			10.36	+
Famphur oxon	327.14	201.00	26	265.00	19	186.01	35	4.91	+
Fenamidone	312.20	236.20	16	264.20	12			13.57	+
Fenamiphos	304.03	217.01	24	234.03	8			17.47	+
Fenamiphos sulfone	336.09	279.87	17	199.98	28			16.95	+
Fenarimol	331.12	268.00	23	81.00	34			16.32	+
Fenazaquin	307.20	57.20	23	160.90	18			20.77	+
Fenbuconazole	337.04	125.14	35	70.41	27			17.8	+
Fenhexamid	302.09	97.00	26	55.00	36			15.84	+
Fenitrothion	277.95	245.95	17	125.10	21			12.76	+
Fenoxycarb	302.17	116.00	13	88.00	20			18.07	+
Fenpiclonil	254.07	172.01	17					7	+
Fenpropathrin	350.20	97.00	34	125.00	16			23.82	+
Fenpropathrin+NH ₄	367.20	125.00	18	97.00	34			25.65	+
Fenpropimorph	304.40	147.10	31	130.10	26			13.16	+
Fenpyroximate	422.21	366.00	15	214.00	34			25.9	+
Fensulfothion	309.18	251.00	21	163.00	18			14.17	+
Fenthion	278.95	247.01	13	169.06	20			12.76	+
Fenthion sulfone	328.09	311.04	9	109.12	37			9.11	+
Fenthion sulfoxide	294.90	108.90	32	114.90	27			8.39	+
Fenuron	165.03	72.10	17	46.30	18			3.53	+
Flonicamid	230.12	174.10	18					13.18	+
Florasulam	360.00	129.00	26	192.00	18			4.98	+
Florasulam+NH ₄	377.00	129.00	30					4.98	+
Fluazinam	463.19	416.00	20	398.00	17			23.95	-
Flubendiamide	681.00	253.94	29	273.93	19	271.89	19	19.03	+
Flucarbazon	397.13	129.90	21	115.00	48			5.01	+
Fludioxinil	266.00	229.00	17	227.10	10			14.74	+
Fludioxonil	246.99	179.99	34	169.06	32	126.15	34	14.74	-
Flufenacet	364.23	194.00	12	152.00	20			16.23	+
Flufenoxuron	487.16	304.00	20	156.00	16			25.95	-
Flumetsulam	326.00	109.00	53					3.46	+
Flumioxazin	355.06	170.81	24	212.82	17	142.87	29	20.84	+
Fluometuron	233.08	72.10	18	46.30	17			8.81	+
Flupicolide	383.01	172.94	23	144.95	47	365.01	17	14.44	+
Fluorochloridone	329.11	302.04	12	188.98	20			17.61	+
Fluoxastrobin	459.20	427.10	18	188.00	37			16.67	+
Fluquinconazole	376.17	349.20	21	307.00	20			15.8	+
Flusiazole	316.18	247.10	19	165.00	34			18.02	+
Flutolanil	324.21	242.00	26	262.00	18			14.84	+
Flutriafol	302.16	70.10	19	123.00	33			10.18	+
Fluvalinate	503.00	181.00	34	208.00	12			28.24	+
Fonophos	246.98	109.10	23	137.10	12			18.44	+
Forchlorfenuron	248.14	129.00	18	93.00	26			10.77	+
Formetanate	222.10	165.00	30					10.01	+
Fosthiazate	284.00	228.00	12	104.00	23			8.77	+
Fuberidazole	185.05	157.05	23	156.03	29	130.18	23	3.41	+
Furalaxyl	302.11	242.10	17	95.00	35			13.23	+
Furathiocarb	383.19	195.00	20	252.00	14			22.38	+
Griseofulvin	353.10	215.00	19	285.06	18	165.03	19	10.97	+
Halofenozide	329.10	121.14	22	77.33	37	155.15	29	13.57	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Haloxyfop-methyl	376.03	315.96	17	287.98	25	91.13	31	20.84	+
Hexaconazole	314.14	70.20	20	159.00	20			19.39	+
Hexaflumuron	458.92	439.00	12	175.00	39			22.79	-
Hexazinone	253.09	171.05	17	85.19	29	71.27	30	7	+
Hexythiazax	353.24	228.20	18	168.10	25			24.03	+
Hydramethylnon	495.27	323.00	35	150.90	55			23.22	+
Imazalil	297.18	159.00	24	201.00	18			10.18	+
Imazamox	306.09	261.10	23	193.10	27			4.05	+
Imazapyr	262.06	216.98	19	201.97	27			9.64	+
Imazaquin	312.00	267.00	22	199.00	30	252.00	27	7.29	+
Imibenconazole	411.00	125.00	36	171.00	21			23.76	+
Imidacloprid	256.12	209.10	18	175.10	20			3.29	+
Inabenfide	339.26	80.20	38	78.90	55			13.09	+
Indanofan	341.00	187.00	14	175.00	17			16.23	+
Indoxacarb	528.30	203.00	40	293.00	15			21.9	+
Ipcnazole	334.13	70.20	22	125.00	42			21.54	+
Iprobenfos	289.02	204.96	11	91.23	24			17.82	+
Iprovalicarb	321.16	119.00	20	203.00	10			15.55	+
Isocarbamid	186.08	145.05	22					21.54	+
Isocarbophos	307.12	230.93	17	171.12	22			10.71	+
Isofenfos	346.04	216.94	23	244.99	12			19.79	+
Isofenfos O-analog	330.15	121.10	43					16.84	+
Isoprocab	194.09	95.00	16	137.00	11			9.5	+
Isopropalin	310.15	225.94	20	222.07	20	210.01	19	26.19	+
Isoprothiolane	291.00	189.00	22	231.00	12			14.5	+
Isoproturon	207.10	72.00	19	165.15	14			10.09	+
Isoxaben	333.13	165.00	20	107.00	61			14.76	+
Isoxaflutole	360.25	220.00	42					19.04	+
Isoxathion	314.00	286.00	10	105.00	18	258.00	12	20.09	+
Isozophos	314.03	162.01	16	97.03	34	120.02	28	15.81	+
Ivermectin B1a +NH ₄	892.50	307.00	28	569.00	17			29.92	+
Kresoxim-methyl	314.07	267.14	8	222.13	15			17.77	+
Lactofen+NH ₄	479.00	344.00	15	223.00	36			23.62	+
Linuron	249.10	182.00	18	160.00	17			12.87	+
Loxynil	369.86	242.95	28		28			11.26	-
Lufenuron	509.21	326.00	18	175.00	37			24.97	-
Malathion	330.97	126.99	13	99.02	25	124.98	32	14.48	+
Mandipropamid	412.10	327.90	15	355.90	11			15.16	+
Matoxuron	229.02	72.22	25	156.03	24			5.25	+
Mefenacet	299.17	148.00	14	120.10	31			15.4	+
Mefluidide	328.09	311.04	14	135.12	30	121.10	41	7.58	+
Mepanipyrim	224.14	106.00	27	77.00	40			15.48	+
Mephospholan	270.03	139.98	25	196.02	14	167.96	17	6.7	+
Mepronil	270.15	228.00	16	119.00	21			14.37	+
Mesotrione	340.16	227.95	16					4.72	+
Metaflumizone	505.15	302.04	22	285.10	52	117.15	34	24.67	-
Metalaxyl	280.11	220.10	16	192.10	16			10.36	+
Metazachlor	278.02	134.07	24	105.11	41			9.96	+
Metconazole	320.20	70.10	22	124.90	41			19.62	+
Methabenzthiazuron	222.13	165.00	17					6.91	+
Methacrifos	258.05	209.01	12	125.04	25	79.21	32	11.44	+
Methamidophos	142.00	94.00	20	125.00	10			1.95	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Methidathion	302.90	85.20	23	144.92	5			10.92	+
Methiocarb	226.09	169.00	10					8.28	+
Methomyl	163.05	106.10	10	88.10	10			2.63	+
Methoprotryne	272.20	240.00	10	198.00	15			9.55	+
Metobromuron	259.10	170.00	20	148.00	25			9.34	+
Metolachlor	284.14	252.10	17	148.20	24			16.14	+
Metominostrobin	285.08	193.96	17	166.02	28	139.95	41	11.15	+
Metosulam	418.00	174.88	27	139.96	45	189.68	24	8.21	+
Metrafenone	409.03	209.10	16	227.10	20			20.13	+
Metribuzin	215.09	187.07	17	130.97	17			6.23	+
Mevinphos1	225.09	127.10	15	192.80	8			3.63	+
Mevinphos2	225.09	127.10	15	192.80	8			4.57	+
Mexacarbate	223.15	151.00	26	166.00	16			3.07	+
Milbemycin A3	511.40	493.20	10	475.20	10			26.77	+
Milbemycin A4+NH ₄	560.40	525.20	10	507.20	12			27.95	+
Milbemycin A4-H ₂ O	525.40	507.20	10	489.20	10			27.96	+
Molinate	188.06	126.20	16	83.10	20			13.75	+
Monocrotophos	224.08	127.05	28	193.10	19			2.83	+
Monolinuron	215.08	126.00	17	99.00	36			8.31	+
Moxidectin	640.20	528.50	15	498.50	20			29.19	+
Myclobutanil	289.13	125.00	31	70.20	19			15.58	+
Naled	396.12	324.13	20	308.15	22			16.22	+
Naphthol	145.11	115.10	18	102.12	22			18.1	+
Napropamide	272.14	171.07	20	129.15	16	114.17	22	16.4	+
Naptalam sodium	331.14	105.16	18	139.04	19			13.57	+
Neburon	275.10	57.20	35	88.00	30			17.82	+
Nitenpyram	271.22	225.00	12	237.00	20			2.53	+
Nitralin	346.12	303.98	15	241.87	17	196.00	36	17.44	+
Nitrothal-isopropyl	313.03	148.95	15	91.14	41			15.23	+
Norflurazon	304.07	284.00	25	88.00	39			11.01	+
Novaluron	493.26	158.00	18	141.00	42			23.17	+
Novaluron	491.23	471.00	15	305.00	19			23.18	-
Noviflumuron	527.00	344.00	15	193.00	35			25.7	+
Nuarimol	315.11	251.90	26	81.00	36			13.33	+
Octhilinone	214.14	102.12	16	57.36	17			16.78	+
Ofurace	299.09	254.05	17	236.04	21	160.09	28	7.25	+
Omethoate	214.07	183.00	13	155.00	18			2.23	+
Orbencarb	258.06	125.05	28	100.15	13	89.13	43	19.38	+
Oryzalin	345.00	281.00	19	147.00	30	78.00	38	16.82	-
Oxadiazon	362.06	302.93	18	219.69	25	184.89	35	23.09	+
Oxadixyl	279.00	219.00	15	132.00	25			5.92	+
Oxamyl+NH ₄	237.10	72.08	15	90.09	10			2.44	+
Paclobutrazole	294.10	70.00	20	125.00	35			14.26	+
Parathion	292.00	236.00	15	97.00	30			17.68	+
Parathion-methyl	263.94	232.07	18	109.13	20	124.90	25	12.11	+
Penconazole	284.12	159.00	35	70.10	17			18.43	+
Pencycuron	329.00	125.00	30	218.00	16			20.49	+
Pendimethalin	282.09	212.00	11	194.11	18	119.07	25	24.1	+
Penoxsulam	484.06	195.20	29	194.70	36			9.33	+
Permethrin+NH ₄	408.00	183.00	22	355.00	10			28.45	+
Phenmediphame	301.17	136.00	22	168.00	10			12.23	+
Phenothrin	368.20	183.00	24	237.04	12	165.03	42	28.24	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Phenthoate	320.93	247.02	11	79.26	46			18.01	+
Phorate	260.97	75.08	14	142.94	19			19.08	+
Phorate oxon sulfone	276.98	142.92	22	97.00	36	152.97	16	9.2	+
Phorate sulfone	276.05	94.15	35	173.97	21			9.85	+
Phosalone	368.00	182.00	17					20	+
Phosmet	317.91	160.05	15	133.15	39			12.18	+
Phosphamiden	317.08	300.01	10	127.04	25	226.93	19	6.07	+
Phoxim	299.00	129.00	10	77.00	20			19.81	+
Phropham	180.00	138.00	10	120.00	15	92.00	26	9.11	+
Picloram	241.00	195.00	24					2.67	+
Picoxystrobin	368.20	145.00	23	205.10	11			18.1	+
Pinoxaden	401.19	317.00	23	57.10	34			20.09	+
Piperonyl butoxide	356.19	177.00	13	119.00	33			22.74	+
Piperophos	354.09	170.85	22	212.83	16	142.90	32	20.84	+
Pirimicarb	239.09	182.00	16	72.00	21			4.59	+
Pirimiphos ethyl	334.07	198.11	24	182.14	26			21.8	+
Pirimiphos-methyl	306.01	164.12	24	108.18	34			18.17	+
Pretilachlor	312.20	252.00	17					22.53	+
Prochloraz	376.21	308.00	14	266.00	18			18.99	+
Profenophos	372.90	302.80	19	143.86	36	127.97	40	22.05	+
Prohexadione	211.07	167.19	17	123.24	17	111.18	23	4.83	+
Promecarb	208.09	151.00	10	109.00	17			13.82	+
Prometon	226.21	184.00	21	141.90	24			7.65	+
Prometryn	242.21	157.90	24	199.90	20			11.65	+
Propachlor	212.06	169.99	15	94.13	25	77.18	41	9.95	+
Propamocarb	189.05	102.10	19	144.05	14			2.32	+
Propanil	215.99	160.02	21					12.9	+
Propargite	368.18	231.00	11	174.90	18			24.9	+
Propazine	230.00	124.00	17					15.09	+
Propetamphos	282.04	138.08	18	156.00	10			15.22	+
Propiconazole	342.20	159.00	29	69.20	21			18.91	+
Propoxur	210.07	111.10	16	168.06	10			6.62	+
Prothioconazole	341.98	306.00	16	100.00	30			19.09	+
Prothoate	286.04	97.02	35					10.73	+
Pymetrozine	218.00	105.00	25	79.00	30			2.18	+
Pyracarbolid	218.20	124.90	21	96.90	31			7.03	+
Pyraclufos	361.10	257.00	23					20	+
Pyraclostrobin	388.22	194.00	14	163.00	26			20.01	+
Pyraflufen-ethyl	413.10	339.00	19					19.46	+
Pyrasulfotole	361.06	159.08	46	64.35	61	79.25	18	24.99	+
Pyrazophos	374.04	222.10	22	194.04	36			19.73	+
Pyridaben	365.20	309.10	13	147.00	23			26.81	+
Pyridalyl	489.95	109.00	29	163.90	38			30.53	+
Pyridaphenthion	340.94	189.09	23	205.04	22			15.62	+
Pyridate	379.20	207.00	19					28.28	+
Pyrifenox	294.97	93.12	26	92.07	52	67.19	50	12.88	+
Pyrimethanil	200.07	107.00	26	82.00	30			9.74	+
Pyriproxyfen	322.22	96.00	16	185.30	27			23.49	+
Pyroquilon	174.10	132.13	23	117.15	31	130.13	38	6.77	+
Pyrosulam	434.95	195.20	28	194.10	39			7.42	+
Quinalphos	299.05	163.01	23	147.06	24	38.00		17.63	+
Quinoxifen	307.88	196.80	33	161.90	47			23.92	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Resmethrin	356.16	171.01	15	143.01	26	128.03	43	27.36	+
Rotenone	395.30	213.20	23	192.10	26			17.69	+
Salfufenacil	518.19	348.94	30	459.00	16			12.36	+
Schradan	287.12	242.02	14	135.08	26	92.15	40	4.25	+
Secbumeton	226.21	169.90	19	99.90	33			7.91	+
Sethoxydim	328.00	178.00	20					7.58	+
Siduron	233.12	137.00	20	94.00	38			12.55	+
Simazine	202.10	132.00	20	104.00	27			6.7	+
Simetryne	214.10	124.00	20	96.00	26			6.56	+
Spinetoram1	748.32	141.92	30	98.03	37			22.65	+
Spinetoram2	760.2	141.88	31					24.11	+
Spinosyn A	732.50	142.00	35	98.00	47			21.19	+
Spinosyn D	746.50	142.00	34	98.00	47			22.6	+
Spirodiclofen	411.00	313.10	15	213.10	25			25.6	+
Spiromefesin	371.30	273.30	15	255.30	25			24.73	+
Spirotetramat	374.20	330.20	17	302.20	19			16.21	+
Spiroxamine	298.22	144.00	21	100.00	35			14.74	+
Sulfentrazone	404.00	387.00	10	307.00	15			7.9	+
Sulfotep-ethyl	323.19	219.00	16	247.10	15			24.39	+
Sulfuramid	525.99	219.02	26	168.94	27	269.07	23	25.97	-
Sulprofos	322.93	218.95	17	246.95	12			24.39	+
Tebuconazole	308.22	70.20	21	125.00	34			18.57	+
Tebufenozide	353.12	133.00	19	297.00	10			17.95	+
Tebufenpyrad	334.21	145.20	28	117.00	36			22.77	+
Tebupirimfos	319.10	210.20	22					14.7	+
Tebuthiuron	229.16	172.06	18	116.10	28			7.29	+
Teflubenzuron	379.16	339.00	13	196.00	22			23.82	-
Tefluthrin	419.03	174.85	27	140.72	47			8.21	+
Temephos	466.95	419.13	20	405.08	14			24.23	+
Tepraloxymid	340.00	220.00	34	248.00	18			8.38	-
Terbufos	288.97	103.10	12	57.50	21			22.23	+
Terbufos sulfone	338.08	171.00	16	115.01	31	97.06	42	12.39	+
Terbumeton	226.22	169.90	20	113.90	25			7.66	+
Terbutryn	242.22	185.90	20	91.00	28			12.03	+
Tetrachlorvinphos-a	365.00	204.00	40	127.00	16			17.79	+
Tetrachlorvinphos-a+NH ₄	382.00	127.00	20					17.79	+
Tetrachlorvinphos-b	366.87	127.03	16	205.96	37	240.74	23	17.79	+
Tetrachlorvinphos-b+NH ₄	383.88	126.95	19	205.81	49	240.88	24	17.79	+
Tetraconazole	372.19	159.00	39	70.00	24			17.13	+
Tetramethrin	332.10	127.04	28	174.03	19	226.92	18	14.29	+
Thiabendazole	202.04	175.05	28	131.05	35			3.2	+
Thiacloprid	253.13	126.10	22	90.20	37			4.68	+
Thiamethoxam	292.15	211.10	14	132.05	24			2.76	+
Thiazopyr	397.05	377.04	22	335.00	26			18.67	+
Thidiazuron	221.13	102.10	16	94.20	14			7.13	+
Thiobencarb	258.07	125.00	18	100.20	15			19.38	+
Thiofanox+NH ₄	236.09	57.20	16	76.10	12			8.52	+
Thiometon+Na	268.88	89.10	25	61.10	36			14.52	+
Thiophanate-methyl	343.21	151.06	24	311.20	12			6.78	+
Tolclofos-methyl	301.00	175.00	22					6.16	+
Tolfenpyrad	384.08	196.95	29	181.69	30			23.59	+
Tralkoxydim	330.00	284.00	13	138.00	22			16.13	+

Compound	Precursor Ion	Quantitation Ion	CE	Confirming Ion 1	CE	Confirming Ion 2	CE	RT (min)	Polarity
Tralomethrin+NH ₄	682.80	440.60	18	665.80	10	412.60	22	27.59	+
Triadimefon	294.17	197.10	16	225.10	16			14.86	+
Triadimenol	296.10	70.00	15					14.26	+
Triazophos	313.99	162.10	21	119.17	36			15.82	+
Trichlamide	340.00	121.00	22					19.14	+
Trichlorfon	256.90	127.00	19	109.10	19			4.57	+
Tricyclazole	190.07	163.06	24	136.10	30			5.33	+
Tridemorph	298.00	130.00	28	98.00	32			19.42	+
Trifloxystrobin	409.30	186.00	21	206.10	16			21.54	+
Triflumizole	346.16	278.10	12	73.00	18			21.4	+
Triflumuron	359.10	156.20	17	139.00	31			20.24	+
Triforine-a	434.90	390.00	12					12.45	+
Triforine-b	432.90	388.00	12					12.46	+
Triforine-c	436.90	392.00	12					12.45	+
Trinexapac-ethyl	253.11	207.02	11	69.27	20	165.02	17	10.28	+
Triconazole	318.12	70.00	25	125.00	30			16.16	+
Uniconazole	292.13	70.20	25	125.00	32			17.32	+
Vamidothion	288.07	146.05	14	118.10	27			3.6	+
Vernolate	204.15	128.21	11	86.22	13	43.47	19	19.47	+
Warfarin	307.03	160.94	20					26.95	+
Zoxamide	336.22	187.00	23	159.00	38			18.7	+

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