Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Validating an Ion Mobility Spectrometry-Quadrupole Time of Flight Mass Spectrometry Method for High-throughput Pesticide Screening

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Table S1. Accurate IM-MS database of 50 pesticides

Pesticide	CAS	Molecular formula	$[M+H]^{+}$ [a]	Major product ion[b]	CE[c]	CCS[d]	Classify
Cadusafos	95465-99-9	C10H23O2PS2	271.0950	158.9698,215.0324,130.9385	10	157.6	organophosphates
Fonofos	944-22-9	C10H15OPS2	247.0375	137.0184,108.9871,124.9821	10	146.4	organophosphates
Diazinon	333-41-5	C12H21N2O3PS	305.1083	169.0794,153.1022,96.9508,277.0770,249.0457	25	168.4	organophosphates
Etrimfos	38260-54-7	C10H17N2O4PS	293.0719	124.9821,265.0406,142.9926,109.0049,78.9943	25	161.9	organophosphates
Pirimiphos-methyl	29232-93-7	C11H20N3O3PS	306.1036	164.1182,108.0556,124.9821,96.9508,67.0291,136.0869	35	165.7	organophosphates
Fenthion	55-38-9	C10H15O3PS2	279.0273	247.0011,169.0140,153.0369,138.0498,124.9821,108.9871	20	157.4	organophosphates
Quinalphos	13593-03-8	C12H15N2O3PS	299.0614	163.0324,242.9988,147.0553,129.0447,96.9508	25	162.3	organophosphates
Fenamiphos	22224-92-6	C13H22NO3PS	304.1131	217.0083,234.0348,201.9848,169.0862,108.0570	20	171.6	organophosphates
Prothiofos	34643-46-4	C11H15Cl2O2PS2	344.9701	240.9041,302.9231,274.8918,204.9274,158.9698,109.9918	10	168.2	organophosphates
Triazophos	24017-47-8	C12H16N3O3PS	314.0723	178.0433,119.0604,96.9508,150.9977	20	171.7	organophosphates
Edifenphos	17109-49-8	C14H15O2PS2	311.0324	201.0134,172.9821,283.0011,111.0263,109.0106	20	161.7	organophosphates
Buprofezin	69327-76-0	C16H23N3OS	306.1635	116.0528,250.1009,106.0651,57.0699,145.0396,208.0539	15	173.2	diazthines
Molinate	2212-67-1	C9H17NOS	188.1104	126.0913,83.0855,98.0964,55.0542	10	138.8	carbamates
Atrazine	1912-24-9	C8H14ClN5	216.1010	146.0228,138.0774,174.0541,132.0323,104.0010,96.0556	25	148.4	triazines
Simeconazole	149508-90-7	C14H20FN3OSi	294.1432	276.1327,135.0605,115.0574,70.0400.73.0468	20	170.0	triazoles
Myclobutanil	88671-89-0	C15H17ClN4	289.1215	70.0400,125.0153,151.0309,220.0888	20	174.5	triazoles
Pyrazophos	13457-18-6	C14H20N3O5PS	374.0934	222.0873,238.0645,194.0560,346.0621,317.0356	20	191.5/ 185.7	organophosphates
Azoxystrobin	131860-33-8	C22H17N3O5	404.1241	372.0979,344.1030,329.0795,316.1081	15	195.7	strobilurins
Fluquinconazole	136426-54-5	C16H8Cl2FN5O	376.0163	349.0054,163.0302,306.9836,287.0256,272.0147	25	177.1/ 184.1	triazoles
Dicrotophos	141-66-2	C8H16NO5P	238.0839	193.0260,127.0155,112.0757,72.0444	10	148.7/ 142.8	organophosphates
Trifluralin	1582-09-8	C13H16F3N3O4	336.1166	276.0591,252.0227,294.0696,236.0278,248.0278	15	168.4	dinitroanilines

Pesticide	CAS	Molecular formula	$[M+H]^+$	Major product ion	CE	CCS	Classify
Triadimefon	43121-43-3	C14H16ClN3O2	294.1004	197.0728,225.0677,155.0258,141.0102,57.0699	5	173.5	triazoles
Penconazole	66246-88-6	C13H15Cl2N3	284.0716	70.0400,158.9763,172.9919	15	165.3	triazoles
Trifloxystrobin	141517-21-7	C20H19F3N2O4	409.1370	186.0525,206.0812,132.0808,116.0495,162.0913	15	188.1	strobilurins
Pyridaben	96489-71-3	C19H25ClN2OS	365.1449	132.0934,105.0699,309.0823,147.1168,119.0855	10	192.5/ 187.0	pyridazinones
Pyrimidifen	105779-78-0	C20H28ClN3O2	378.1943	169.0401,124.0883,184.0636,89.0386	30	178.0/ 188.2	pyrimidines
Dimethenamid	87674-68-8	C12H18ClNO2S	276.0820	244.0557,168.0841,111.0263,73.0648,138.0372	10	154.8	amides
Metalaxyl	57837-19-1	C15H21NO4	280.1543	220.1332,192.1383,248.1281,160.1121,148.1121	10	160.5	amides
Diphenamid	957-51-7	C16H17NO	240.1383	134.0964,91.0542,72.0444,239.1305,118.0651	20	153.9	amides
Cyprodinil	121552-61-2	C14H15N3	226.1339	93.0573,108.0808,119.0604,91.0542,210.1026	40	152.6	pyrimidines
Napropamide	15299-99-7	C17H21NO2	272.1645	129.1148,199.0754,171.0804,114.0913,100.0757,74.0964	15	164.3	amides
Pretilachlor	51218-49-6	C17H26ClNO2	312.1725	252.1150,176.1434,146.0964,238.0993,162.1277	15	171.5	amides
Benalaxyl	71626-11-4	C20H23NO3	326.1751	208.1332,266.1539,148.1121,121.0886,91.0542	10	172.1	amides
Tebuconazole	107534-96-3	C16H22ClN3O	308.1524	70.0400,151.0309,138.9945,125.0153	25	167.0	triazoles
Indoxacarb	173584-44-6	C22H17ClF3N3O7	528.0780	249.0425,218.0423,293.0324,190.0054,150.0105,203.0189	15	206.1	carbamates
Esprocarb	85785-20-2	C15H23NOS	266.1573	148.1121,91.0542,71.0855,196.0791	15	160.7	carbamates
Fenbuconazole	114369-43-6	C19H17ClN4	337.1215	70.0400,125.0153,91.0542,194.0480	25	183.5	triazoles
Butylate	2008-41-5	C11H23NOS	218.1573	57.0699,156.1383,162.0947,134.0998,100.0757	10	150.5	carbamates
Sulfotep	3689-24-5	C8H20O5P2S2	323.0300	171.0239,142.9844,182.9971,96.9508,294.9987,266.9674	10	160.5	organophosphates
Pyrimethanil	53112-28-0	C12H13N3	200.1182	107.0604,183.0917,181.0760,182.0838,168.0682,82.0651	40	142.9	pyrimidines
Fenpropimorph	67564-91-4	C20H33NO	304.2635	147.1168,130.1226,132.0934,119.0855,116.1070,57.0699	35	173.0/ 178.1	morpholines
Ethychlozate	27512-72-7	C11H11ClN2O2	239.0582	165.0214,138.0105,107.0604	15	152.7	indoles
Quizalofop-ethyl	76578-14-8	C19H17ClN2O4	373.0950	287.0469,271.0633,299.0582,255.0320,243.0684	25	191.6/ 199.2	phenoxyalkanoic acids
Flutriafol	76674-21-0	C16H13F2N3O	302.1099	70.0400,123.0241,109.0448,233.0772,137.0397	20	167.2	triazoles

Pesticide	CAS	Molecular formula	$[M+H]^+$	Major product ion	CE	CCS	Classify
Carboxine	5234-68-4	C12H13NO2S	236.0740	143.0161,86.9899,124.0215,93.0573,132.0444,117.0369	15	150.5	amides
Acetamiprid	135410-20-7	C10H11ClN4	223.0745	126.0105,56.0495,98.9996,90.0338	20	153.7	nicotiniums
Picolinafen	137641-05-5	C19H12F4N2O2	377.0908	238.0474,359.0802,256.0580,337.0783,266.0423	20	188.9	pyridines
Fenamidone	161326-34-7	C17H17N3OS	312.1165	92.0495,236.1182,165.0481,120.0808,103.0542	15	172.6	pyrroles
Fluridone	59756-60-4	C19H14F3NO	330.1100	309.0960,242.0964,294.0725,259.0992,290.0976,287.0916	55	179.0	pyridines
Spiroxamine	118134-30-8	C18H35NO2	298.2741	100.1121,144.1383,72.0808,126.1277,58.0651	25	182.0/ 176.9	morpholines

a: accurate mass of $[M+H]^+$ and its unit is Da;

b: accurate mass of major product ion;

c: optimized collision energy for each pesticide in MS^2 mode;

d: CCS reference value of $[M+H]^+$ and its unit is $Å^2$.

Table S2. Measured results of 50 pesticides in scallion samples

Pesticide	$[M+H]^+$	CCS_1	CCS_2	CCS_3	Average [a]	SD[b]	Deviation[c]	LOD [d] (APCI)	LOD [d] (ESI)
Cadusafos	271.0950	157.9	157.7	157.6	157.7	0.15	0.1	5	100
Fonofos	247.0375	146.6	146.5	146.4	146.5	0.10	0.1	20	10
Diazinon	305.1083	167.6	167.6	167.8	167.7	0.12	-0.7	10	5
Etrimfos	293.0719	161.7	161.8	161.7	161.7	0.06	-0.1	5	5
Pirimiphos-methyl	306.1036	165.6	165.5	165.5	165.5	0.06	-0.2	5	5
Fenthion	279.0273	157.2	157.3	157.1	157.2	0.10	-0.2	10	50
Quinalphos	299.0614	162.1	162.1	162.1	162.1	0.00	-0.2	20	50
Fenamiphos	304.1131	170.9	170.9	170.8	170.9	0.06	-0.8	5	10
Prothiofos	344.9701	167.9	167.8	167.8	167.8	0.06	-0.3	5	50
Triazophos	314.0723	170.9	170.9	170.8	170.9	0.06	-0.8	5	5
Edifenphos	311.0324	161.6	161.6	161.5	161.6	0.06	-0.1	10	10
Buprofezin	306.1635	173.3	173.2	173.2	173.2	0.06	0.0	5	5
Molinate	188.1104	138.9	139.2	139.0	139.0	0.15	0.2	5	100
Atrazine	216.1010	148.4	148.4	148.3	148.4	0.06	0.0	5	5
Dimethenamid	276.0820	154.7	154.6	154.6	154.6	0.06	-0.2	20	100
Simeconazole	294.1432	169.8	169.7	169.7	169.7	0.06	-0.2	10	20
Fluquinconazole	376.0163	176.7	176.6	176.6	176.6	0.06	-0.4	20	50
		183.5	183.9	183.2	183.5	0.35	-0.6		
Dicrotophos	238.0839	148.9	148.7	148.9	148.8	0.12	0.2	100	50
		142.7	143.0	143.1	142.9	0.21	0.1		
Trifluralin	336.1166	168.0	168.0	168.3	168.1	0.17	-0.3	10	200
Triadimefon	294.1004	172.9	172.9	172.9	172.9	0.00	-0.6	50	50
Penconazole	284.0716	165.2	165.3	165.3	165.3	0.06	0.0	10	50
Trifloxystrobin	409.1370	187.2	187.2	187.3	187.2	0.06	-0.8	5	50
Pyridaben	365.1449	191.5	191.6	191.6	191.6	0.06	-0.9	50	50
		186.5	187.4	186.0	186.6	0.71	0.4		
Pyrimidifen	378.1943	177.1	177.1	177.2	177.1	0.06	-0.9	5	5
		187.5	187.4	187.5	187.5	0.06	-0.7		
Metalaxyl	280.1543	160.2	160.3	160.2	160.2	0.06	-0.2	5	5
Diphenamid	240.1383	153.7	153.7	153.6	153.7	0.06	-0.2	20	10
Cyprodinil	226.1339	152.6	152.6	152.5	152.6	0.06	-0.1	10	5
Napropamide	272.1645	164.0	164.0	164.0	164.0	0.00	-0.3	5	20
Pretilachlor	312.1725	170.8	170.8	170.8	170.8	0.00	-0.7	20	5
Benalaxyl	326.1751	171.3	171.3	171.3	171.3	0.00	-0.8	5	5
Myclobutanil	289.1215	174.1	174.1	174.0	174.1	0.06	-0.4	5	50
Pyrazophos[e]	374.0934	191.2	191.1	191.1	191.1	0.06	-0.3	5	10
		185.7	185.6	186.0	185.8	0.21	0.1		
Esprocarb	266.1573	160.5	160.4	160.3	160.4	0.10	-0.3	20	50
Fenbuconazole	337.1215	182.8	182.8	182.7	182.8	0.06	-0.7	50	50
Butylate	218.1573	150.4	150.2	150.0	150.2	0.20	-0.3	5	5
Tebuconazole	308.1524	166.4	166.4	166.4	166.4	0.00	-0.6	5	5
Indoxacarb	528.0780	205.7	205.7	205.6	205.7	0.06	-0.4	10	100
Azoxystrobin	404.1241	195.4	195.3	195.2	195.3	0.10	-0.4	10	20

Pesticide	$[M+H]^+$	CCS_1	CCS_2	CCS_3	Average	SD	Deviation	LOD (APCI)	LOD (ESI)
Sulfotep	323.0300	160.6	160.4	160.3	160.4	0.15	-0.1	5	5
Ethychlozate	239.0582	152.2	152.1	152.1	152.1	0.06	-0.6	5	5
Pyrimethanil	200.1182	142.8	142.6	142.6	142.7	0.12	-0.2	5	5
Fenpropimorph	304.2635	172.6	172.5	172.4	172.5	0.10	-0.5	5	5
		177.6	177.4	177.3	177.4	0.15	-0.7		
Quizalofop-ethyl	373.0950	191.2	191.0	190.8	191.0	0.20	-0.6	20	10
		198.9	198.8	198.8	198.8	0.06	-0.4		
Flutriafol	302.1099	166.7	166.7	166.6	166.7	0.06	-0.5	20	50
Carboxine	236.0740	150.4	150.5	150.5	150.5	0.06	-0.1	10	50
Acetamiprid	223.0745	153.6	153.5	153.6	153.6	0.06	-0.1	20	100
Picolinafen	377.0908	188.4	188.4	188.4	188.4	0.00	-0.5	5	50
Fenamidone	312.1165	171.9	171.9	171.9	171.9	0.00	-0.7	10	10
Fluridone	330.1100	178.5	178.6	178.7	178.6	0.10	-0.4	5	10
Spiroxamine	298.2741	181.2	181.1	181.0	181.1	0.10	-0.9	5	5
		175.9	175.9	175.9	175.9	0.00	-1.0		

a: the average of measured CCS values (CCS_1，CCS_2，CCS_3) in three consecutive injection;

b: the standard deviation of measured CCS values in three consecutive injection;

c: the deviation between the average CCS value in table 2 and the reference in database;

d: the unit of LOD (limit of detection) is ng/mL;

e: each pesticide has two CCS values, each CCS value is corresponding to its one isomeric ion.