

Supplementary

Assessment of Pesticide Content in Apples and Selected Citrus Fruits Subjected to Simple Culinary Processing

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Both transitions were used for quantification and confirmation purposes (Table S1, Table S2).

Table S1. List of pesticides determined in the positive ionization mode.

No.	ID	RT (min)	Q1	Q3	DP	EP	CE	CXP
1.	3 hydroxycarbofuran 1	7.9	238.1	220.1	50	10	9	9
2.	3 hydroxycarbofuran 2	7.9	238.1	181.1	50	10	11	11
3.	3,5-Dichloroaniline 1	12.2	162	127	56	10	29	22
4.	3,5-Dichloroaniline 2	12.2	164	129	51	10	29	6
5.	Abamectin 1	13.9	890.5	567.4	81	10	29	10
6.	Abamectin 2	13.9	890.5	305.3	81	10	37	8
7.	Acephate 1	3.7	184	143	51	10	13	10
8.	Acephate 2	3.7	184	125	51	10	25	5
9.	Acetamiprid 1	7.4	223	126	71	10	31	6
10.	Acetamiprid 2	7.4	223	99	71	10	51	6
11.	Acrinathrin 1	15.2	559.1	208.1	66	10	23	10
12.	Acrinathrin 2	15.2	559.1	181.1	66	10	43	8
13.	Alachlor 1	12.7	270.1	238.1	31	10	15	8
14.	Alachlor 2	12.7	270.1	162.2	31	10	25	8
15.	Aldicarb 1	8.9	208.2	116	50	10	20	10
16.	Aldicarb 2	8.9	208.2	89	50	10	20	10
17.	Aldicarb Sulfoxide 1	4.4	207.3	132	56	10	11	10
18.	Aldicarb Sulfoxide 2	4.4	207.3	89	56	10	19	6
19.	Aldicarb Sulphone 1	4.8	223.1	86.2	66	10	25	4
20.	Aldicarb Sulphone 2	4.8	223.1	148	66	10	13	14
21.	Ametryn 1	11.7	228	186	50	10	35	10
22.	Ametryn 2	11.7	228	116	50	10	35	10
23.	Amitraz 1	17.4	294.2	163.1	50	10	21	9
24.	Amitraz 2	17.4	294.2	122.1	50	10	41	10
25.	Atrazine 1	11.2	216.1	104	76	10	41	10
26.	Atrazine 2	11.2	216.1	174	76	10	25	12
27.	Azinophos-Et 1	12.4	346.3	160	50	10	15	10
28.	Azinophos-Et 2	12.4	346.3	132	50	10	20	10
29.	Azinphos-Me 1	11.3	318	160	50	10	15	10
30.	Azinphos-Me 2	11.3	318	132	50	10	20	10
31.	Azoxystrobin 1	11.3	404	344.2	50	10	35	10
32.	Azoxystrobin 2	11.3	404	372	50	10	20	10
33.	Benfuracarb 1	14.2	411.4	252	36	10	19	12
34.	Benfuracarb 2	14.2	411.4	195	36	10	31	12

35.	Benzoylprop ethyl 1	13.5	368.098	105.088	61	10	19	9
36.	Benzoylprop ethyl 2	13.5	368.097	77.159	61	10	75	12
37.	Bifenazate 1	12.6	301.2	170	60	10	20	9
38.	Bifenazate 2	12.6	301.2	152	60	10	40	7
39.	Bromacil 1	9.9	261.2	188	41	10	41	10
40.	Bromacil 2	9.9	261.2	205	41	10	19	12
41.	Bromuconazole 1	12.5	378	159	50	10	35	10
42.	Bromuconazole 2	12.5	378	70	50	10	35	10
43.	Buprofezine 1	14.7	306.2	116	50	10	20	10
44.	Buprofezine 2	14.7	306.2	201	50	10	35	10
45.	Butoxycarboxin 1	5.2	223.1	106.1	40	10	9	9
46.	Butoxycarboxin 2	5.2	223.1	86.2	40	10	10	9
47.	Carbaryl 1	10.4	202.1	127.1	50	10	35	10
48.	Carbaryl 2	10.4	202.1	145.1	50	10	20	10
49.	Carbendazim 1	8.4	192.1	132.1	50	10	50	10
50.	Carbendazim 2	8.4	192.1	160.1	50	10	20	10
51.	Carbetamide 1	9.3	237.1	118.1	21	10	19	8
52.	Carbetamide 2	9.3	237.1	192	21	10	13	8
53.	Carbofuran 1	9.8	222.1	165	61	10	20	10
54.	Carbofuran 2	9.8	222.1	123	61	10	31	10
55.	Carbosulfan 1	18.2	381.2	118	50	10	35	10
56.	Carbosulfan 2	18.2	381.2	160	50	10	20	10
57.	Carboxin 1	10.2	236	142.9	50	10	20	10
58.	Carboxin 2	10.2	236	93.1	50	10	35	10
59.	Chlorantraniliprole 1	11.6	482.1	450.9	66	10	21	9
60.	Chlorantraniliprole 2	11.6	482.1	283.8	66	10	19	11
61.	Chloridazon 1	7.7	222	104.2	56	10	31	8
62.	Chloridazon 2	7.7	222	92.2	56	10	35	8
63.	Chlorotoluron 1	10.7	213.1	72	66	10	33	8
64.	Chlorotoluron 2	10.7	215.1	72	66	10	33	8
65.	Chlorpyrifos 1	15.4	349.9	115.1	66	10	33	8
66.	Chlorpyrifos 2	15.4	349.9	197.9	66	10	25	14
67.	Chlorsulfuron 1	6.6	358	141	51	10	23	8
68.	Chlorsulfuron 2	6.6	358	167	51	10	25	8
69.	Clofentezine 1	13.4	303	102.1	51	10	53	8
70.	Clofentezine 2	13.4	303	138	51	10	21	8
71.	Clomazone 1	11.5	240.1	125	56	10	27	8
72.	Clomazone 2	11.5	240.1	89.1	56	10	65	8
73.	Clothianidin 1	6.9	250	132	50	10	30	8
74.	Clothianidin 2	6.9	250	169	50	10	30	8
75.	Coumaphos 1	13	363	227	66	10	35	8
76.	Coumaphos 2	13	363	307	66	10	23	8
77.	Cyanazine 1	9.3	241.1	214.1	41	10	23	8
78.	Cyanazine 2	9.3	241.1	104.1	41	10	41	8
79.	Cyanofenophos 1	13.1	304	276	66	10	17	6
80.	Cyanofenophos 2	13.1	304	157	66	10	27	6
81.	Cycloate 1	14.7	216	154	41	10	17	6
82.	Cycloate 2	14.7	216	83	56	10	23	4
83.	Cymoxanil 1	8.4	199.2	128	46	10	13	8

84.	Cymoxanil 2	8.4	199.2	111	46	10	27	8
85.	Cyphenothrin 1	17.0	393	151	71	10	21	12
86.	Cyphenothrin 2	17.0	393	123	71	10	33	8
87.	Cyprofuram 1	10.7	280.1	166.2	23	10	22	8
88.	Cyprofuram 2	10.7	280.1	184.1	23	10	27	9
89.	DEF 1	17.3	315.2	169.2	28	10	23	8
90.	DEF 2	17.3	315.2	259.3	28	10	20	13
91.	Demeton-S-methyl 1	10	248	89.1	6	10	17	10
92.	Demeton-S-methyl 2	10	248	61	6	10	47	10
93.	Demeton-S-methylsulphon 1	5.6	263	169.1	71	10	23	10
94.	Demeton-S-methylsulphon 2	5.6	263	108.9	71	10	41	6
95.	Desethyl atrazin 1	8.3	188.1	104	56	10	33	8
96.	Desethyl atrazin 2	8.3	188.1	146	56	10	25	8
97.	Desisopropyl atrazin 1	6.7	174.07	103.85	56	10	31	8
98.	Desisopropyl atrazin 2	6.7	174.07	95.95	56	10	27	8
99.	Desmedipham 1	11.1	301.2	136	66	10	33	8
100.	Desmedipham 2	11.1	301.2	182.1	66	10	13	12
101.	Desmetryn 1	11.5	214.1	82.1	65	10	44	6
102.	Desmetryn 2	11.5	214.1	116.1	65	10	43	6
103.	Diafenthiuron 1	16	385.3	329.3	60	10	29	17
104.	Diafenthiuron 2	16	385.3	278.3	60	10	45	14
105.	Dialifos 1	14.5	394	208.1	46	10	23	9
106.	Dialifos 2	14.5	394	186.9	46	10	17	9
107.	Diazinon 1	13.7	305.1	169.1	60	10	29	9
108.	Diazinon 2	13.7	305.1	96.6	60	10	41	10
109.	Dichlofluanid 1	13.1	333	123	56	10	24	9
110.	Dichlofluanid 2	13.1	333	224	56	10	17	10
111.	Diclorovos 1	9.7	221	109	76	10	27	6
112.	Diclorovos 2	9.7	221	127	76	10	25	10
113.	Dicrotophos 1	6.4	238.1	127.1	16	10	23	8
114.	Dicrotophos 2	6.4	238.1	112.1	16	10	17	8
115.	Dimefuron 1	11.2	339.1	167	61	10	29	8
116.	Dimefuron 2	11.2	339.1	256	61	10	21	8
117.	Dimethachlor 1	11.4	256.1	224.2	26	10	19	10
118.	Dimethachlor 2	11.4	256.1	148.1	26	10	33	10
119.	Dimethenamide 1	12	276.1	244.1	11	10	19	8
120.	Dimethenamide 2	12	276.1	168.1	11	10	33	8
121.	Dimethoate 1	7.6	230	171	50	10	20	10
122.	Dimethoate 2	7.6	230	199	50	10	20	10
123.	Dimethomorph 1	11.8	388	301	50	10	35	10
124.	Dimethomorph 2	11.8	388	165	50	10	50	10
125.	Diniconazole 1	14.0	326.1	70.2	60	10	25	9
126.	Diniconazole 2	14.0	326.1	159	60	10	34	10
127.	Diphenamide 1	11.6	240.1	134.1	50	10	20	9
128.	Diphenamide 2	11.6	240.1	167.1	50	10	22	10
129.	Diphenylamine 1	12.4	170.144	93.1	66	10	37	6
130.	Diphenylamine 2	12.4	170.144	152	66	10	35	10
131.	Disulfoton 1	14.2	275	89.2	6	10	17	10
132.	Disulfoton 2	14.2	275	61.1	6	10	43	4

133.	Ditalimfos 1	12.9	300.1	148	60	10	20	9
134.	Ditalimfos 2	12.9	300.1	130.1	60	10	34	10
135.	Diuron 1	11.1	233.2	160	71	10	35	10
136.	Diuron 2	11.1	233.2	72	71	10	37	12
137.	DMF (2,4-Dimethyl-phenyl-formamidine) 1	9.9	151	107	66	10	43	6
138.	DMF (2,4-Dimethyl-phenyl-formamidine) 2	9.9	151	106	66	10	27	6
139.	Dodine 1	13	228.305	57	70	10	43	8
140.	Dodine 2	13.1	228.305	60	70	10	41	10
141.	Epoxiconazole 1	12.5	330.2	101.1	51	10	71	4
142.	Epoxiconazole 2	12.5	330.2	121.1	51	10	31	8
143.	Etaconazole 1	13	329.476	161	46	10	53	14
144.	Etaconazole 2	13	329.476	55.163	46	10	57	8
145.	Ethiofencarb 1a	10.6	226.1	106.901	61	10	21	4
146.	Ethiofencarb 2a	10.6	226.1	164.1	61	10	11	4
147.	Ethirimol 1	11.6	210.2	140.1	55	10	23	9
148.	Ethirimol 2	11.6	210.2	98.1	55	10	28	9
149.	Ethofenprox 1	19	394.24	177.07	16	10	23	12
150.	Ethofenprox 2	19	394.24	107.1	16	10	53	10
151.	Etoxazole 1	15.8	360	113	66	10	79	8
152.	Etoxazole 2	15.8	360	141	66	10	37	8
153.	Etrimphos 1	13.6	293.1	125	60	10	33	9
154.	Etrimphos 2	13.6	293.1	265.1	60	10	21	10
155.	Fenamidon 1	12.1	312.1	92.2	50	10	33	9
156.	Fenamidon 2	12.1	312.1	236.1	50	10	19	10
157.	Fenamiphos 1	13	304.1	217.1	55	10	31	9
158.	Fenamiphos 2	13	304.1	202	55	10	45	10
159.	Fenazaquin 1	17.6	307	161	51	10	31	8
160.	Fenazaquin 2	17.6	307	147	51	10	25	8
161.	Fenbuconazole 1	12.4	337.3	125	56	10	39	6
162.	Fenbuconazole 2	12.4	337.3	69.9	56	10	47	2
163.	Fenhexamid 1	12.2	302	55	86	10	63	10
164.	Fenhexamid 2	12.2	302	97	86	10	35	10
165.	Fenoxap-p-ethyl 1	11	362	121	46	10	37	10
166.	Fenoxap-p-ethyl 2	11	362	288.1	46	10	23	10
167.	Fenoxycarb 1	12.7	302.3	116.1	46	10	17	8
168.	Fenoxycarb 2	12.7	302.3	88.1	46	10	29	6
169.	Fenpropimorph 1	19.5	304.241	147.1	51	10	41	12
170.	Fenpropimorph 2	19.5	304.241	117.1	51	10	77	6
171.	Fenpyroximate 1	16.2	422	135.1	76	10	45	10
172.	Fenpyroximate 2	16.2	422	366	76	10	20	10
173.	Fenthion 1	13.1	279	169	66	10	35	10
174.	Fenthion 2	13.1	279	247.1	66	10	19	16
175.	Fenthion sulfon 1	10.5	311.1	125	60	10	22	9
176.	Fenthion sulfon 2	10.5	311.1	109	60	10	28	9
177.	Fenuron 1	8.0	165.00	72.1	60	10	17	9
178.	Fenuron 2	8.0	165.00	46.3	60	10	18	9
179.	Flazasulfuron 1	7.7	408.1	182.1	41	10	25	8

180.	Flazasulfuron 2	7.7	408.1	226.9	41	10	25	8
181.	Florosulam 1	6.6	360	191.9	50	10	35	10
182.	Florosulam 2	6.6	360	129.1	71	10	23	8
183.	Fluazifop-p-butyl 1	14	384.1	282.1	50	10	35	10
184.	Fluazifop-p-butyl 2	14	384.1	328	50	10	20	10
185.	Flufenacet 1	12.4	364.1	194.2	11	10	17	8
186.	Flufenacet 2	12.4	364.1	152.1	11	10	27	8
187.	Flufenoxuron 1	15	489.1	141.1	50	10	50	10
188.	Flufenoxuron 2	15	489.1	158	50	10	35	10
189.	Fluometuron 1	10.5	233	160	61	10	39	8
190.	Fluometuron 2	10.5	233	72	61	10	57	2
191.	Fluroxypyr 1	5.8	255.015	209	56	10	23	12
192.	Fluroxypyr 2	5.8	255.015	181	56	10	33	12
193.	Flurtamon 1	11.8	335.541	179.181	61	10	59	10
194.	Flurtamon 2	11.8	335.541	178.187	61	10	71	14
195.	Fluthiacet methyl 1	11.9	404.768	344.777	60	10	33	18
196.	Fluthiacet methyl 2	11.9	404.768	214.909	60	10	57	12
197.	Flutriafol 1	11.1	302.1	122.9	50	10	39	9
198.	Flutriafol 2	11.1	302.1	109	50	10	43	10
199.	Fonofos 1	13.8	247	109.1	50	10	25	9
200.	Fonofos 2	13.8	247	137	50	10	15	9
201.	Fosthiazate 1	10.5	284.2	104	51	10	29	6
202.	Fosthiazate 2	10.5	284.2	228	51	10	15	14
203.	Fuberidazol 1	9.9	185	157	50	10	22	9
204.	Fuberidazol 2	9.9	185	156	50	10	27	10
205.	Furathiocarb 1	14.7	383.2	195	51	10	23	8
206.	Furathiocarb 2	14.7	383.2	251.9	51	10	19	8
207.	Halfenprox 1	20	494.1	183.1	46	10	27	9
208.	Halfenprox 2	20	494.1	168	46	10	53	10
209.	Haloxypyr methyl 1	13.8	376.1	315.9	91	10	23	8
210.	Haloxypyr methyl 2	13.8	376.1	287.8	91	10	33	8
211.	Haloxypyr-2-ethoxyethyl 1	14.5	434	316	81	10	25	8
212.	Haloxypyr-2-ethoxyethyl 2	14.5	434	288	81	10	35	9
213.	Heptenophos 1	11.1	251	109	51	10	45	6
214.	Heptenophos 2	11.1	251	127	51	10	31	8
215.	Hexazinone 1	10.2	253.2	171.1	16	10	21	8
216.	Hexazinone 2	10.2	253.2	71.1	16	10	47	8
217.	Hexythiazox 1	15.5	353.1	167.9	66	10	37	10
218.	Hexythiazox 2	15.5	353.1	228	66	10	23	16
219.	Imazalil 1	13.2	297	159	26	10	31	10
220.	Imazalil 2	13.2	297	201	26	10	23	10
221.	Imazamox 1	4.7	306.164	264	66	10	27	14
222.	Imazamox 2	4.7	306.164	193.1	66	10	37	10
223.	Imazapyr 1	3.9	262.1	217.1	56	10	27	8
224.	Imazapyr 2	3.9	262.1	149.1	56	10	35	8
225.	Imidacloprid 1	7.1	256.2	175.1	50	10	35	10
226.	Imidacloprid 2	7.1	256.2	209.2	50	10	35	10
227.	Indoxacarb 1	13.5	528	203.1	86	10	57	12
228.	Indoxacarb 2	13.5	528	56	86	10	79	10

229.	Iprodione 1	12.8	330	245.1	121	10	53	9
230.	Iprodione 2	12.8	330	288.1	121	10	53	9
231.	Iprovalicarb 1	12.3	321.2	119.1	46	10	23	6
232.	Iprovalicarb 2	12.3	321.2	203.1	46	10	13	14
233.	Isazofos 1	12.7	314	162	61	10	21	7
234.	Isazofos 2	12.7	314	120	61	10	35	6
235.	Isocarbamide 1	8.8	186.1	87.1	50	10	16	6
236.	Isocarbamide 2	8.8	186.1	130.1	50	10	12	6
237.	Isomethiozin 1	13.9	269.1	200.2	34	10	23	10
238.	Isomethiozin 2	13.9	269.1	172.2	34	10	33	8
239.	Isoproturon 1	11	207.3	165.1	76	10	17	8
240.	Isoproturon 2	11	207.3	72	76	10	33	12
241.	Isoxaflutole 1	11	377	251	46	10	27	8
242.	Isoxaflutole 2	11	360.1	251	81	10	21	8
243.	Lenacil 1	11	235.1	153.1	56	10	21	8
244.	Lenacil 2	11	235.1	136.1	56	10	43	8
245.	Linuron 1	11.7	249.1	160	50	10	20	10
246.	Linuron 2	11.7	249.1	182.1	50	10	20	10
247.	Lufenuron 1	14.3	511	141	50	10	35	10
248.	Lufenuron 2	14.3	511	158	86	10	35	10
249.	Malaoxon 1	10	315.1	127	86	10	20	10
250.	Malaoxon 2	10	315.1	99	50	10	35	10
251.	Malathion 1	12	331	99	50	10	20	10
252.	Malathion 2	12	331	211.1	50	10	20	10
253.	Mecarbam 1	12.5	330.2	227.1	36	10	13	14
254.	Mecarbam 2	12.5	330.2	96.9	36	10	55	4
255.	Mepanipyrim 1	12.5	224.1	106.1	46	10	37	6
256.	Mepanipyrim 2	12.5	224.1	77.1	96	10	37	6
257.	Metalaxyl 1	11.2	280.2	160.1	96	10	59	12
258.	Metalaxyl 2	11.2	280.2	220.2	50	10	20	10
259.	Metalaxyl-M 1	11.5	280.1	220.2	55	10	21	11
260.	Metalaxyl-M 2	11.5	280.1	160.3	49	10	22	7
261.	Metamitron 1	7.9	203.1	77.1	76	10	47	12
262.	Metamitron 2	7.9	203.1	175.1	76	10	25	12
263.	Metazachlor 1	11.2	278.3	134	36	10	29	8
264.	Metazachlor 2	11.2	278.3	210	36	10	15	14
265.	Metconazole 1	13.7	320.1	125	61	10	49	6
266.	Metconazole 2	13.7	320.1	70.1	56	10	45	6
267.	Methabenzthiazuron 1	10.9	222.1	165.1	11	10	23	8
268.	Methabenzthiazuron 2	10.9	222.1	150	11	10	23	8
269.	Methacrifos 1	11.7	241.1	209.1	41	10	15	9
270.	Methacrifos 2	11.7	241.1	125.1	41	10	25	9
271.	Methamidophos 1	3.3	142.2	112	41	10	43	8
272.	Methamidophos 2	3.3	142.2	94	51	10	21	16
273.	Methidathion 1	11.7	302.9	145.1	46	10	15	9
274.	Methidathion 2	11.7	302.9	85.1	46	10	27	9
275.	Methiocarb 1	11.9	243	121.1	50	10	35	10
276.	Methiocarb 2	11.9	243	169.1	50	10	20	10
277.	Methoprotetryne 1	12.2	272.2	170.2	50	10	28	9

278.	Methoprottryne 2	12.2	272.2	198.2	50	10	22	10
279.	Methoxyfenozide 1	12.1	369	133	50	10	35	10
280.	Methoxyfenozide 2	12.1	369	149	50	10	20	10
281.	Metobromuron 1	11	259.2	148.1	61	10	21	10
282.	Metobromuron 2	11	259.2	170.2	61	10	25	10
283.	Metolachlor 1	12.9	284.2	252.2	60	10	21	18
284.	Metolachlor 2	12.9	284.2	176.2	60	10	33	18
285.	Metolachlor S 1	13.2	285	131	36	10	75	10
286.	Metolachlor S 2	13.2	285	134	36	10	47	8
287.	Metosulam 1	8.7	418	174.9	80	10	35	10
288.	Metosulam 2	8.7	418	140.1	80	10	79	10
289.	Metoxuron 1	9.1	229.2	72	66	10	37	12
290.	Metoxuron 2	9.1	229.2	156.2	66	10	35	10
291.	Metrafenon 1	13.9	409.1	209.1	41	10	21	9
292.	Metrafenon 2	13.9	409.1	226.9	41	10	25	9
293.	Monocrotophos 1	6.2	224	127	50	10	20	10
294.	Monocrotophos 2	6.2	224	98	50	10	20	10
295.	Monolinuron 1	10.7	215.2	126	51	10	25	8
296.	Monolinuron 2	10.7	215.2	148.1	51	10	21	10
297.	Monuron 1	9.9	199.1	72	51	10	29	8
298.	Monuron 2	9.9	199.1	126	51	10	35	8
299.	Myclobutanil 1	12	289	125	50	10	50	10
300.	Myclobutanil 2	12	289	70	50	10	50	10
301.	Nicosulfuron 1	6.1	411	182	56	10	31	10
302.	Nicosulfuron 2	6.1	411	106	61	10	51	6
303.	Nitenpyram 1	5.2	271.1	126.1	51	10	39	8
304.	Nitenpyram 2	5.2	271.1	237.2	51	10	25	8
305.	Norflurazon 1	11.4	304	284.1	81	10	31	10
306.	Norflurazon 2	11.4	304	160.1	81	10	41	11
307.	Novaluron 1	13.7	492.948	141.132	81	10	65	8
308.	Novaluron 2	13.7	492.948	158.111	81	10	29	10
309.	Omethoate 1	4.2	214	125	60	10	33	10
310.	Omethoate 2	4.2	214	183	60	10	15	10
311.	Oxamyl 1	5.2	237	72	50	10	35	10
312.	Oxamyl 2	5.2	237	90.1	50	10	20	10
313.	Oxycarboxin 1	8.6	268	175.1	56	10	19	6
314.	Oxycarboxin 2	8.6	268	147	56	10	29	6
315.	Oxydemeton methyl 1	5.4	247	108.9	66	10	37	6
316.	Oxydemeton methyl 2	5.4	247	169	66	10	21	16
317.	Paraoxon ethyl 1	11	276.1	220	66	10	25	9
318.	Paraoxon ethyl 2	11	276.1	94.2	66	10	45	9
319.	Paraoxon methyl 1	9.4	248	109.1	70	10	35	9
320.	Paraoxon methyl 2	9.4	248	202.1	70	10	25	9
321.	Parathion ethyl 1	13.3	292	236.1	66	10	21	9
322.	Parathion ethyl 2	13.3	292	97	66	10	39	9
323.	Pebulat 1	14.3	204.1	57.2	50	10	16	6
324.	Pebulat 2	14.3	204.1	128	50	10	11	6
325.	Penconazole 1	13.1	284	159	41	10	39	10
326.	Penconazole 2	13.1	284	70	41	10	29	10

327.	Pencycuron 1	13.6	329.1	125	41	10	33	10
328.	Pencycuron 2	13.6	329.1	99	41	10	83	10
329.	Phenkapton 1	17	378.977	192.971	36	10	25	16
330.	Phenkapton 2	17	378.977	199.019	36	10	15	10
331.	Phenmedipham 1	11.1	301.3	136	71	10	27	8
332.	Phenmedipham 2	11.1	301.3	168.1	71	10	13	12
333.	Phenothrin 1	18.4	351.1	183.2	81	10	31	10
334.	Phenothrin 2	18.4	351.1	128	81	10	77	10
335.	Phenthoate 1	13	321	79	50	10	50	10
336.	Phenthoate 2	13	321	247.2	50	10	20	10
337.	Phorate 1	14.0	261	75	56	10	31	9
338.	Phorate 2	14.0	261	47.152	56	10	47	9
339.	Phosalone 1	13.5	368	111	50	10	50	10
340.	Phosalone 2	13.5	368	182	50	10	20	10
341.	Phosmet 1	11.8	317.9	160	46	10	19	6
342.	Phosmet 2	11.8	317.9	133.1	49	10	49	6
343.	Phosphamidon 1	9.4	300	127.1	56	10	27	9
344.	Phosphamidon 2	9.4	300	174.1	56	10	19	9
345.	Phoxim 1	13.4	299	129.1	26	10	17	8
346.	Phoxim 2	13.4	299	77.1	26	10	41	8
347.	Picoxystrobin 1	12.7	368.1	145	36	10	27	8
348.	Picoxystrobin 2	12.7	368.1	205.2	36	10	15	8
349.	Pirimicarb 1	11	239.2	182.3	50	10	20	10
350.	Pirimicarb 2	11	239.2	72	50	10	20	10
351.	Pirimiphos methyl 1	14.0	306.1	164.1	46	10	29	9
352.	Pirimiphos methyl 2	14.0	306.1	108.1	46	10	39	9
353.	Prochloraz 1	13.5	376	308	50	10	30	10
354.	Prochloraz 2	13.5	376	70.1	50	10	50	10
355.	Profenofos 1	14.7	372.9	302.9	56	10	25	9
356.	Profenofos 2	14.7	372.9	97	56	10	43	9
357.	Prometryn 1	12.7	242	158	50	10	35	10
358.	Prometryn 2	12.7	242	200	50	10	35	10
359.	Propamocarb 1	6.4	189	102	50	10	20	10
360.	Propamocarb 2	6.4	189	144.1	50	10	20	10
361.	Propanil 1	12.2	218	162	50	10	35	9
362.	Propanil 2	12.2	218	127	50	10	23	10
363.	Propaquizafop 1	14.9	444.1	299.1	76	10	31	8
364.	Propaquizafop 2	14.9	444.1	100	76	10	27	8
365.	Prophos 1	13.3	243.1	97.1	60	10	33	9
366.	Prophos 2	13.3	243.1	131.1	60	10	23	9
367.	Prosulfuron 1	9.3	420.1	141.1	56	10	27	8
368.	Prosulfuron 2	9.3	420.1	167	56	10	25	8
369.	Pyraclostrobin 1	13.3	388	163	41	10	33	10
370.	Pyraclostrobin 2	13.3	388	194	46	10	33	12
371.	Pyraflufen ethyl 1	13.2	413	339	91	10	25	10
372.	Pyraflufen ethyl 2	13.2	413	253	91	10	43	9
373.	Pyridaphenthion 1	12.4	341	189	46	10	29	9
374.	Pyridaphenthion 2	12.4	341	205.1	46	10	27	9
375.	Pyridate 1	17.9	379.135	207	51	10	25	12

376.	Pyridate 2	17.9	379.135	351.2	51	10	15	20
377.	Pyrimiphos ethyl 1	15.2	334.1	198.1	50	10	29	9
378.	Pyrimiphos ethyl 2	15.2	334.1	182.2	50	10	27	9
379.	Pyriproxyfen 1	15.4	322.2	185.1	50	10	29	10
380.	Pyriproxyfen 2	15.4	322.2	96	50	10	20	10
381.	Quinmerac 1	5.6	222	204.1	21	10	23	8
382.	Quinmerac 2	5.6	222	141	21	10	43	8
383.	Quizalofop-p-ethyl 1	14.6	373	255	50	10	50	10
384.	Quizalofop-p-ethyl 2	14.6	373	299	50	10	20	10
385.	Resmethrine 1	17.6	356.2	171.2	21	10	21	8
386.	Resmethrine 2	17.6	356.2	128.1	21	10	57	8
387.	Rimsulfuron 1	6.5	432.1	182	71	10	29	8
388.	Rimsulfuron 2	6.5	432.1	324.9	71	10	21	8
389.	Sebuthylazine 1	12	230.1	174.2	21	10	25	8
390.	Sebuthylazine 2	12	230.1	104.2	21	10	41	8
391.	Sethoxydim 1	9.7	328.1	282.201	51	10	17	8
392.	Sethoxydim 2	9.7	328.1	178.101	51	10	25	8
393.	Silthiofam 1	13.2	269.06	253.111	36	10	17	14
394.	Silthiofam 2	13.2	269.06	139.033	36	10	51	10
395.	Simazine 1	10.1	202.2	131.9	61	10	27	8
396.	Simazine 2	10.1	202.2	124	61	10	27	2
397.	Simetryn 1	11.2	214.1	124.2	31	10	27	8
398.	Simetryn 2	11.2	214.1	144	31	10	27	8
399.	Spinosad A 1	19.2	732.472	142.1	101	10	41	8
400.	Spinosad A 2	19.2	732.472	98.1	101	10	103	6
401.	Spinosad D 1	20.2	746.476	142.1	96	10	43	10
402.	Spinosad D 2	20.2	746.476	98.2	96	10	105	6
403.	Spirotetramat 1	12.7	374.2	330.2	60	10	17	9
404.	Spirotetramat 2	12.7	374.2	302.2	60	10	19	9
405.	Spiroxamin 1	17	298.3	100.3	56	10	45	6
406.	Spiroxamin 2	17	298.3	144.2	56	10	29	8
407.	Sulfotep 1	13.3	323	115	46	10	39	9
408.	Sulfotep 2	13.3	323	97.1	46	10	45	9
409.	Sulprofos 1	7.8	323	247.1	50	10	17	9
410.	Sulprofos 2	7.8	323	219	50	10	21	9
411.	Tebuconazole 1	13.1	308	125	50	10	35	10
412.	Tebuconazole 2	13.1	308	70.1	50	10	35	10
413.	Tebufenozide 1	12.6	353	133	50	10	20	10
414.	Tebufenozide 2	12.6	353	297.2	50	10	20	10
415.	Tebufenpyrad 1	14.8	334.3	145	66	10	37	8
416.	Tebufenpyrad 2	14.8	334.3	117	66	10	74	10
417.	Tebutam 1	13.2	234.2	91	46	10	29	9
418.	Tebutam 2	13.2	234.2	192.2	46	10	19	9
419.	Tepraloxydim 1	7.5	342	166.001	46	10	31	12
420.	Tepraloxydim 2	7.5	342	250.001	46	10	19	24
421.	Terbumeton 1	12.3	226.1	170.1	50	10	15	9
422.	Terbumeton 2	12.3	226.1	114.1	50	10	25	9
423.	Terbuthialzine desethyl 1	10.4	202.1	145.9	26	10	23	10
424.	Terbuthialzine desethyl 2	10.4	202.1	104.2	26	10	37	10

425.	Terbutylazine 1	12	230	104	50	10	50	10
426.	Terbutylazine 2	12	230	174	50	10	20	10
427.	Tetramethrin 1	15.0	349.2	164.2	50	10	29	9
428.	Tetramethrin 2	15.0	349.2	135.2	50	10	23	9
429.	Thiabendazole 1	9.4	202.1	131	50	10	50	10
430.	Thiabendazole 2	9.4	202.1	175	50	10	35	10
431.	Thiacloprid 1	8.3	253.2	126	50	10	20	10
432.	Thiacloprid 2	8.3	253.2	186	50	10	20	10
433.	Thiamethoxam 1	6	292	211	50	10	20	10
434.	Thiamethoxam 2	6	292	181.2	50	10	35	10
435.	Thiodicarb 1	10.2	355.072	88.1	61	10	31	6
436.	Thiodicarb 2	10.2	355.072	107.9	61	10	23	6
437.	Thiophanate methyl 1	9.8	343.077	151.1	50	10	20	8
438.	Thiophanate methyl 2	9.8	343.077	192.2	50	10	20	8
439.	Tolclofos methyl 1	14	301	268.9	46	10	23	9
440.	Tolclofos methyl 2	14	301	175	46	10	35	9
441.	Tolyfluanid 1	12.9	364	137	50	10	35	10
442.	Tolyfluanid 2	12.9	364	238	50	10	20	10
443.	Triadimefon 1	12.5	294	197.2	55	10	21	9
444.	Triadimefon 2	12.5	294	225.1	55	10	19	10
445.	Tri-allate 1	16.0	307.997	85.026	86	10	73	4
446.	Tri-allate 2	16.0	307.997	146.947	86	10	37	6
447.	Triamiphos 1	14.3	295.122	278.03	36	10	11	14
448.	Triamiphos 2	14.3	295.122	109.101	36	10	37	6
449.	Triazophos 1	12.1	314.2	119	50	10	50	10
450.	Triazophos 2	12.1	314.2	162	50	10	20	10
451.	Trichlorofon 1	7.6	274	108.9	26	10	31	10
452.	Trichlorofon 2	7.6	274	221	26	10	21	10
453.	Trifloxystrobin 1	13.8	409	186	50	10	20	10
454.	Trifloxystrobin 2	13.8	409	206.2	50	10	20	10
455.	Triforine 1	11.2	434.961	389.9	50	10	17	22
456.	Triforine 2	11.2	432.961	388	50	10	17	12

ID—compound (1—quantifier ion, 2—qualifier ion); RT—retention time; Q1—pseudo-molecular ion; Q3—fragment ion; DP—declustering potential; EP—entrance potential; CE—collision energy; CXP—collision cell exit potential.

Table S2. List of pesticides determined in the negative ionization mode.

No.	ID	RT (min)	Q1	Q3	DP	EP	CE	CXP
1.	2,4 D 1	6.9	219	161	-40	-10	-18	-9
2.	2,4 D 2	6.9	219	125	-40	-10	-36	-7
3.	2,4 DB 1	8.1	247	161	-20	-10	-12	-9
4.	2,4 DB 2	8.1	249	163	-20	-10	-12	-9
5.	2,4,5 T 1	7.7	253.1	195.1	-50	-10	-16	-13
6.	2,4,5 T 2	7.7	255	197	-50	-10	-16	-13
7.	Bentazon 1	5.2	239	132	-70	-10	-36	-7
8.	Bentazon 2	5.2	239	197	-70	-10	-30	-11
9.	Bromoxynil 1	6.1	276	79	-60	-10	-52	-3
10.	Bromoxynil 2	6.1	276	81	-60	-10	-52	-3
11.	CAP 1	5.9	186.931	128.8	-45	-10	-18	-17

12.	CAP 2	5.9	184.903	126.7	-45	-10	-24	-7
13.	Dicamba 1	5.4	219	175	-25	-10	-10	-9
14.	Dicamba 2	5.4	221	177	-25	-10	-10	-9
15.	Dichloprop 2,4 DP 1	7.5	233	161	-40	-10	-18	-11
16.	Dichloprop 2,4 DP 2	7.5	235	163	-40	-10	-16	-11
17.	Diflubenzuron 1	10.8	309	155.9	-36	-10	-12	-8
18.	Diflubenzuron 2	10.8	309	288.9	-36	-10	-8	-8
19.	Fipronil 1	4.6	435.00	330.00	-18	-10	-20	-6
20.	Fipronil 2	4.6	435.00	250.00	-18	-10	-20	-6
21.	Fluazifop 1	7.5	326.1	253.8	-31	-10	-18	-8
22.	Fluazifop 2	7.5	326.1	108.1	-31	-10	-50	-8
23.	Fluazinam 1	12.3	462.9	415.8	-11	-10	-24	-8
24.	Fluazinam 2	12.3	462.9	397.9	-11	-10	-20	-8
25.	Fludioxonil 1	9.4	247	125.9	-56	-10	-42	-8
26.	Fludioxonil 2	9.4	247	169	-56	-10	-42	-8
27.	Haloxifop 2	8.7	360	196	-55	-10	-54	-9
28.	Haloxifop 1	8.7	360	288	-55	-10	-22	-15
29.	Hexaflumuron 1	12.2	459	438.8	-6	-10	-14	-8
30.	Hexaflumuron 2	12.2	459	275.9	-6	-10	-22	-8
31.	Ioxynil 1	6.8	370	127	-60	-10	-44	-5
32.	Ioxynil 2	6.8	370	215	-60	-10	-48	-11
33.	MCPA 1	6.9	199	141	-45	-10	-20	-9
34.	MCPA 2	6.9	201	143	-45	-10	-14	-9
35.	MCPB 1	8.1	227	141	-30	-10	-12	-9
36.	MCPB 2	8.1	229	143	-30	-10	-12	-9
37.	MCPB Mecoprop 1	7.4	213	141	-15	-10	-18	-1
38.	MCPB Mecoprop 2	7.4	215	143	-15	-10	-18	-7
39.	Teflubenzuron 1	13.5	379	338.9	-6	-10	-12	-8
40.	Teflubenzuron 2	13.5	379	358.8	-6	-10	-8	-8
41.	Triflumuron 1	11.6	357	154	-16	-10	-14	-8
42.	Triflumuron 2	11.6	357	175.9	-16	-10	-22	-8
43.	Triclopyr 1	7.5	253.9	196	-35	-10	-16	-18
44.	Triclopyr 2	7.5	255.9	198	-35	-10	-16	-18

ID—compound (1—quantifier ion, 2—qualifier ion); RT—retention time; Q1—pseudo-molecular ion; Q3—fragment ion; DP—declustering potential; EP—entrance potential; CE—collision energy; CXP—collision cell exit potential.