

Table S1. Analytical method validation and optimized MRM transitions of n=108 pesticides, n=18 PCBs and n=13 PAHs under analysis.

Nº	Compound	Transition 1 (m/z)	CE 1 (eV)	Transition 2 (m/z)	CE 2 (eV)	R ²	LOD (µg/Kg)	LOQ (µg/Kg)
Pesticides								
<i>Carbamates</i>								
1	(±)-Indoxacarb	218 → 203	10	218 → 134	20	0.993	0.15	0.56
2	Bendiocarb	166 → 151	10	166 → 109	20	0.999	0.03	0.10
3	Carbaryl	144 → 115	20	115 → 89	20	0.997	0.09	0.33
4	Carbofuran	164 → 149	15	164 → 103	20	0.995	0.06	0.18
5	Carbophenothion	157 → 121	20	157 → 77	20	0.996	0.06	0.20
6	Diethofencarb	267 → 225	10	267 → 168	20	1.000	0.05	0.17
7	Ethiofencarb	168 → 107	10	168 → 77	25	0.999	0.08	0.27
8	Furathiocarb	194 → 105	20	194 → 165	15	0.988	0.06	0.22
9	Phenoxy carb	116 → 88	15	186 → 109	15	0.996	0.13	0.42
10	Pirimicarb	238 → 166	10	206 → 166	15	0.992	0.03	0.09
<i>Carbamates /Acaricides</i>								
11	Mecarbam	296 → 196	10	296 → 168	10	0.996	1.16	4.17
<i>Fungicides</i>								
12	Azoxystrobin	344 → 329	20	344 → 183	20	0.990	0.07	0.25
13	Boscalid	342 → 140	10	342 → 112	25	0.986	0.15	0.56
14	Bupirimate	208 → 165	15	108 → 140	15	0.999	0.96	3.81
15	Captafol	151 → 79	20	151 → 122	10	0.994	0.04	0.12
16	Captan	107 → 79	10	107 → 77	20	0.987	1.30	4.79
17	Cyproconazole isomer II	222 → 125	20	224 → 127	20	0.999	0.06	0.19
18	Diclobutrazol	270 → 159	10	270 → 137	25	0.962	0.11	0.30
19	Fenarimol	251 → 139	20	251 → 111	25	0.973	0.31	1.10
20	Fenhexamid	177 → 78	20	177 → 113	20	0.929	2.58	8.04
21	Fluodioxonil	248 → 127	20	248 → 154	25	0.965	0.40	1.27
22	Flusilazole	233 → 165	20	233 → 152	20	0.982	2.55	8.36
23	Imazalil	215 → 173	15	215 → 145	25	0.987	0.28	0.92
24	Kresoxim methyl	206 → 131	10	206 → 116	10	1.000	1.38	4.23
25	Metalaxyl-M	160 → 130	20	160 → 144	20	0.993	0.08	0.25
26	Mepronil	269 → 119	10	210 → 181	20	0.996	0.07	0.23
27	Penconazole	248 → 157	20	248 → 192	20	0.990	0.41	1.34
28	Prochloraz	180 → 138	15	180 → 69	20	0.990	1.07	3.05
29	Procymidone	283 → 96	10	285 → 96	15	0.991	0.13	0.48
30	Pyrimethanil	198 → 118	30	199 → 198	25	0.983	0.25	0.82
31	Quintozen	237 → 143	20	237 → 119	20	0.999	0.12	0.36
32	Tebuconazole	250 → 125	15	125 → 89	25	1.000	0.15	0.49
33	Tolchlophos methyl	265 → 250	20	265 → 93	24	0.966	0.38	1.26
34	Triadimefon	208 → 181	10	208 → 127	15	0.997	0.09	0.34
35	Trifloxystrobin	190 → 130	15	190 → 102	25	0.988	0.31	1.06
36	Vinclozolin	212 → 177	15	212 → 145	20	0.997	2.48	8.18
<i>Herbicides</i>								
37	Amandryn	227 → 170	10	227 → 185	10	0.993	2.53	8.26
38	Atrazine	200 → 122	15	215 → 200	10	0.998	0.11	0.45
39	Diflufenican	266 → 183	25	246 → 218	25	0.995	5.09	14.57
40	Linuron	160 → 133	15	160 → 125	15	0.979	5.54	18.74
41	Methabenzthiazuron	164 → 136	15	127 → 109	20	0.997	0.06	0.22
42	Oxyfluorfen	300 → 223	20	252 → 170	25	0.981	0.36	1.38

43	Propazine	214 → 172	15	214 → 94	20	0.973	0.07	0.20
44	Propyzamide	173 → 145	15	173 → 109	25	0.997	0.04	0.10
45	Simazine	201 → 173	7	201 → 186	8	0.999	0.06	0.22
46	Terbuthilazine	214 → 104	15	214 → 132	10	0.998	0.13	0.40
47	Trifluralin	264 → 160	15	264 → 206	10	0.975	5.28	17.89
<i>Insect growth regulators</i>								
48	Buprofezin	175 → 132	15	175 → 117	20	0.952	0.17	0.63
49	Cyromazine	151 → 109	15	165 → 123	20	0.994	0.05	0.17
50	Pyriproxyfen	136 → 78	20	136 → 96	20	0.997	0.18	0.64
<i>Organochlorine pesticides</i>								
51	2,4'-DDD	235 → 165	20	237 → 165	20	0.991	0.09	0.33
52	2,4'-DDE	246 → 176	20	318 → 248	20	0.963	0.55	1.62
53	2,4'-DDT	235 → 165	20	237 → 165	20	0.994	0.26	0.79
54	4,4'-DDD	235 → 165	20	237 → 165	20	0.999	0.11	0.35
55	4,4'-DDE	246 → 176	30	318 → 248	30	0.997	0.16	0.56
56	4,4'-DDT	235 → 165	20	237 → 165	20	0.999	2.31	8.17
57	Alachlor	188 → 160	15	161 → 146	15	0.987	0.04	0.12
58	Aldrin	263 → 193	20	293 → 258	20	0.992	0.76	2.88
59	cis-Chlordane	373 → 266	20	373 → 264	20	0.997	0.20	0.64
60	Dicofol	250 → 139	20	250 → 215	10	0.993	0.12	0.38
61	Dieldrin	263 → 193	20	263 → 228	20	0.992	0.19	0.73
62	Endosulfan sulfate	272 → 237	15	274 → 239	15	0.997	0.09	0.37
63	Endosulfan α	241 → 206	25	241 → 170	25	0.994	0.15	0.46
64	Endosulfan β	195 → 160	10	195 → 125	20	0.999	0.07	0.20
65	Endrin	263 → 193	20	281 → 245	15	0.984	0.13	0.49
66	Methoxychlor	227 → 169	20	227 → 141	25	0.973	0.14	0.46
67	trans-Chlordane	373 → 266	20	373 → 264	20	0.972	0.12	0.47
68	α-HCH	181 → 145	10	219 → 183	10	0.988	0.04	0.13
69	β-HCH	181 → 145	15	219 → 183	10	0.985	0.22	0.82
70	γ-HCH	181 → 145	15	219 → 183	10	0.996	0.11	0.43
<i>Organophosphorous pesticides</i>								
71	Acephate	136 → 94	10	136 → 119	8	0.989	0.33	1.15
72	Andhion	231 → 175	15	231 → 129	20	0.972	0.34	1.09
73	Azinphos ethyl	160 → 132	5	160 → 77	10	0.994	0.29	0.95
74	Chlorpyriphos	197 → 169	15	197 → 169	15	0.999	1.58	5.71
75	Chlorpyriphos methyl	286 → 93	25	286 → 271	20	0.984	0.76	2.78
76	cis-Chlorfenvinphos	267 → 159	20	269 → 161	20	0.984	0.09	0.31
77	Coumaphos	226 → 163	20	226 → 135	25	0.999	0.26	0.92
78	Diazinon	137 → 84	15	179 → 137	20	0.992	0.09	0.35
79	Dimethoate	125 → 79	20	125 → 79	8	1.000	0.11	0.37
80	Fenamiphos	303 → 154	15	303 → 195	10	0.988	0.10	0.33
81	Fenchlorphos	285 → 270	20	285 → 240	20	0.990	0.06	0.21
82	Fenitrothion	125 → 79	15	277 → 125	18	0.998	0.07	0.26
83	Fenthion	278 → 109	20	278 → 125	22	0.995	0.19	0.58
84	Fenthion Sulfone	310 → 105	20	310 → 109	30	0.976	0.74	2.79
85	Fenthion Sulfoxide	278 → 109	15	278 → 169	25	0.998	0.04	0.15
86	Malathion	173 → 99	15	173 → 117	15	1.000	0.09	0.28
87	Methidathion	145 → 85	10	145 → 58	20	0.992	0.07	0.20
88	Omethoate	156 → 110	10	156 → 79	30	0.994	0.14	0.45
89	Parathion methyl	263 → 109	15	263 → 246	6	1.000	0.06	0.15
90	Phentoate	274 → 125	15	274 → 121	15	0.999	0.11	0.33

91	Phosalone	182 → 111	20	182 → 75	30	0.995	0.06	0.17
92	Phosmet	160 → 77	25	160 → 133	15	0.997	0.04	0.15
93	Phoxim	109 → 81	15	109 → 91	15	1.000	0.10	0.34
94	Quinalphos	146 → 118	15	146 → 91	30	0.994	0.07	0.22
95	<i>trans</i> -Chlorfenvinphos	267 → 159	20	269 → 161	20	0.996	0.08	0.29
96	Triphenyl phosphate	325 → 169	20	325 → 77	25	0.998	0.09	0.34
<i>Pyrethroid insecticides</i>								
97	Carbophenothion	157 → 121	20	157 → 77	20	0.999	0.10	0.37
98	Pirimiphos-methyl	290 → 125	15	290 → 151	15	0.992	0.14	0.46
99	<i>cis</i> -Fluvalinate	250 → 55	15	252 → 55	20	0.997	0.39	1.18
100	<i>cis</i> -Permethrin	183 → 153	15	183 → 168	15	1.000	0.06	0.20
101	Cypermethrin isomer I	181 → 152	20	163 → 91	15	0.995	0.06	0.22
102	Cypermethrin isomer II	181 → 152	20	163 → 91	15	0.998	0.09	0.30
103	Cypermethrin isomer III	181 → 152	20	163 → 91	15	0.997	0.07	0.24
104	Deltamethrin	181 → 152	20	253 → 93	15	1.000	0.08	0.27
105	<i>trans</i> -Fluvalinate	250 → 55	15	252 → 55	20	0.996	0.08	0.29
106	<i>trans</i> -Permethrin	183 → 153	20	183 → 168	20	0.984	0.10	0.36
107	Λ-Cyhalothrin	181 → 152	25	197 → 141	10	0.989	0.13	0.41
<i>Synergists</i>								
108	Piperonyl butoxide	176 → 131	15	176 → 103	20	0.999	0.05	0.18
<i>PCBs</i>								
1	PCB28	256 → 186	15	258 → 186	15	1.000	0.15	0.48
2	PCB52	290 → 220	15	292 → 222	15	0.998	0.07	0.22
3	PCB77	290 → 220	20	292 → 222	20	1.000	0.12	0.41
4	PCB81	290 → 220	20	292 → 222	20	0.999	0.06	0.22
5	PCB101	324 → 254	20	326 → 256	20	0.997	0.08	0.24
6	PCB105	324 → 254	20	326 → 256	20	0.990	0.04	0.15
7	PCB114	324 → 254	20	326 → 256	20	0.992	0.12	0.39
8	PCB118	324 → 254	20	326 → 256	20	0.998	0.12	0.35
9	PCB123	324 → 254	20	326 → 256	20	1.000	0.04	0.14
10	PCB126	324 → 254	20	326 → 256	20	0.987	0.03	0.10
11	PCB138	360 → 290	25	362 → 292	25	0.980	0.10	0.36
12	PCB153	360 → 290	25	362 → 292	25	0.999	0.05	0.19
13	PCB156	360 → 290	30	362 → 292	30	0.998	0.04	0.15
14	PCB157	360 → 290	30	362 → 292	30	0.975	0.16	0.55
15	PCB167	360 → 290	30	362 → 292	30	0.997	0.11	0.43
16	PCB169	360 → 290	30	362 → 292	30	0.995	0.07	0.24
17	PCB180	394 → 324	20	396 → 326	20	0.993	0.03	0.11
18	PCB189	394 → 324	25	396 → 326	25	0.999	0.04	0.12
<i>PAHs</i>								
1	Acenaphthylene	152 → 126	30	152 → 102	30	0.992	0.06	0.19
2	Anthracene	178 → 152	25	176 → 150	25	0.993	0.07	0.20
3	Benzo[a]anthracene	228 → 226	30	228 → 202	20	0.991	0.06	0.21
4	Benzo[a]pyrene	252 → 250	35	252 → 226	20	0.998	0.08	0.25
5	Benzo[b]fluoranthene	252 → 250	35	126 → 113	10	0.989	0.28	0.89
6	Benzo[g,h,i]perylene	276 → 274	45	276 → 272	50	0.999	0.07	0.21
7	Benzo[k]fluoranthene	252 → 250	35	126 → 113	10	0.994	0.14	0.48
8	Chrysene	228 → 226	30	228 → 202	20	0.990	0.06	0.17
9	Dibenzo[a,h]anthracene	278 → 276	30	278 → 252	20	0.998	0.06	0.23
10	Fluorene	166 → 165	15	165 → 164	20	0.996	0.04	0.15
11	Indeno[1,2,3-cd]pyrene	276 → 274	30	137 → 136	15	0.995	0.09	0.29

12	Phenanthrene	178 → 152	25	176 → 150	25	1.000	0.05	0.16
13	Pyrene	202 → 200	20	202 → 152	30	0.996	1.28	4.19

CE, Collision Energy; R², determination coefficient; LOD, Limit of Detection; LOQ, Limit of Quantification

Table S2. Analytical method validation and monitored ions of n=10 PAEs and n=8 NPPs under analysis.

<i>Nº</i>	<i>Compound</i>	<i>Abbreviation</i>	<i>Monitored ions (m/z)</i>	<i>R²</i>	<i>LOD (mg/Kg)</i>	<i>LOQ (mg/Kg)</i>
<i>PAEs</i>						
1	Dimethyl Phthalate	DMP	<u>163</u> , 92, 164	0.996	0.007	0.021
2	Diethyl Phthalate	DEP	<u>149</u> , 177, 176	0.995	0.003	0.010
3	Dipropyl Phthalate	DPrP	<u>149</u> , 150, 209	0.991	0.004	0.013
4	Dibutyl Phthalate	DBP	<u>149</u> , 150, 223	0.990	0.006	0.021
5	Diisobutyl Phthalate	DiBP	<u>149</u> , 150, 223	0.997	0.007	0.027
6	Butyl Benzyl Phthalate	BBP	<u>149</u> , 91, 206	0.999	0.004	0.012
7	Diphenyl Phthalate	DPhP	<u>225</u> , 226, 104	0.992	0.018	0.062
8	Dicyclohexyl Phthalate	DcHexP	<u>149</u> , 167, 150	0.999	0.028	0.087
9	Diheptyl Phthalate	DHepP	<u>149</u> , 99, 265	0.997	0.177	0.555
10	Di(2-ethylhexyl) Phthalate	DEHP	<u>149</u> , 167, 279	0.999	0.007	0.025
<i>NPPs</i>						
1	Dimethyl Adipate	DMA	<u>114</u> , 101, 111	0.998	0.011	0.033
2	Diethyl Adipate	DEA	<u>111</u> , 157, 128	0.992	0.003	0.010
3	Benzyl Benzoate	BB	<u>105</u> , 91, 212	0.987	0.012	0.043
4	Dibutyl Adipate	DBA	<u>129</u> , 185, 111	0.989	0.023	0.071
5	Diisobutyl Adipate	DiBA	<u>129</u> , 185, 111	0.993	0.009	0.029
6	Di(2-ethylhexyl) Adipate	DEHA	<u>129</u> , 112, 147	0.982	0.014	0.044
7	Di(2-ethylhexyl) Terephthalate	DEHT	<u>149</u> , 112, 261	0.988	0.009	0.033
8	Di(2-ethylhexyl) Sebacate	DEHS	<u>185</u> , 149, 112	0.997	0.048	0.182

R², coefficient of determination; LOD, Limit of Detection; LOQ, Limit of Quantification.

Underlined ions were considered for quantitative analysis.

Table S3. Analytical method validation and MS/MS condition of n=9 BPs under analysis.

Nº	Compound	Abbreviation	Transition 1 (m/z)	CE 1 (eV)	Transition 2 (m/z)	CE 2 (eV)	R ²	LOD (µg/Kg)	LOQ (µg/Kg)
1	4,4'-Sulfonyldiphenol	BPS	249.2 → 107.9	15	249.27 → 156.0	12	0.998	0.297	1.142
2	4,4'-Methylenediphenol	BPF	199.2 → 93.1	13	199.23 → 105.1	14	0.993	0.385	1.362
3	1,1-Bis(4-hydroxyphenyl)ethane	BPE	213.3 → 198.0	38	213.26 → 194.9	40	0.992	0.328	1.168
4	4,4'-(propan-2,2-diyl)diphenol	BPA	227.3 → 212.1	17	227.29 → 133.0	18	0.988	0.431	1.457
5	4-[2-(4-hydroxyphenyl)butan-2-yl] phenol	BPB	241.3 → 212.0	20	241.31 → 211.0	21	0.995	0.289	0.945
6	2,2-Bis(4-hydroxyphenyl)hexafluoropropane	BPAF	335.3 → 265.0	35	335.30 → 177.0	33	0.996	0.276	0.839
7	1,1-Bis(4-hydroxyphenyl)-1-phenyl-ethane	BPAP	289.4 → 274.1	10	289.36 → 273.1	10	0.994	0.462	1.591
8	1,1-Bis(4-hydroxyphenyl)-cyclohexane	BPZ	267.3 → 145.0	17	267.30 → 173.1	18	0.997	0.435	1.483
9	1,4-Bis(2-(4-hydroxyphenyl)-2-propyl)benzene	BPP	345.5 → 330.1	33	345.46 → 133.1	34	0.989	0.414	1.436

CE, Collision Energy; R², coefficient of determination; LOD, Limit of Detection; LOQ, Limit of Quantification.