

Supplementary Material

Table S1. Optimized MRM transitions and parameters of analytical validation for $n=139$ organic contaminants under analysis, including pesticides ($n=108$), PCBs ($n=18$) and PAHs ($n=13$). CE, Collision Energy; R^2 , coefficient of determination; LOD, Limit of Detection; LOQ, Limit of Quantification.

No.	Compound	Transition 1 (m/z)	CE 1 (V)	Transition 2 (m/z)	CE 2 (V)	R^2	LOD (ng/g)	LOQ (ng/g)
<i>Pesticides</i>								
1	(±)-Indoxacarb	218 → 203	10	218 → 134	20	0.995	0.14	0.51
2	Bendiocarb	166 → 151	10	166 → 109	20	1.000	0.02	0.04
3	Carbaryl	144 → 115	20	115 → 89	20	0.996	0.08	0.21
4	Carbofuran	164 → 149	15	164 → 103	20	0.996	0.05	0.11
5	Carbophenothion	157 → 121	20	157 → 77	20	0.998	0.05	0.15
6	Diethofencarb	267 → 225	10	267 → 168	20	0.994	0.04	0.12
7	Ethiofencarb	168 → 107	10	168 → 77	25	0.997	0.08	0.23
8	Furathiocarb	194 → 105	20	194 → 165	15	0.980	0.10	0.29
9	Phenoxycarb	116 → 88	15	186 → 109	15	0.990	0.15	0.56
10	Pirimicarb	238 → 166	10	206 → 166	15	0.998	0.04	0.14
11	Mecarbam	296 → 196	10	296 → 168	10	0.992	1.14	4.21
12	Azoxystrobin	344 → 329	20	344 → 183	20	0.989	0.06	0.2
13	Boscalid	342 → 140	10	342 → 112	25	0.987	0.13	0.42
14	Bupirimate	208 → 165	15	108 → 140	15	0.994	0.93	3.61
15	Captafol	151 → 79	20	151 → 122	10	1.000	0.03	0.09
16	Captan	107 → 79	10	107 → 77	20	0.986	1.32	4.37
17	Cyproconazole isomer II	222 → 125	20	224 → 127	20	0.998	0.06	0.17
18	Diclobutrazol	270 → 159	10	270 → 137	25	0.955	0.12	0.38
19	Fenarimol	251 → 139	20	251 → 111	25	0.985	0.32	1.05
20	Fenhexamid	177 → 78	20	177 → 113	20	0.922	2.54	8.38
21	Fluodioxonil	248 → 127	20	248 → 154	25	0.972	0.42	1.31
22	Flusilazole	233 → 165	20	233 → 152	20	0.980	2.55	8.36
23	Imazalil	215 → 173	15	215 → 145	25	0.989	0.26	0.86
24	Kresoxim methyl	206 → 131	10	206 → 116	10	0.990	1.38	4.23
25	Metalaxyl-M	160 → 130	20	160 → 144	20	0.995	2.32	8.22
26	Mepronil	269 → 119	10	210 → 181	20	0.992	0.07	0.23
27	Penconazole	248 → 157	20	248 → 192	20	0.992	0.41	1.22
28	Prochloraz	180 → 138	15	180 → 69	20	0.982	0.82	2.92

No.	Compound	Transition 1 (<i>m/z</i>)	CE 1 (V)	Transition 2 (<i>m/z</i>)	CE 2 (V)	<i>R</i> ²	LOD (ng/g)	LOQ (ng/g)
29	Procymidone	283 → 96	10	285 → 96	15	0.996	0.13	0.48
30	Pyrimethanil	198 → 118	30	199 → 198	25	0.986	0.25	0.82
31	Quintozen	237 → 143	20	237 → 119	20	1.000	0.12	0.36
32	Tebuconazole	250 → 125	15	125 → 89	25	0.999	0.15	0.47
33	Tolchlophos methyl	265 → 250	20	265 → 93	24	0.972	0.35	1.17
34	Triadimefon	208 → 181	10	208 → 127	15	0.994	0.11	0.34
35	Trifloxystrobin	190 → 130	15	190 → 102	25	0.992	0.31	0.99
36	Vinclozolin	212 → 177	15	212 → 145	20	0.998	2.45	8.24
37	Amandryn	227 → 170	10	227 → 185	10	0.994	2.49	8.18
38	Atrazine	200 → 122	15	215 → 200	10	0.996	0.12	0.4
39	Diflufenican	266 → 183	25	246 → 218	25	0.999	5.09	14.5
40	Linuron	160 → 133	15	160 → 125	15	0.984	5.51	19.3
41	Methabenzthiazuron	164 → 136	15	127 → 109	20	0.992	4.85	15.8
42	Oxyfluorfen	300 → 223	20	252 → 170	25	0.978	0.32	1.29
43	Propazine	214 → 172	15	214 → 94	20	0.952	0.54	1.62
44	Propyzamide	173 → 145	15	173 → 109	25	0.999	0.11	0.33
45	Simazine	201 → 173	7	201 → 186	8	0.998	0.05	0.17
46	Terbuthilazine	214 → 104	15	214 → 132	10	1.000	0.12	0.38
47	Trifluralin	264 → 160	15	264 → 206	10	0.961	5.11	17.08
48	Buprofezin	175 → 132	15	175 → 117	20	0.989	0.18	0.65
49	Cyromazine	151 → 109	15	165 → 123	20	0.999	0.06	0.18
50	Pyriproxyfen	136 → 78	20	136 → 96	20	0.990	0.16	0.54
51	2,4'-DDD	235 → 165	20	237 → 165	20	0.996	0.09	0.31
52	2,4'-DDE	246 → 176	20	318 → 248	20	0.962	0.52	1.62
53	2,4'-DDT	235 → 165	20	237 → 165	20	0.996	0.21	0.65
54	4,4'-DDD	235 → 165	20	237 → 165	20	0.998	0.09	0.29
55	4,4'-DDE	246 → 176	30	318 → 248	30	0.996	0.16	0.55
56	4,4'-DDT	235 → 165	20	237 → 165	20	0.998	2.33	8.23
57	Alachlor	188 → 160	15	161 → 146	15	0.985	0.26	0.95
58	Aldrin	263 → 193	20	293 → 258	20	0.986	0.82	2.85
59	<i>cis</i> -Chlordane	373 → 266	20	373 → 264	20	0.992	0.19	0.62
60	Dicofol	250 → 139	20	250 → 215	10	0.998	0.12	0.36
61	Dieldrin	263 → 193	20	263 → 228	20	0.996	0.12	0.53
62	Endosulfan sulfate	272 → 237	15	274 → 239	15	0.998	0.09	0.31

No.	Compound	Transition 1 (<i>m/z</i>)	CE 1 (V)	Transition 2 (<i>m/z</i>)	CE 2 (V)	<i>R</i> ²	LOD (ng/g)	LOQ (ng/g)
63	Endosulfan α	241 \rightarrow 206	25	241 \rightarrow 170	25	0.998	0.15	0.46
64	Endosulfan β	195 \rightarrow 160	10	195 \rightarrow 125	20	1.000	0.07	0.23
65	Endrin	263 \rightarrow 193	20	281 \rightarrow 245	15	0.972	0.09	0.29
66	Methoxychlor	227 \rightarrow 169	20	227 \rightarrow 141	25	0.978	0.12	0.38
67	<i>trans</i> -Chlordane	373 \rightarrow 266	20	373 \rightarrow 264	20	0.980	0.14	0.42
68	α -HCH	181 \rightarrow 145	10	219 \rightarrow 183	10	0.985	0.04	0.14
69	β -HCH	181 \rightarrow 145	15	219 \rightarrow 183	10	0.986	0.28	0.94
70	γ -HCH	181 \rightarrow 145	15	219 \rightarrow 183	10	0.998	0.12	0.42
71	Acephate	136 \rightarrow 94	10	136 \rightarrow 119	8	0.987	0.35	1.13
72	Andhion	231 \rightarrow 175	15	231 \rightarrow 129	20	0.969	0.36	1.15
73	Azinphos ethyl	160 \rightarrow 132	5	160 \rightarrow 77	10	0.999	0.29	0.91
74	Chlorpyrifos	197 \rightarrow 169	15	197 \rightarrow 169	15	0.996	1.68	6.04
75	Chlorpyrifos methyl	286 \rightarrow 93	25	286 \rightarrow 271	20	0.984	0.76	2.64
76	<i>cis</i> -Chlorfenvinphos	267 \rightarrow 159	20	269 \rightarrow 161	20	0.999	0.08	0.27
77	Coumaphos	226 \rightarrow 163	20	226 \rightarrow 135	25	0.984	0.29	0.92
78	Diazinon	137 \rightarrow 84	15	179 \rightarrow 137	20	0.992	0.09	0.28
79	Dimethoate	125 \rightarrow 79	20	125 \rightarrow 79	8	0.999	0.11	0.35
80	Fenamiphos	303 \rightarrow 154	15	303 \rightarrow 195	10	0.986	0.09	0.29
81	Fenchlorphos	285 \rightarrow 270	20	285 \rightarrow 240	20	0.998	0.07	0.21
82	Fenitrothion	125 \rightarrow 79	15	277 \rightarrow 125	18	0.990	0.07	0.23
83	Fenthion	278 \rightarrow 109	20	278 \rightarrow 125	22	0.998	0.19	0.58
84	Fenthion Sulfone	310 \rightarrow 105	20	310 \rightarrow 109	30	0.970	0.69	2.55
85	Fenthion Sulfoxide	278 \rightarrow 109	15	278 \rightarrow 169	25	0.995	0.04	0.13
86	Malathion	173 \rightarrow 99	15	173 \rightarrow 117	15	0.992	0.09	0.28
87	Methidathion	145 \rightarrow 85	10	145 \rightarrow 58	20	1.000	0.07	0.20
88	Omethoate	156 \rightarrow 110	10	156 \rightarrow 79	30	0.994	0.12	0.35
89	Parathion methyl	263 \rightarrow 109	15	263 \rightarrow 246	6	0.999	0.06	0.16
90	Phenthoate	274 \rightarrow 125	15	274 \rightarrow 121	15	1.000	0.11	0.30
91	Phosalone	182 \rightarrow 111	20	182 \rightarrow 75	30	0.997	0.04	0.10
92	Phosmet	160 \rightarrow 77	25	160 \rightarrow 133	15	1.000	0.04	0.10
93	Phoxim	109 \rightarrow 81	15	109 \rightarrow 91	15	0.998	0.10	0.29
94	Quinalphos	146 \rightarrow 118	15	146 \rightarrow 91	30	0.999	0.07	0.18
95	<i>trans</i> -Chlorfenvinphos	267 \rightarrow 159	20	269 \rightarrow 161	20	1.000	0.11	0.29
96	Triphenyl phosphate	325 \rightarrow 169	20	325 \rightarrow 77	25	0.997	0.13	0.30

No.	Compound	Transition 1 (<i>m/z</i>)	CE 1 (V)	Transition 2 (<i>m/z</i>)	CE 2 (V)	<i>R</i> ²	LOD (ng/g)	LOQ (ng/g)
97	Carbophenothion	157 → 121	20	157 → 77	20	1.000	0.11	0.37
98	Pirimiphos-methyl	290 → 125	15	290 → 151	15	0.998	0.14	0.46
99	<i>cis</i> -Fluvalinate	250 → 55	15	252 → 55	20	0.990	0.39	1.18
100	<i>cis</i> -Permethrin	183 → 153	15	183 → 168	15	0.994	0.52	1.76
101	Cypermethrin isomer I	181 → 152	20	163 → 91	15	0.992	0.08	0.26
102	Cypermethrin isomer II	181 → 152	20	163 → 91	15	1.000	0.1	0.3
103	Cypermethrin isomer III	181 → 152	20	163 → 91	15	0.999	0.05	0.14
104	Deltamethrin	181 → 152	20	253 → 93	15	0.999	0.1	0.33
105	<i>trans</i> -Fluvalinate	250 → 55	15	252 → 55	20	0.994	0.1	0.32
106	<i>trans</i> -Permethrin	183 → 153	20	183 → 168	20	0.986	0.09	0.29
107	Λ-Cyhalothrin	181 → 152	25	197 → 141	10	0.988	0.11	0.37
108	Piperonyl butoxide	176 → 131	15	176 → 103	20	1.000	0.06	0.18
PCBs								
1	PCB28	256 → 186	15	258 → 186	15	0.999	0.12	0.38
2	PCB52	290 → 220	15	292 → 222	15	0.999	0.09	0.30
3	PCB77	290 → 220	20	292 → 222	20	1.000	0.08	0.22
4	PCB81	290 → 220	20	292 → 222	20	1.000	0.08	0.24
5	PCB101	324 → 254	20	326 → 256	20	0.996	0.06	0.22
6	PCB105	324 → 254	20	326 → 256	20	0.989	0.12	0.35
7	PCB114	324 → 254	20	326 → 256	20	0.996	0.14	0.49
8	PCB118	324 → 254	20	326 → 256	20	0.999	0.09	0.32
9	PCB123	324 → 254	20	326 → 256	20	0.998	0.08	0.24
10	PCB126	324 → 254	20	326 → 256	20	0.982	0.34	1.15
11	PCB138	360 → 290	25	362 → 292	25	0.982	0.13	0.46
12	PCB153	360 → 290	25	362 → 292	25	1.000	0.24	0.92
13	PCB156	360 → 290	30	362 → 292	30	1.000	0.06	0.19
14	PCB157	360 → 290	30	362 → 292	30	0.978	0.74	2.75
15	PCB167	360 → 290	30	362 → 292	30	0.996	0.33	1.13
16	PCB169	360 → 290	30	362 → 292	30	0.996	0.14	0.34
17	PCB180	394 → 324	20	396 → 326	20	0.992	0.15	0.52
18	PCB189	394 → 324	25	396 → 326	25	0.998	0.04	0.14
PAHs								
1	Acenaphthylene	152 → 126	30	152 → 102	30	0.990	0.11	0.24
2	Anthracene	178 → 152	25	176 → 150	25	0.990	0.13	0.38

No.	Compound	Transition 1 (<i>m/z</i>)	CE 1 (V)	Transition 2 (<i>m/z</i>)	CE 2 (V)	<i>R</i> ²	LOD (ng/g)	LOQ (ng/g)
3	Benzo[a]anthracene	228 → 226	30	228 → 202	20	0.994	0.12	0.41
4	Benzo[a]pyrene	252 → 250	35	252 → 226	20	0.996	0.09	0.28
5	Benzo[b]fluoranthene	252 → 250	35	126 → 113	10	0.990	0.28	0.86
6	Benzo[g,h,i]perylene	276 → 274	45	276 → 272	50	1.000	0.1	0.31
7	Benzo[k]fluoranthene	252 → 250	35	126 → 113	10	0.994	0.17	0.48
8	Chrysene	228 → 226	30	228 → 202	20	0.990	0.1	0.34
9	Dibenzo[a,h]anthracene	278 → 276	30	278 → 252	20	1.000	0.11	0.32
10	Fluorene	166 → 165	15	165 → 164	20	0.996	0.12	0.42
11	Indeno[1,2,3-cd]pyrene	276 → 274	30	137 → 136	15	0.997	0.09	0.38
12	Phenanthrene	178 → 152	25	176 → 150	25	0.999	2.42	8.02
13	Pyrene	202 → 200	20	202 → 152	30	0.996	2.38	8.21

Table S2. Main figures of merit of analytical validation and monitored ions for investigated plasticizers, including $n=10$ PAEs and $n=8$ NPPs. R^2 , coefficient of determination; LOD, Limit of Detection; LOQ, Limit of Quantification.

No.	Compound	Abbreviation	Monitored ions (m/z)	R^2	LOD (mg/Kg)	LOQ (mg/Kg)
<i>PAEs</i>						
1	Dimethyl Phthalate	DMP	<u>163</u> , 92, 164	0.995	0.007	0.023
2	Diethyl Phthalate	DEP	<u>149</u> , 177, 176	0.992	0.005	0.017
3	Dipropyl Phthalate	DPrP	<u>149</u> , 150, 209	0.993	0.007	0.020
4	Dibutyl Phthalate	DBP	<u>149</u> , 150, 223	0.994	0.007	0.023
5	Diisobutyl Phthalate	DiBP	<u>149</u> , 150, 223	0.992	0.007	0.023
6	Butyl Benzyl Phthalate	BBP	<u>149</u> , 91, 206	0.988	0.037	0.121
7	Diphenyl Phthalate	DPhP	<u>225</u> , 226, 104	0.994	0.015	0.051
8	Dicyclohexyl Phthalate	DcHexP	<u>149</u> , 167, 150	0.998	0.027	0.087
9	Diheptyl Phthalate	DHepP	<u>149</u> , 99, 265	0.995	0.177	0.553
10	Di(2-ethylhexyl) Phthalate	DEHP	<u>149</u> , 167, 279	0.998	0.007	0.020
<i>NPPs</i>						
1	Dimethyl Adipate	DMA	<u>114</u> , 101, 111	0.996	0.010	0.030
2	Diethyl Adipate	DEA	<u>111</u> , 157, 128	0.994	0.013	0.037
3	Benzyl Benzoate	BB	<u>105</u> , 91, 212	0.989	0.012	0.033
4	Dibutyl Adipate	DBA	<u>129</u> , 185, 111	0.985	0.023	0.068
5	Diisobutyl Adipate	DiBA	<u>129</u> , 185, 111	0.995	0.008	0.027
6	Di(2-ethylhexyl) adipate	DEHA	<u>129</u> , 112, 147	0.986	0.013	0.037
7	Di(2-ethylhexyl) terephthalate	DEHT	<u>149</u> , 112, 261	0.988	0.070	0.233
8	Di(2-ethylhexyl) sebacate	DEHS	<u>185</u> , 149, 112	0.993	0.018	0.053

Underlined ions were considered for quantitative analysis

Table S3. Optimized MRM transitions and parameters of analytical validation for $n=9$ BPs under analysis. R^2 , coefficient of determination; LOD, Limit of Detection; LOQ, Limit of Quantification

No.	Compound	Abbreviat ion	Transition 1 Quantifier ion (m/z)	CE 1 (V)	Transition 2 Qualifier ion (m/z)	CE 2 (V)	R^2	LOD (ng/g)	LOQ (ng/g)
1	4,4'-Sulfonyldiphenol	BPS	249.27 \rightarrow 107.9	25	249.27 \rightarrow 92.0	30	0.9993	0.30	1.0
2	4,4'-Methylenediphenol	BPF	199.23 \rightarrow 93.1	15	199.23 \rightarrow 105.1	25	0.9911	0.45	1.5
3	1,1-Bis(4-hydroxyphenyl) ethane	BPE	213.26 \rightarrow 198.0	20	213.26 \rightarrow 176.9	30	0.9931	0.30	1.0
4	4,4'-(propan-2,2-diyl) diphenol	BPA	227.29 \rightarrow 212.1	10	227.29 \rightarrow 133.0	20	0.9907	0.45	1.5
5	4-[2-(4-hydroxyphenyl) butan-2-yl] phenol	BPB	241.31 \rightarrow 212.0	20	241.31 \rightarrow 211.0	15	0.9944	0.30	1.0
6	2,2-Bis(4-hydroxyphenyl) hexafluoropropane	BPAF	335.30 \rightarrow 265.0	30	335.30 \rightarrow 177.0	20	0.9995	0.30	1.0
7	1,1-Bis(4-hydroxyphenyl)-1-phenyl-ethane	BPAP	289.36 \rightarrow 274.1	35	289.36 \rightarrow 211.0	25	0.9954	0.45	1.5
8	1,1-Bis(4-hydroxyphenyl)-cyclohexane	BPZ	267.30 \rightarrow 145.0	15	267.30 \rightarrow 222.9	30	0.9984	0.45	1.5
9	1,4-Bis(2-(4-hydroxyphenyl)-2-propyl)benzene	BPP	345.46 \rightarrow 330.1	25	345.46 \rightarrow 314.9	10	0.9992	0.45	1.5

Table S4. Main figures of merit of analytical validation for $n=15$ inorganic elements under analysis. R^2 , coefficient of determination; LOD, Limit of Detection; LOQ, Limit of Quantification.

No.	Inorganic element	R^2	LOD ($\mu\text{g/kg}$)	LOQ ($\mu\text{g/kg}$)
1	Na	0.9978	1.533	5.059
2	Mg	0.9990	0.433	1.429
3	K	0.9980	0.501	1.653
4	Ca	0.9981	1.322	4.363
5	Mn	0.9998	0.003	0.010
6	Fe	0.9996	0.015	0.050
7	Co	0.9997	0.001	0.003
8	Ni	0.9997	0.007	0.023
9	Cu	0.9994	0.005	0.017
10	Zn	0.9993	0.038	0.125
11	Cr	0.9995	0.007	0.023
12	Al	0.9993	0.067	0.221
13	As	0.9998	0.001	0.003
14	Cd	0.9999	0.001	0.003
15	Pb	0.9999	0.001	0.003

Table S5. Daily intake limits and Oral Reference Dose (mg/Kg_{bw}/day) for each element. TDI: Tolerable Daily Intake; TWI: Tolerable Daily Intake; BMDL01: Benchmark dose at 1% level of extra risk (lower confidence level); BMDL05: Benchmark dose at 5% level of extra risk (lower confidence level).

Contaminant	Adequate intake (mg/Kg _{bw} /day)	Guideline value and reference	RfD (mg/Kg _{bw} /day)	Reference
DEHP	0.05	TDI [1]	0.02	[8]
DEP	5	TDI [1]	0.8	
DBP	0.01	TDI [1]	0.1	
DEHA	0.30	TDI [2]	0.6	
BPA*	4	TDI [3]	0.05	
Al	1	TWI [4]	0.1	
Ni	22	TDI [5]	0.02	
Pb	0.5	BMDL01 [6]	0.0035	
As*	3	BMDL05 [7]	0.0003	

*Expressed as µg/Kg_{bw}/day