

# Multi-class analysis for simultaneous determination of pesticides, mycotoxins, process-induced toxicants and packaging contaminants in tea

Cladière, M.<sup>\*</sup>, Delaporte, G., Le Roux, E., Camel, V.

UMR Ingénierie Procédés Aliments, AgroParisTech, Inra, Université Paris-Saclay, 91300 Massy, France

Corresponding author<sup>\*</sup>: [mathieu.cladiere@agroparistech.fr](mailto:mathieu.cladiere@agroparistech.fr)

## Analytical parameters

Table S1: Ionization parameters for ESI<sup>+</sup> and ESI<sup>-</sup>.

Parameter	ESI <sup>+</sup>	ESI <sup>-</sup>
Capillary (kV)	1.5	1.0
Sampling cone (V)	20	35
Source offset (V)	20	80
Source temperature (°C)	130	130
Desolvation temperature (°C)	500	500
Cone gas flow (L/h)	50	20
Desolvation gas flow (L/h)	1,200	600

## Recoveries and RSDs in tea brew

Table S2 : Recoveries, RSDs and estimated MLOQs in tea brew for compounds spiked between 10 and 100 µg/kg extracted by LLE or D&S method

N°	Name	Liquid- liquid extraction					Dilute and shoot				
		Level 1 10 µg/L a = 50 µg/L		Level 2 100 µg/L a = 500 µg/L		MLOQ (µg/L)	Level 1 10 µg/L a = 50 µg/L		Level 2 100 µg/L a = 500 µg/L		MLOQ (µg/L)
		Recovery (%)	RSD (%)	Recovery (%)	RSD (%)		Recovery (%)	RSD (%)	Recoveries (%)	RSD (%)	
1	Acrylamide <sup>a</sup>	66	4.2	98	22.1	500	49	33.3	83	1.0	500
2	Hydroxymethylfurfural <sup>a</sup>	116	9.2	124	7.3	50	132	26.0	108	8.5	500
3	Deoxynivalenol <sup>a</sup>	134	22.6	102	8.9	500	83	7.9	74	15.7	50
4	Imidacloprid	125	40.7	116	4.5	100	121	5.2	125	8.0	(10)
5	Dimethoate	102	5.9	94	3.4	10	95	5.3	95	3.2	10
6	Acetamiprid	118	8.6	111	3.8	10	117	8.8	116	7.4	10
7	Fumonisin B1	48	20.1	49	47.9	-	109	2.9	178	9.7	10
8	Aldicarb	144	0.3	161	25.5	-	135	0.2	165	6.5	-
9	Ametryn	113	6.3	111	3.1	10	109	7.5	104	5.2	10
10	Dichlorvos	92	12.3	99	4.3	10	95	8.0	109	4.0	10
11	Fumonisin B2	85	4.8	32	113	10	109	7.5	161	8.7	10
12	Atrazine	136	4.8	110	7.3	100	114	7.5	119	5.4	10
13	Diuron	120	13.1	105	5.8	100	97	2.5	95	5.3	10
14	Ochratoxin A	106	12.0	107	2.5	10	96	8.5	100	2.9	10
15	BFDGE	ND	-	112.8	7.1	100	91	27	91.3	19.6	100
16	Malathion	97	17.8	99	1.6	10	96	4.5	96	1.9	10
17	Diffubenzuron	25	61.1	85	15.6	100	119	7.6	119	6.3	10
18	BADGE	ND	-	57.5	34	-	120.0	21	118.3	18.7	(10)
19	Pirimiphos-methyl	27	19.2	63	43.6	-	119	4.4	114	4.3	10
20	2,4-D	ND	-	99	20.9	100	117	32.5	114	7.5	100
21	Bisphenol S	50	11.4	57	16.6	-	58	1.6	84	4.0	100
22	Tolfenpyrad	ND	-	ND	-	-	86	5.4	92	3.3	10
23	MCPA	77	25.3	106	16.9	100	128	10.9	101	3.9	100
24	Propargite	ND	-	ND	-	-	91	4.6	92	7.5	10
25	Dichloprop	27	53.7	55	15.4	-	89	12.6	107	5.1	10
26	Mecoprop	67	21.2	109	16.9	100	98	7.8	97	4.8	10
27	2,4,5-T	15	30.1	66	10.5	(100)	78	8.8	90	4.3	10
29	Fenoprop	55	25.0	71	12.2	100	99	6.2	101	7.0	10
28	Bisphenol F	52	13.6	52	16.9	-	70	0.5	61	8.5	10
30	Dinoseb	64	23.3	75	5.9	100	113	3.7	109	5.8	10
31	Bisphenol A	62	9.3	62	5.4	(10)	71	14.8	71	28.3	10
32	2,4-DB	79	20.5	57	8.2	-	102	19.0	100	8.6	10