Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary data

Development and optimisation of home-made stir bar sorptive extraction for analysis of plastic additives: application in human urine

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Table S1: Analytes and UHPLC-MS/MS settings (ionization mode, retention time (RT), precursor ion, quantification transition (T1) [precursor ion>product ion], confirmation ion (T2) [precursor ion>product ion], MRM ratio (T1/T2), declustering potential (DP), collision energy (CE)

Analytes	RT (min)	Precursor ion	T1 (m/z)	T2 (m/z)	T1/T2	Dwell time (msec)	DP (T1 / T2) (V)	CE (T1 / T2) (eV)
				Positive mode				
Tinuvin 622	0.48	$[M+H]^+$	316 > 102	316 > 216	2.20	9	36 / 36	29 / 25
Cyasorb UV 9	2.66	$[M+H]^+$	229 > 151	229 > 105	1.70	9	46 / 46	25 / 27
Hostanox 03	4.61	$[M+NH_4]^+$	813 > 325	813 > 217	1.15	9	56 / 56	65 / 45
Oleamide	4.80	$[M+H]^+$	282 > 83	282 > 97	1.00	9	41 / 41	27 / 31
Chimassorb 81	5.10	$[M+H]^+$	327 > 137	327 > 215	2.10	9	51 / 51	39 / 25
Glycerol monostearate	5.15	$[M+H]^+$	359 > 341	359 > 267	1.70	9	41 / 41	15 / 15
Isonox 129	5.38	$[M+NH_4]^+$	456 > 233	456 > 177	3.40	9	21 / 21	21 / 27
Tinuvin 326	5.48	$[M+H]^+$	316 > 260	316 > 107	2.10	9	51 / 51	25 / 37
Irganox 3114	5.56	$[M+NH_4]^+$	802 > 219	802 > 203	3.30	9	46 / 46	51 / 107
Tinuvin 327	5.72	$[M+H]^+$	358 > 302	358 > 246	4.45	9	61 / 61	29 / 35
Tinuvin 328	5.73	$[M+H]^+$	352 > 282	352 > 212	3.90	9	71 / 71	27 / 39
Vitamin E	5.6	$[M+H-H_2]^+$	429 > 165	429 > 91	4.10	9	41 / 41	29 / 95
Irganox 1010	5.93	$[M+NH_4]^+$	1194 > 219	1194 > 163	1.40	9	96 / 96	101 / 129
Irganox 1330	6.01	$[M+NH_4]^+$	793 > 219	793 > 203	3.80	9	61 / 61	45 / 101
Naugard DLTDP	6.16	$[M+H]^+$	515 > 143	515 > 329	2.80	9	71 / 71	25 / 19
Irganox 1076	5.5	$[M+NH_4]^+$	548 > 107	548 > 149	1.10	9	66 / 66	63 / 33
Irgafos 168	6.85	$[M+H]^+$	648 > 235	648 > 147	1.00	9	96 / 96	73 / 63
Naugard DSTDP	8.92	$[M+H]^+$	684 > 143	684 > 89	2.50	9	96 / 96	35 / 57
				Negative mode				
Diphenyl phosphate	2.78	$[M-H]^-$	249 > 93	249 > 155	14.00	33	1	1,1875
3,5-di-tert-butyl-4-hydroxybenzoic acid	4.53	$[M-H]^-$	249 > 205	249 > 189	50.00	33	1	34 / 42
2,4-di-tertbutyl-phenol	5.09	$[M-H]^-$	205 > 189	-	-	33	-60	-36