

Supplementary Information

Multi-Residue Method for Determination of Thirty-Five Pesticides, Pharmaceuticals and Personal Care Products in Water Using Ionic Liquid-Dispersive Liquid-Liquid Microextraction Combined with Liquid Chromatography-Tandem Mass Spectrometry

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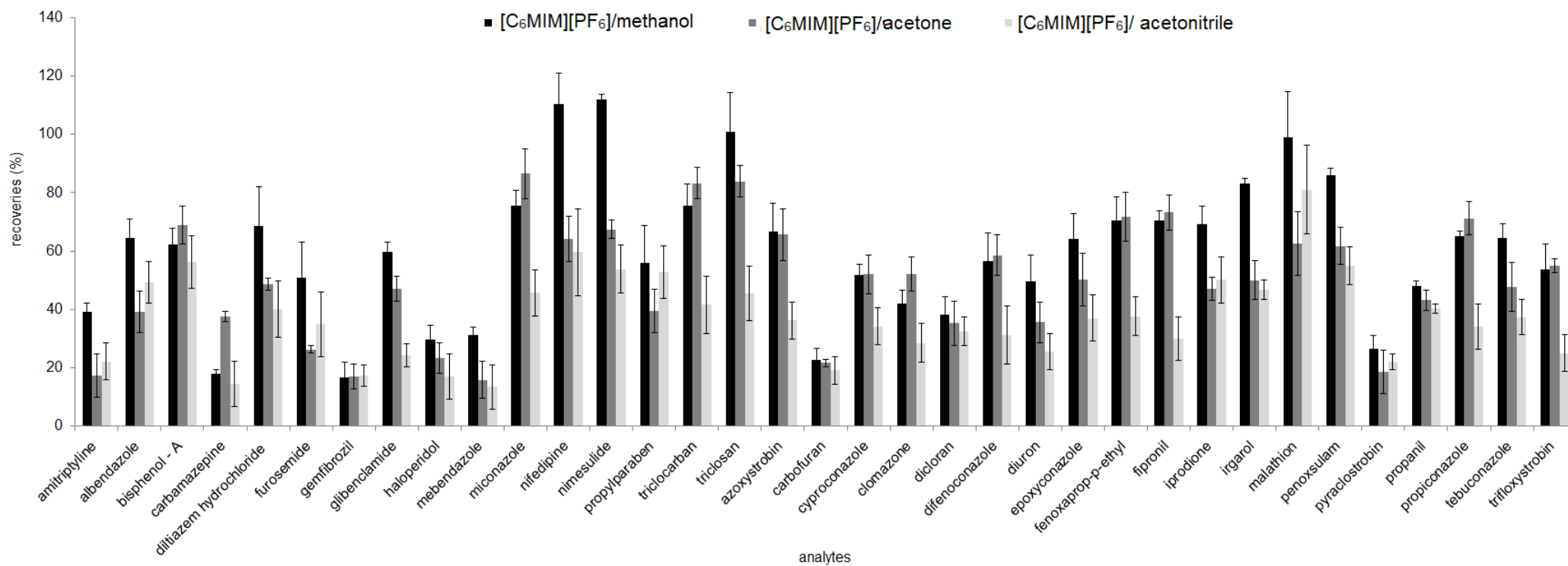


Figure S1. Effect of the type of extractor solvent and disperser in IL-DLLME step on the recovery of pesticides and PPCPs from drinking water (water sample volume: 10.0 mL; extractor solvent volume: 100 μ L; disperser solvent: 500 μ L). Bars indicate RSD values.

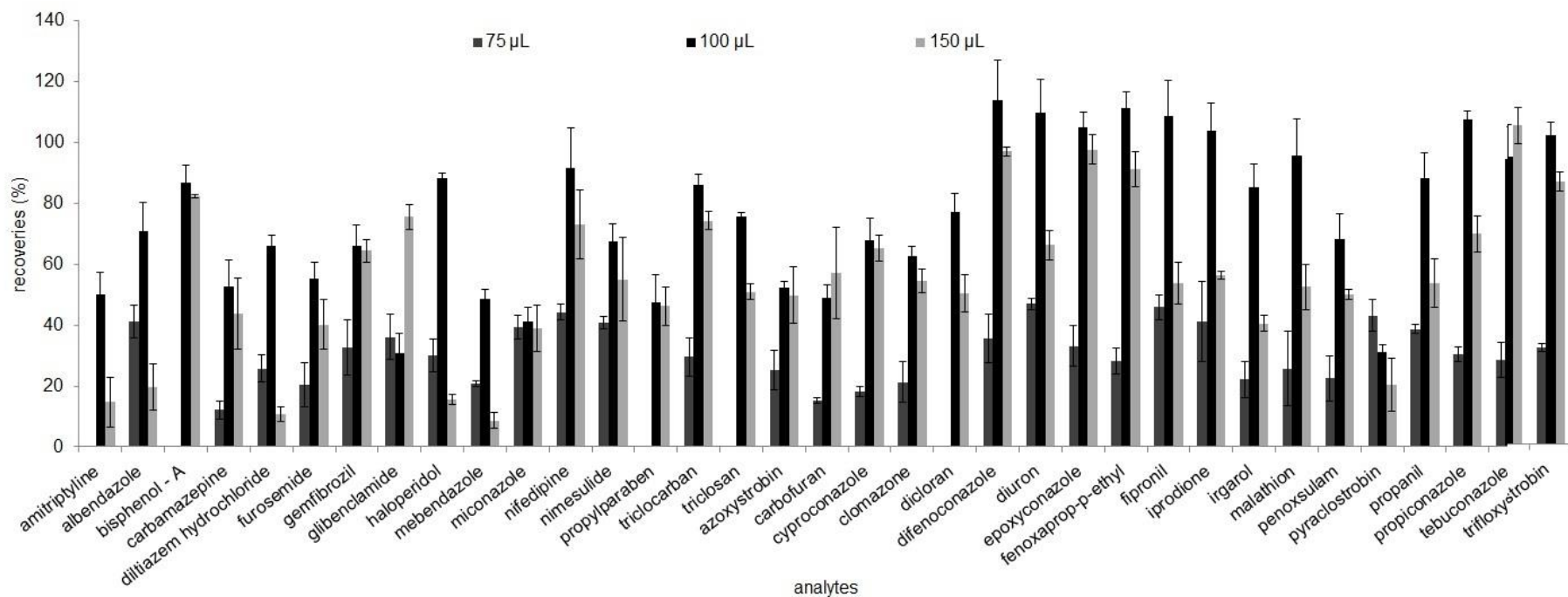


Figure S2. Effect of the volume of extractor solvent ($[C_6MIM][PF_6]$) in the IL-DLLME step on the recovery of pesticides and PPCPs from drinking water (water sample volume: 10.0 mL; extractor solvent: $[C_6MIM][PF_6]$; disperser solvent: 500 μ L of methanol). Error bars indicate RSD values.

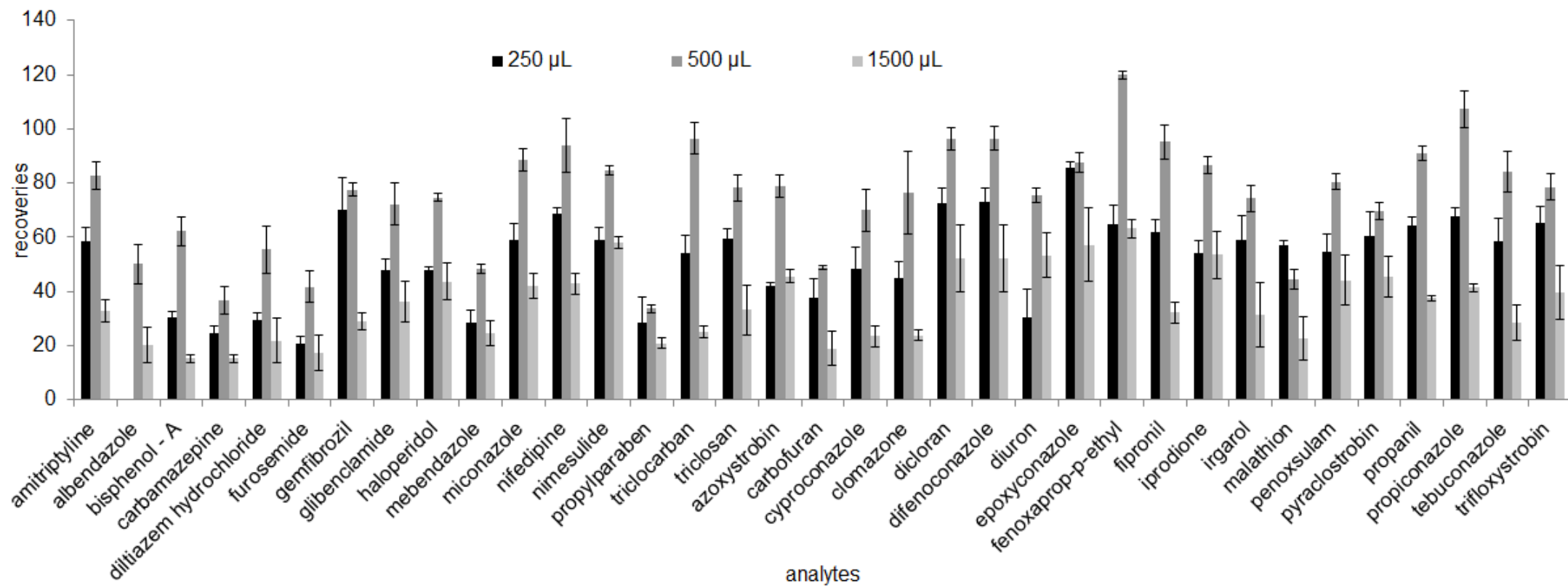


Figure S3. Effect of the volume of disperser solvent (methanol) on the IL-DLLME step on the recovery of pesticides and PPCPs from drinking water (water sample volume: 10.0 mL; extractor solvent volume of [C₆MIM][PF₆]: 100 µL). Bars indicate RSD values.

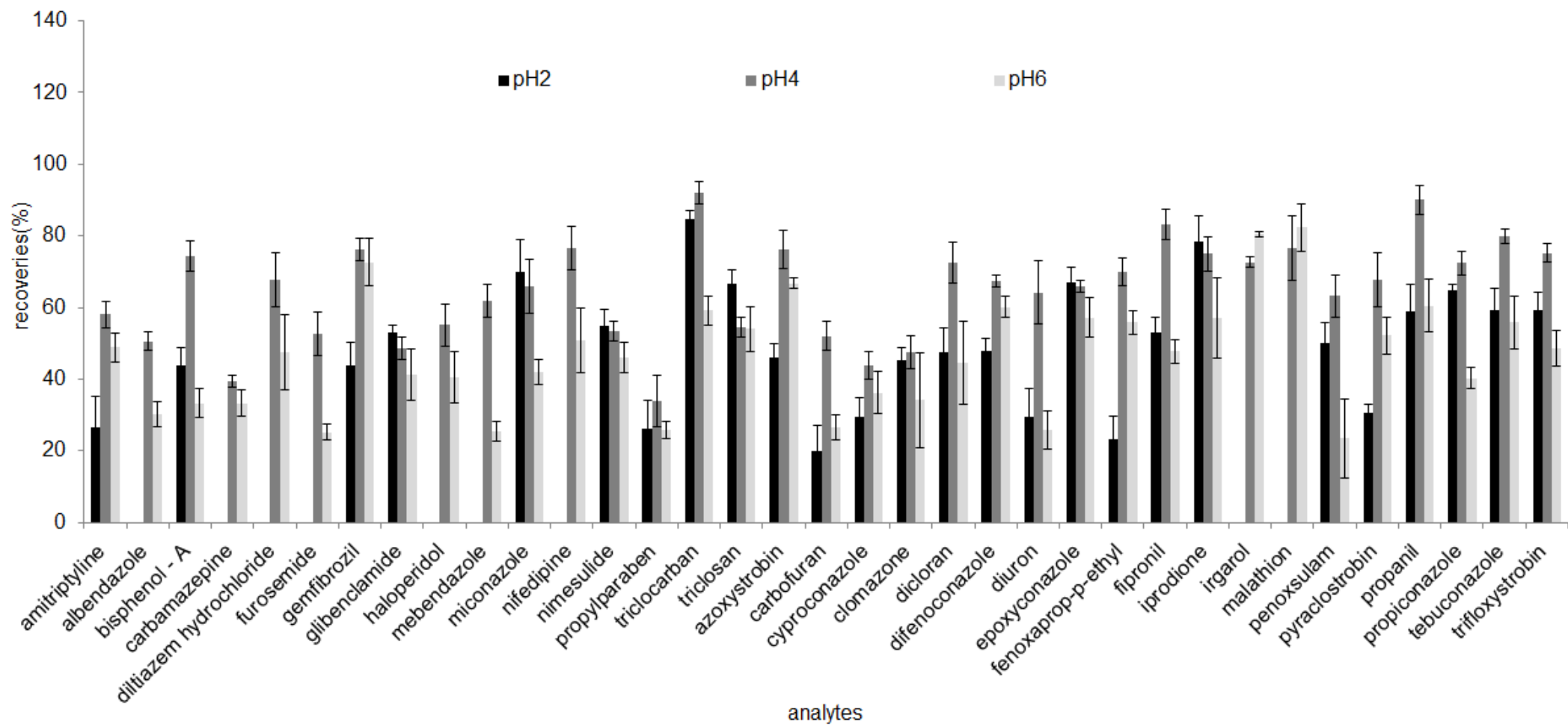


Figure S4. Effect of the pH of the sample in the IL-DLLME step on the recovery of pesticides and PPCPs from tap water (water sample volume: 10.0 mL; volume of extractor solvent: 100 μ L of $[C_6MIM][PF_6]$; disperser solvent: 500 μ L of methanol). Bars indicate RSD values.

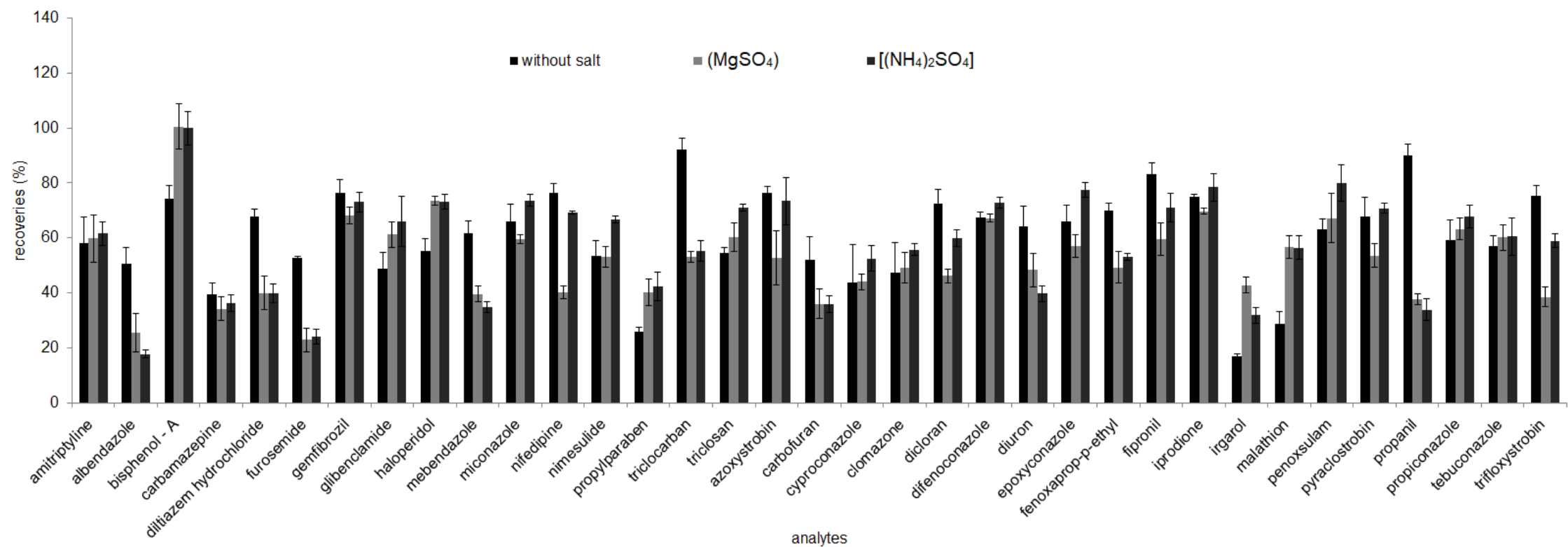


Figure S5. Effect of different salts in the IL-DLLME step on the recovery of pesticides and PPCPs from drinking water (water sample volume (pH 4): 10.0 mL; volume of extractor solvent: 100 μ L of [C₆MIM][PF₆]; disperser solvent: 500 μ L of methanol). Bars indicate RSD values.

Table S1. Mass spectrometric parameters for LC-MS/MS determination of pesticides and PPCPs, octanol/water partition coefficient (K_{ow})^{1,2}

Analyte	Use	ESI	MRM transition (m/z)	Cone voltage / V	Collision energy / eV	log Kow
Albendazole	anthelmintic	+	266 > 234 ^a	30	20	2.7
			266 > 191	33	32	
Amitriptyline	antidepressant	+	278.3 > 233.3 ^a	35	15	4.92
			278.3 > 116.9	35	15	
Bisphenol A	plasticizer	-	227 > 212.2 ^a	43	19	3.18-3.7
			227 > 133	43	25	
Carbamazepine	anticonvulsant	+	237 > 194.1 ^a	26	12	2.45
			237 > 167.4	35	40	
Diltiazem hydrochloride	antihypertensive	+	415 > 178 ^a	35	20	2.8
			415 > 310	35	20	
Furosemide	diuretic	-	328.8 > 284.9 ^a	30	15	2.03
			328.8 > 205	30	20	
Gemfibrozil	hypolipidemic	-	249 > 121 ^a	20	30	3.4
Glibenclamide	antidiabetic	+	494 > 169 ^a	30	18	4.7
			494 > 369	30	38	
Haloperidol	antipsychotic	+	376 > 165 ^a	30	21	4.3
			376 > 123	35	25	
Mebendazole	antiparasitic	+	296.2 > 104.9 ^a	30	30	2.83
			296.2 > 264.2	35	30	
Miconazole nitrate	antifungal	+	417.1 > 161 ^a	45	25	6.1
			417.1 > 159	45	30	
nifepidine	antihypertensive	?	347.4 > 315.2 ^a	20	20	2.49
			347.4 > 271.3	8	8	
Nimesulide	anti-inflammatory	-	307 > 229 ^a	33	20	2.6
			307 > 198.1	30	25	
Propylparaben	preservative	-	179.1 > 91.8 ^a	30	15	2.94
			179.1 > 137.1	30	20	
Triclocarban	antibacterial, antifungal	-	313 > 160.1 ^a	30	25	3.5
			315 > 125.7	30	15	
Triclosan	antiseptic	-	287 > 35 ^a	18	7	5.3
			289 > 35	18	9	
Azoxystrobin	fungicide	+	404 > 372 ^a	20	20	2.5
			404 > 329	15	30	

Table S1. Mass spectrometric parameters for LC-MS/MS determination of pesticides and PPCPs, octanol/water partition coefficient (K_{ow})^{1,2} (cont.)

Analyte	Use	ESI	MRM transition (m/z)	Cone voltage / V	Collision energy / eV	log Kow
Carbofuran	insecticide	+	222 > 123 ^a	20	25	1.52
			222 > 165			
Cyproconazole	fungicide	+	292 > 70 ^a	35	20	3.1
			292 > 125	35	20	
Clomazone	herbicide	+	240 > 125 ^a	30	20	2.5
			240 > 219	26	20	
Dichloran	fungicide	-	205 > 175.2 ^a	40	15	2.8
			205 > 138.9	40	20	
Difenoconazole	fungicide	+	406 > 251 ^a	31	32	4.4
			406 > 337	32	20	
Diuron	herbicide	+	233 > 72 ^a	28	20	2.85
			233 > 160	28	25	
Epoxiconazole	fungicide	+	330 > 121 ^a	27	30	3.44
			330 > 123	27	30	
Fenoxaprop-p-ethyl	herbicide	+	362.1 > 288.1 ^a	22	23	4.58
			362.1 > 121	22	37	
Fipronil	insecticide	-	435 > 330 ^a	30	15	4
			435 > 250	25	26	
iprodione	fungicide	+	330 > 101 ^a	20	20	3.1
			330 > 143.2	33	21	
Irgarol	antifouling	+	254 > 198 ^a	30	30	3.9
			254 > 108	30	19	
Malathion	insecticide	+	331 > 127 ^a	24	30	2.75
			331 > 199	24	10	
Penoxsulam	herbicide	-	482 > 179 ^a	35	40	-0.35
			482 > 109	35	25	
Pyraclostrobin	fungicide	+	388.1 > 163 ^a	20	19	3.99
			388.1 > 194	20	19	
Propanil	herbicide	+	218 > 127 ^a	25	28	3.3
			218 > 162	30	14	
Propiconazole	fungicide	+	342 > 159 ^a	32	22	3.72
			342 > 69	30	20	
Tebuconazole	fungicide	+	308 > 70 ^a	40	20	3.7
			308 > 125	28	22	
Trifloxystrobin	fungicide	+	409 > 145 ^a	35	15	4.5
			409 > 206	25	40	

Table S1. Mass spectrometric parameters for LC-MS/MS determination of pesticides and PPCPs, octanol/water partition coefficient (K_{ow})^{1,2} (cont.)

Analyte	Use	ESI	MRM transition (m/z)	Cone voltage / V	Collision energy / eV	log K_{ow}
Carbofuran- d_3	insecticide	+	225 > 121.1 ^a	20	25	2.3
			225 > 140.5	20	25	
Diuron- d_6	herbicide	+	239.33 > 78.1	29	15	2.7
			239.33 > 52.1	29	17	

^aQuantification transition.

References

1. <http://www.drugbank.ca/>, accessed in May 2017.
2. Tomlin, C.; British Crop Protection Council (BCPC); *The Pesticide Manual: A World Compendium*, Tomlin, C., ed.; BCPC: Alton, UK, 2003.