

Supplementary Information

Occurrence of Pesticides and PPCPs in Surface and Drinking Water in Southern Brazil: Data on 4-Year Monitoring

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Table S1. SRM conditions, limit of quantification (LOQ), partition coefficient octanol/water (Kow) and guideline value for the PPCPs and pesticides under study

PPCP/pesticide	ESI mode	Transition (<i>m/z</i>)	Cone / V	Collision / eV	log Kow ^{1,2}	LOQ / (ng L ⁻¹)	Guideline value ³ / (ng L ⁻¹)
Atenolol	+	267 > 145 ^a	15	30	0.16	40	
		267 > 190.2	25	25			
Avobenzon	+	310.4 > 135 ^a	20	30	4.51	40	
		310.4 > 161	20	30			
Benzofenone	-	307.1 > 211.1 ^a	55	35	3.18	40	
		307.1 > 182.2	55	35			
Caffeine	+	195.3 > 110	25	20	-0.07	40	
		195.3 > 138 ^a	25	20			
Carbamazepine	+	236.9 > 194.1 ^a	26	12	2.45	4	
		237.4 > 167.4	35	40			
Clorpropamide	+	277 > 175 ^a	27	22	2.27	40	
		277 > 110.9	27	29			
Diclofenac	-	293.6 > 250.2 ^a	20	10	4.51	8	
		294 > 214	20	25			
Eusolex - 6300 (methybenzylidene camphor)	+	255.4 > 157.2	25	20	4.95	40	
		255.4 > 105 ^a	25	30			
Gemfibrozil	-	249 > 121 ^a	20	30	3.4	8	
Furosemide	-	328.8 > 284.9	30	15	2.03	40	
		328.8 > 205 ^a	30	20			
Glibenclamide	+	494 > 369	30	18	4.7	40	
		494 > 169 ^a	30	38			
Mebendazole	+	296.2 > 264.2	35	30	2.83	8	
		296.2 > 104.9 ^a	35	30			

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Methylparaben	+	151 > 135.9	35	15	1.96	8	
		151 > 91.6 ^a	35	20			
Nimesulide	-	307 > 229 ^a	33	20	2.6	4	
		307.2 > 198.1	30	25			
Miconazole nitrate	+	417.1 > 161	45	25	6.1	8	
		417.1 > 159 ^a	45	30			
Propylparaben	-	179.1 > 137.1	30	15	3.04	8	
		179.1 > 91.8 ^a	30	20			
Triclocarban	-	313 > 160.1 ^a	30	15	4.9	0.8	
		315 > 125.7	30	20			
Triclosan	-	289 > 35	18	7	5.53	80	
		287 > 35 ^a	18	9			
2,4-d	-	219 > 161 ^a	15	20	0.04-0.33 (pH 5)	40	30000
		219 > 89	15	30			
3,4-dca	+	162 > 127	35	15		40	
		162 > 109 ^a	25	25			
3-hidroxy-carbofuran	+	238 > 163 ^a	25	15		80	
		238 > 135	25	20			
Atrazine	+	216 > 174	33	20	2.5	4	100 000
		216 > 146 ^a	35	22			
Azoxystrobin	+	404 > 372 ^a	20	20	2.5	40	
		404 > 329	15	30			

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Bentazone	–	239 > 132 ^a 239 > 197	35 35	25 20	0.77 (pH 5)	8	occurs in drinking-water at concentrations well below those of health concern
Bispyribac-sodium	+	453 > 297 ^a 453 > 275	35 35	25 22	–1.03	8	
Carbendazin	+	192 > 160 192 > 132 ^a	28 28	28 29	1.51 (pH 7)	8	
Carbofuran	+	222 > 165 222 > 123	20 20	25 25	1.52	8	7000
Ciproconazole	+	292 > 125 292 > 70 ^a	35 35	20 20	3.1	8	
Clomazone	+	240 > 125 ^a 240 > 219	30 26	20 20	2.5	40	
Difenoconazole	+	406 > 251 ^a 406 > 337	31 32	32 20	4.4	8	
Diuron	+	233 > 72 ^a 233 > 160	28 28	20 25	2.85	40	
Epoxiconazole	+	330 > 123 330 > 121 ^a	27 27	30 30	3.44	40	
Fipronil	–	435 > 330 ^a 435 > 250	30 25	15 26	4.0	0.8	
Imazapic	+	276 > 231 ^a 276 > 185	40 40	20 30	0.393	8	
Imazethapyr	+	290 > 230 290 > 177 ^a	40 40	20 20	0.22	8	

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Iprodione	+	330 > 101 ^a	20	33	3.0	40	
		330 > 143.2	20	21			
Irgarol	+	254 > 108	30	30	3.95	4	
		254 > 198 ^a	30	19			
Malathion	+	331 > 199	24	30	2.75	4	
		331 > 127 ^a	24	10			
Methalaxyl-M	+	280 > 220	16	17	1.71	4	
		280 > 192 ^a	16	17			
Metsulfuron-methyl	-	380 > 139 ^a	30	15	0.018	40	
		380 > 214	30	10			
Molinate	+	188 > 126 ^a	25	10	3.21	8	
		188 > 83	25	20			
Penoxsulan	-	482 > 109	35	40	-0.354	40	
		482 > 179 ^a	35	25			
Pyrazosulfuron-ethyl	-	413 > 232	35	15	3.16	4	
		413 > 154 ^a	35	26			
Pirimiphos-methyl	+	306 > 136	40	33	4.2	8	
		306 > 108 ^a	40	20			
Propanil	+	218 > 127	25	28	3.3	8	readily transformed into metabolites that are more toxic; a guideline value for the parent compound is considered inappropriate, and there are inadequate data to enable the derivation of guideline values for the metabolites
		218 > 162 ^a	30	14			

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Propiconazole	+	342 > 159 ^a	32	22	3.72	4	
		342 > 69	30	20			
Quinclorac	-	240 > 196	15	6	-1.15	80	
Simazine	+	202 > 132 ^a	35	18	2.1	4	2000
		202 > 124	35	18			
Tebuconazole	+	308 > 70 ^a	40	20	3.7	40	
		308 > 125	28	22			
Tiabendazole	+	202 > 131	47	25	2.47	8	
		202 > 158 ^a	47	25			
Trifloxystrobin	+	409 > 206	35	15	4.5	8	
		409 > 145 ^a	25	40			

^aQuantification ions.

References

1. Tomlin, C. D.; *The Pesticide Manual: a World Compendium*; British Crop Production Council: Alton, 2009.
2. <https://www.drugbank.ca/>, accessed in March 2016.
3. World Health Organization (WHO); *Guidelines for Drinking-Water Quality*, 4th ed.; WHO Press: Geneva, Switzerland, 2011. Available at http://apps.who.int/iris/bitstream/10665/44584/1/9789241548151_eng.pdf, accessed in August 2018.

