Supplementary Data (SD)

Occurrence of pharmaceuticals in surface waters: Analytical method development and environmental risk assessment

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Table SD1. Levels of pharmaceuticals in surface waters worldwide

Therapeutic group	Compound	Concentration (ng/L)	Reference
Analgesics/ Non-steroidal anti- inflammatory drugs (NSDAIDs)]	Paracetamol	250 (max)	[1]
		10000 (max)	[2]
		154 - 634	[3]
		n.d. - 872	[4]
	Phenazone	950 (max)	[5]
		bql-13	[6]
		27 (max)	[7]
	Salicylic acid	8800 (max)	[8]
		4100 (max)	[5]
		7.8 - 9.6	[9]
		<1.6-85.8	[10]
		<0.3-302	[11]
		n.d.	[12]
	Diclofenac	1200 (max)	[5]
		156±6.0	[7]
		45.5 (mean)	[13]
	Ibuprofen	144-2370	[14]
		280-530	[5]
		29.4- 490.4	[15]
		29.1 (mean)	[13]
		2796 (max)	[16]
	Ketoprofen	7 (mean), 9808 (max)	[17]
		n.d. - 22	[18]
		0.4 - 39.5	[19]
		10 - 190	[20]
		0.5 - 14	[21]
		n.d.	[12]
	Indomethacin	n.d. - 33.5±8	[22]
		n.d. - 62.5	[4]
		<7 (mean), 2323(max)	[17]
	Mefenamic acid	n.d. - 39.8	[23]
		0–326	[22]
Lipid regulators	Gemfibrozil	0.3 - 169	[21]
		29.1-59.2	[23]
		41 (mean)	[17]
		1.9 - 3.5	[20]
	Fenofibrate	26-1014	[24]
		9 (max)	[6]
		1200 (max)	[5]
		n.d.	[3]
	Bezafibrate	29±2.5	[7]
		bql - 16	[25]

Antibiotics	Sulfamethazine	16 - 43	[3]
		<LOQ - 52	[3]
		n.d. - <LOQ	[4]
		<4(mean), 1626 (max)	[17]
	Sulfamethoxazole	93±4.4	[7]
		10 - 79	[25]
		11 (mean), 56 (max)	[17]
		n.d. - 5.1	[18]
		0.3 - 60	[20]
		0.5 - 4	[21]
	Ciprofloxacin	<31 (mean), 740 (max)	[17]
		<LOQ - 822, 30.4 (mean)	[26]
		n.d. - 13.6	[27]
	Erythromycin	n.d. - 137±15	[22]
		16 - 23	[3]
		75 - 100	[28]
		1.1 - 20.7	[29]
Antiepileptic	Carbamazepine	16 - 23	[3]
		n.d. - 595±14	[22]
		6300 (max)	[30]
		1100	[5]
		1238	[16]
		1.3 - 2.6	[7]
		0.5 - 684	[21]
		<4 - 595	[22]
		n.d. - 31.6	[18]
		0.088 ± 0.066 / 0.017 ± 0.008	[31]
Antipsychotic	Risperidone	0.34	[32]
Psychomotor stimulant	Caffeine	29.1 - 659	[29]
		6000 (max)	[2]
		4275	[16]
		24 (mean)	[17]
		1 - 1813	[20]
Disinfectant	Triclosan	220 (mean)	[33]
		35 - 1023	[34]
		11, 263 (max)	[17]
		3-39	[19]
		5-95	[21]
Estrogen	Estriol	n.d.	[3]
		n.d. - 1	[34]
		<LOD - 16	[26]
Beta- blocker	Atenolol	n.d. - 690±26	[22]
		0 -34	[18]
		1 - 560	[21]
H ₂ receptor antagonist	Cimetidine	n.d. - <1237	[4]
		n.d. - <LOQ	[4]

Table SD2. Physicochemical properties of the target pharmaceuticals.

Therapeutic group	Compound	Molecular formula	MW	pKa ^[35]	LogK _{ow} ^[35]
Analgesics/ Non-steroidal anti-inflammatory drugs (NSDAIDs)	Paracetamol	C ₈ H ₉ NO ₂	151.17	9.4	0.46
	Phenazone	C ₁₁ H ₁₂ N ₂ O	188.23	1.5	0.38
	Salicylic acid	C ₇ H ₆ O ₃	138.12	2.3/3.5 ^[36]	1.13/2.26/- 2.42 ^[36]
	Diclofenac	C ₁₄ H ₁₁ Cl ₂ NO ₂	296.15	4.2	4.51/0.7 ^[36]
	Ibuprofen	C ₁₃ H ₁₈ O ₂	206.28	4.9	3.97/0.45 ^[36]
	Ketoprofen	C ₁₆ H ₁₄ O ₃	254.28	4.45	3.12
	Indomethacin	C ₁₉ H ₁₆ ClNO ₄	357.79	4.5	4.27
	Mefenamic acid	C ₁₅ H ₁₅ NO ₂	241.28	4.3	5.12
Lipid regulators	Gemfibrozil	C ₁₅ H ₂₂ O ₃	250.34	4.7	4.77
	Fenofibrate	C ₂₀ H ₂₁ ClO ₄	360.83	4.5	5.19
	Bezafibrate	C ₁₉ H ₂₀ ClNO ₄	361.82	3.6 ^[36]	4.25 ^[36]
Antibiotics	Sulfamethazine	C ₁₂ H ₁₄ N ₄ O ₂ S	278.33	7.59	0.89
	Sulfamethoxazole	C ₁₀ H ₁₁ N ₃ O ₃ S	253.28	5.7 ^[36]	0.89 ^[36]
	Ciprofloxacin	C ₁₇ H ₁₈ FN ₃ O ₃	331.37	6.09 ^[37]	0.00 ^[37]
	Erythromycin	C ₃₇ H ₆₇ NO ₁₃	733.93	8.88 ^[37]	2.47 ^[37]
Antiepileptic	Carbamazepine	C ₁₅ H ₁₂ N ₂ O	236.27	7/13.9 ^[36]	2.47
Antipsychotic	Risperidone	C ₂₃ H ₂₇ FN ₄ O ₂	410.45	8.76	2.5
Psychomotor stimulant	Caffeine	C ₈ H ₁₀ N ₄ O ₂	194.20	10.4	-0.007
Glucocorticoid steroid	Budesonide	C ₂₅ H ₃₄ O ₆	430.53	7.9	2.18
Disinfectant	Triclosan	C ₁₂ H ₇ Cl ₃ O ₂	289.54	4.5/8.1 ^[36]	4.80/5.34 ^[36]
Estrogen	Estriol	C ₁₈ H ₂₄ O ₃	288.38	10.4	2.45
Beta- blocker	Atenolol	C ₁₄ H ₂₂ N ₂ O ₃	266.34	9.6	0.16
H ₂ receptor antagonist	Cimetidine	C ₁₀ H ₁₆ N ₆ S	252.34	6.8	0.4

Literature data from: Kosma *et al.* [36], Verlicchi *et al.* [37] and Rivera *et al.* [38].

Table SD3. Instrumental parameters for target pharmaceuticals using LC-ESI-MS in SIM mode.

Compound	Polarity (ESI)	Retention time (min)	<i>m/z</i> ions*	Relative ion intensity (%)
Cimetidine	+	6.47	253 , 159	100.0, 60.1
Paracetamol	+	6.52	152 , 110	100.0, 40.0
Atenolol	+	6.75	267 , 190, 145	100.0, 21.0, 19.3
Caffeine	+	8.20	195 , 138	100.0, 60.2
Sulfamethazine	+	10.83	279 , 156, 186	100.0, 84.3, 60.1
Phenazone	+	11.48	189 , 147, 56	100.0, 86.5, 12.3
Ciprofloxacin	+	12.30	332 , 288	100.0, 44.5
Sulfamethoxazole	+	13.78	254 , 156, 92	100.0, 40.2, 12.3
Carbamazepine	+	17.77	237 , 194, 192	100.0, 80.4, 48.6
Bezafibrate	+	22.74	362 , 276, 316	100.0, 25.9, 14.9
Erythromycin	+	22.85	734 , 576	100.0, 20.6
Budesonide	+	23.39	431 , 413, 323	100.0, 98.3, 29.8
Fenofibrate	+	26.05	319	100.0
Risperidone	+	30.28	411 , 110	100.0, 81.9
Estriol	-	3.12	287 , 171	100.0, 92.4
Salicylic acid	-	12.21	137 , 93	100.0, 97.8
Ibuprofen	-	12.58	205 , 160, 161	100.0, 90.2, 71.1
Ketoprofen	-	18.89	253 , 209	100.0, 81.9
Indomethacin	-	23.67	356 , 312, 314	100.0, 75.3, 68.8
Diclofenac	-	23.84	294 , 295, 250	100.0, 40.9, 12.7
Gemfibrozil	-	24.04	249 , 121	100.0, 82.63
Mefenamic acid	-	27.08	240 , 196, 180	100.0, 94.0, 90.8
Triclosan	-	29.64	288 , 287	100.0, 90.9

*Quantitation ions in bold

Table SD4. Limits of detection (LODs), limits of quantification (LOQs), precision in the same day (RSD_r) and in different days (RSD_R) in distilled, river and lake water.

Compound	IDL (ng/L)	LOD (ng/L)			LOQ (ng/L)			RSD _r (%) (n=5)			RSD _R (%) (n=5)		
		DW	RW	LW	DW	RW	LW	DW	RW	LW	DW	RW	LW
Cimetidine	4.9	3.5	3.7	5.1	11.6	14.4	19.9	4.5	6.7	5.8	5.2	7.1	7.4
Paracetamol	12.9	12.3	12.8	12.7	40.6	42.2	41.9	9.8	10.0	11.3	13.0	14.1	14.5
Atenolol	15.1	17.0	18.1	20.3	56.1	56.1	62.9	6.1	5.7	6.1	6.8	7.1	6.9
Caffeine	14.1	9.4	9.8	13.1	30.6	32.3	43.2	5.1	9.0	10.1	9.2	9.0	8.8
Sulfamethazine	5.2	4.7	5.2	8.9	15.5	15.6	26.7	2.9	2.1	3.2	5.1	6.9	8.5
Phenazone	2.8	2.7	2.9	5.6	8.9	11.3	21.8	1.9	5.5	5.9	4.3	5.2	6.1
Ciprofloxacin	8.9	9.9	10.8	27.1	32.7	33.5	84.0	7.5	8.9	9.0	7.9	8.3	10.1
Sulfamethoxazole	5.7	3.8	4.7	6.8	12.5	17.4	25.2	2.5	6.1	6.8	3.7	5.1	5.1
Carbamazepine	5.2	4.8	5.2	7.3	17.8	16.6	23.4	2.1	3.6	4.1	4.2	6.7	7.2
Bezafibrate	4.2	5.9	6.2	6.1	18.3	23.6	23.2	3.5	3.5	4.1	7.9	8.5	9.2
Erythromycin	9.8	9.3	10.1	9.8	32.6	30.3	29.4	4.3	7.1	8.8	5.1	5.9	6.7
Budesonide	20.1	26.1	28.1	29.9	96.6	95.5	101.7	4.6	7.8	9.4	10	11.1	13.1
Fenofibrate	9.0	9.3	9.7	10.3	30.7	32.0	34.0	5.3	6.9	6.4	16.1	18.5	21.5
Risperidone	65.1	73.5	87.0	101.0	220.5	304.5	353.5	7.5	8.9	10.4	8.1	9.7	9.9
Estriol	29.4	29.7	31.6	40.0	98.0	101.1	128.0	6.0	9.0	10.8	7.1	8.9	9.1
Salicylic acid	40.0	46.0	47.1	47.6	147.2	141.3	142.8	3.0	5.1	7.4	6.1	6.5	6.9
Ibuprofen	76.9	81.7	83.0	91.0	318.6	307.1	336.7	4.1	7.3	7.4	4.7	6.1	6.9
Ketoprofen	14.1	10.0	12.5	12.9	37.0	41.3	42.6	3.9	4.5	4.2	5.7	8.9	8.1
Indomethacin	22.3	25.0	25.8	24.9	82.5	85.1	82.2	4.6	4.9	5.7	5.1	5.8	5.8
Diclofenac	15.4	15.9	17.1	18.5	52.5	56.4	61.1	5.4	7.9	7.1	11.2	13.2	15.2
Gemfibrozil	37.9	38.1	40.0	45.7	125.7	124.0	141.7	9.7	10.7	10.4	10.9	10.1	10.9
Mefenamic acid	7.9	6.2	7.1	8.2	21.7	23.4	27.1	4.9	5.7	5.2	6.1	8.3	9.4
Triclosan	28.7	34.5	37.0	41.3	113.9	111.0	123.9	4.8	7.1	8.6	5.0	9.1	11.7

Table SD5. Mean recoveries (%) and RSD (%) in distilled, river and lake water, after spiking with 0.2 and 2 µg/L (n=3).

Compound	% Recoveries after spiking with 0.2 µg/L (RSD %)			% Recoveries after spiking with 2 µg/L (RSD %)		
	DW	RW	LW	DW	RW	LW
Cimetidine	86.1 (5.8)	82.7 (4.1)	79.1 (4.4)	89.5 (4.7)	87.3 (4.1)	85.1 (4.8)
Paracetamol	76.7 (5.1)	78.2 (5.2)	74.9 (5.6)	83.8 (5.7)	81.7 (6.1)	80.4 (5.7)
Atenolol	70.1 (7.8)	69.6 (7.2)	67.2 (8.1)	71.3 (6.5)	74.8 (8.9)	73.1 (8.6)
Caffeine	89.1 (5.8)	88.1 (5.2)	86.2 (3.2)	98.1 (2.7)	95.3 (2.9)	95.3 (2.9)
Sulfamethazine	78.4 (6.8)	75.4 (6.5)	73.2 (6.1)	81.1 (4.3)	81.9 (5.1)	81.9 (5.1)
Phenazone	89.1 (3.7)	89.1 (3.5)	86.7 (3.9)	98.7 (11.2)	96.7 (10.5)	94.3 (9.3)
Ciprofloxacin	80.1 (7.6)	78.1 (7.3)	75.4 (7.1)	83.1 (6.4)	81.1 (4.4)	82.5 (4.9)
Sulfamethoxazole	93.1 (4.1)	90.4(4.7)	91.5 (3.8)	100.1 (2.9)	91.1 (3.9)	89.7 (3.2)
Carbamazepine	93.7 (9.4)	91.9 (9.2)	93.4 (9.1)	99.1 (10.5)	95.2 (8.7)	91.4 (8.9)
Bezafibrate	77.7 (7.9)	75.3 (8.1)	75.1(7.8)	97.1 (8.1)	79.9 (7.2)	78.7 (7.4)
Erythromycin	95.0 (15.1)	92.1(13.2)	90.8(11.1)	97.4 (12.1)	94.2 (12.9)	92.2 (13.1)
Budesonide	69.7 (9.0)	64.9 (9.3)	61.3(9.5)	74.8 (8.9)	69.1 (8.9)	70.8 (8.2)
Fenofibrate	52.1 (3.5)	51.0 (3.2)	53.0 (3.8)	60.8 (8.9)	55.3 (3.9)	52.1 (3.7)
Risperidone	30.0 (19.1)	27.5 (17.1)	25.2(16.3)	34.9 (13.9)	32.1 (11.8)	30.6 (10.6)
Estriol	43.4(9.1)	47.8 (9.9)	46.8 (9.7)	50.2 (3.9)	50.1 (3.0)	49.3 (3.2)
Salicylic acid	57.9 (3.1)	56.7 (3.6)	52.4 (3.1)	60.0 (2.7)	60.1 (3.3)	68.3 (4.1)
Ibuprofen	67.3 (4.2)	64.1 (3.8)	60.8 (3.2)	81.4 (2.9)	69.2 (4.0)	67.1 (4.9)
Ketoprofen	52.1 (2.4)	57.7 (2.9)	54.2 (2.3)	61.7 (4.2)	57.2 (5.0)	52.7 (5.1)
Indomethacin	74.2 (5.1)	70.1 (5.3)	70.3 (5.0)	75.1 (5.9)	74.1 (5.1)	72.1 (5.9)
Diclofenac	100.4 (9.1)	100.0 (8.5)	98.2 (7.9)	111.1 (3.4)	104.6 (8.3)	102.1 (7.1)
Gemfibrozil	58.3 (9.7)	56.0 (8.7)	53.1 (8.1)	59.1 (4.0)	58.0 (8.1)	56.1 (8.6)
Mefenamic acid	89.1 (8.0)	78.3 (7.2)	81.2 (7.1)	94.4 (3.2)	92.1 (3.1)	91.8 (3.0)
Triclosan	44.2 (11.1)	48.1 (11.3)	47.7 (10.2)	57.4 (6.0)	57.4 (6.0)	55.5 (6.7)

Table SD6. Ecotoxicological data of the analysed pharmaceuticals, for acute toxicity (lowest values in bold)

Compounds	Species	Test	Toxicity (mg/L)	Reference
Cimetidine	Fish	EC ₅₀	571	[38]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	35	[38]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	271.3	[39]
	Algae	EC ₅₀	40	[38]
Paracetamol	Fish	EC ₅₀	40	[38]
	Fish (<i>B. rerio</i>)	EC ₅₀	378	[40]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	41	[38]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	136 (24 h)	[41]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	9.2 (48 h)	[41]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	50	[40]
	Algae	EC ₅₀	2549	[38]
	Algae (<i>S. subcapitata</i>)	EC ₅₀	134	[40]
	Invertebrates	EC ₅₀	30	[36]
Atenolol	Invertebrates (<i>Daphnid</i>)	LC ₅₀	33.4 (48h)	[42]
	Algae	LC ₅₀	620 (24h)	[42]
	Fish	EC ₅₀	805	[38]
Caffeine	Fish	LC ₅₀	87 (<96h)	[42]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	46	[38]
	Fish	LC ₅₀	182 (48h)	[42]
	Algae	EC ₅₀	46	[38]
	Fish	EC ₅₀	517	[38]
Sulfamethazine	Invertebrates (<i>Daphnid</i>)	EC ₅₀	4	[38]
	Algae	EC ₅₀	38	[38]
	Fish	EC ₅₀	3	[43]
Phenazone	Invertebrates (<i>D. magna</i>)	EC ₅₀	6.7	[43]
	Algae	EC ₅₀	1.1	[43]
	Fish	EC ₅₀	246000	[38]
Ciprofloxacin	Fish (<i>B. rerio</i>)	EC ₅₀	>100	[40]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	991	[38]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	>60	[40]
	Algae	EC ₅₀	938	[38]
	Algae (<i>P. subcapitata</i>)	EC ₅₀	2.97	[40]
	Fish	EC ₅₀	562.5	[44]
Sulfamethoxazole	Fish	EC ₅₀	890	[38]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	25.2	[44]
	Invertebrates (<i>B. Calyciflorus</i>)	EC ₅₀	26	[40]
	Invertebrates (<i>C. dubia</i>)	EC ₅₀	15.5	[40]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	25	[40]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	4.5	[38]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	10 (48h)	[42]
	Algae (<i>S. leopoliensis</i>)	EC ₅₀	0.027	[44]
	Algae (<i>P. subcapitata</i>)	EC ₅₀	0.146	[40]
	Algae (<i>C. meneghiniana</i>)	EC ₅₀	2.4	[40]
	Algae (<i>P. subcapitata</i>)	EC ₅₀	0.57	[40]
	Algae	EC ₅₀	51	[38]

Carbamazepine	Fish	EC ₅₀	101	[38]
	Fish	EC ₅₀	35.4	[43]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	111	[38]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	76.3	[43]
	Algae	EC ₅₀	70	[38]
	Algae	EC ₅₀	85	[43]
Bezafibrate	Fish	EC ₅₀	5.3	[45]
	Fish	LC ₅₀	>100 (<96h)	[42]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	30	[45]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	25	[38]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	>100 (48h)	[42]
	Algae	EC ₅₀	18	[45]
Erythromycin	Algae	EC ₅₀	>100 (24h)	[42]
	Fish	EC ₅₀	900	[36]
	Invertebrates	EC ₅₀	15	[36]
	Algae	EC ₅₀	0.02	[36]
Budesonide	Fish	LC ₅₀	19 (<96h)	[42]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	20 (48h)	[42]
Fenofibrate	Algae	EC ₅₀	0.8	[45]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	50	[45]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	0.35	[38]
	Algae	EC ₅₀	0.1	[45]
Risperidone	Fish	LC ₅₀	6 (<96h)	[42]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	6 (48h)	[42]
	Algae	LC ₅₀	N.A.	[42]
Salicylic acid	Fish	EC ₅₀	1.29	[43]
	Fish	LC ₅₀	37 (<96h)	[42]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	59	[43]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	118 (48h)	[42]
	Algae	EC ₅₀	48	[43]
	Algae	LC ₅₀	>100 (24h)	[42]
Ibuprofen	Fish	EC ₅₀	5	[43]
	Fish	LC ₅₀	173 (<96h)	[42]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	9.02	[43]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	9.06 (48h)	[41]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	101	[40]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	9.1 (48h)	[42]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	38	[38]
	Algae	EC ₅₀	4	[43]
	Algae (<i>S.costatum</i>)	EC ₅₀	7.1 (96h)	[41]
	Algae (<i>D. subspicatus</i>)	EC ₅₀	342	[40]
	Algae	LC ₅₀	7.1 (24h)	[42]
Ketoprofen	Algae	EC ₅₀	26	[38]
	Fish	EC ₅₀	32	[38]
	Fish	EC ₅₀	157.7	[46]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	248	[38]
	Invertebrates	EC ₅₀	9.05	[46]
	Algae	EC ₅₀	164	[38]
Indomethacin	Algae	EC ₅₀	7.87	[46]
	Fish	EC ₅₀	3.9	[38]

Diclofenac	Invertebrates (<i>Daphnid</i>)	EC ₅₀	26	[38]
	Algae	EC ₅₀	18	[38]
	Fish	EC ₅₀	531	[43]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	22	[43]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	5057	[38]
Diclofenac	Invertebrates (<i>D. magna</i>)	EC ₅₀	68	[40]
	Invertebrates (<i>T. Platyurus</i>)	EC ₅₀	41	[40]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	80	[40]
	Invertebrates (<i>C. dubia</i>)	EC ₅₀	23	[40]
	Algae	EC ₅₀	14.5	[40]
Gemfibrozil	Algae	EC ₅₀	2911	[38]
	Algae (<i>D. subspicatus</i>)	EC ₅₀	72	[40]
	Algae (<i>P. subcapitata</i>)	EC ₅₀	16	[40]
	Algae (<i>C. meneghiniana</i>)	EC ₅₀	19	[40]
	Fish	EC ₅₀	0.9	[43]
Triclosan	Invertebrates (<i>D. magna</i>)	EC ₅₀	10.4	[43]
	Invertebrates (<i>Daphnid</i>)	EC ₅₀	6	[38]
	Algae	EC ₅₀	4	[43]
	Fish (<i>P. Promelas</i>)	EC ₅₀	0.26 (96h)	[47]
	Fish (<i>L. macrochirus</i>)	EC ₅₀	0.37 (96h)	[47]
	Invertebrates (<i>D. magna</i>)	EC ₅₀	0.39 (48 h)	[47]
	Invertebrates (<i>Daphnid</i>)	LC ₅₀	0.13 (48h)	[42]
	Algae (<i>Scenedesmus</i>)	EC ₅₀	0.0014	[47]
	Algae	LC ₅₀	0.0045 (48h)	[42]

Table SD7. Ecotoxicological data of the analyzed pharmaceuticals, for chronic toxicity (lowest values in bold)

Compounds	Species	Test	Toxicity (mg/L)	Reference
Ciprofloxacin	Algae (<i>P. subcapitata</i>)	NOEC	1.09	[48]
	Fish (<i>D. Rerio</i>)	NOEC	>8	[49]
	Invertebrates (<i>B. calyciflorus</i>)	NOEC	0.25	[49]
	Invertebrates (<i>C. dubia</i>)	NOEC	0.25	[49]
Sulfamethoxazole	Invertebrates (<i>C. dubia</i>)	NOEC	0.21	[40]
	Invertebrates (<i>B. calyciflorus</i>)	NOEC	9.63	[40]
	Algae (<i>P. subcapitata</i>)	NOEC	0.09	[49]
	Algae (<i>C. meneghiniana</i>)	NOEC	0.25	[49]
	Algae (<i>L. gibba</i>)	NOEC	0.01	[40]
Carbamazepine	Fish (<i>D. Rerio</i>)	NOEC	25	[49]
	Invertebrates (<i>B. calyciflorus</i>)	NOEC	0.377	[49]
	Invertebrates (<i>C. dubia</i>)	NOEC	0.025	[49]
	Algae (<i>P. subcapitata</i>)	NOEC	>100	[49]
	Algae (<i>C. meneghiniana</i>)	NOEC	10	[49]
Bezafibrate	Algae (<i>S. leopoliensis</i>)	NOEC	17.5	[49]
	Fish	NOEC	3.8	[45]

Erythromycin	Algae (<i>P. Subcapitata</i>)	NOEC	0.0103 (144h)	[50]
	Algae (<i>P. Subcapitata</i>)	NOEC	0.0103 (72h)	[50]
Budesonide	Invertebrates (<i>Daphnid</i>)	NOEC	10	[42]
Fenofibrate	Fish	NOEC	0.048	[45]
Ibuprofen	Algae (<i>Synechocystis</i>)	NOEC	>1	[40]
	Algae (<i>D. subspicatus</i>)	NOEC	103	[40]
	Fish (<i>D. Rerio</i>)	NOEC	4	[49]
	Fish (<i>D. Rerio</i>)	NOEC	0.5	[40]
	Fish (<i>S. trutta</i>)	NOEC	0.0015	[40]
	Fish (<i>O. mykiss</i>)	NOEC	0.005	[40]
	Invertebrates (<i>B. calyciflorus</i>)	NOEC	12.5	[49]
	Invertebrates (<i>C. dubia</i>)	NOEC	1	[49]
Diclofenac	Invertebrates (<i>D. magna</i>)	NOEC	10	[40]
	Algae (<i>P. subcapitata</i>)	NOEC	10	[49]
	Algae (<i>C. meneghiniana</i>)	NOEC	10	[49]
	Algae (<i>S. leopoliensis</i>)	NOEC	10	[49]
	Algae (<i>D. subspicatus</i>)	NOEC	49	[40]
	Fish	NOEC	0.93	[45]
Gemfibrozil	Fish (<i>O. mykiss</i>)	NOEC	0.034	[51]
	Algae (<i>S. subspicatus</i>)	NOEC	0.0007	[51]
Triclosan	Algae (<i>Scenedesmus</i>)	NOEC	0.00069	[47]

Figure SD1 (a)

Figure SD1 (b)

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