

Table 1. PNEC_{ecotox} values obtained from Tell et al. (2019), PNEC_{resistance} calculated according to Bengtsson-Palme et al. (2016) and PNEC_{resistance} calculated according to Rico et al. (2017), and lowest PNEC considering potential ecotoxicological and antibiotic resistance effects. The table also shows the percentage of samples that exceed the different PNECs for each antibiotic as well as the removal efficiency targets that should be further implemented to achieve antibiotic emissions below the proposed environmental threshold (lowest PNEC).

Antibiotic	PNEC _{ecotox}		PNEC _{resistance} Bengtsson-Palme et al. (2016)		PNEC _{resistance} Rico et al. (2017)		Lowest PNEC		Removal efficiency target (%)
	Value (ng L ⁻¹)	Exceedance (%)	Value (ng L ⁻¹)	Exceedance (%)	Value (ng L ⁻¹)	Exceedance (%)	Value (ng L ⁻¹)	Exceedance (%)	
Azithromycin	20	100	250	100	110	100	20	100	99
Ciprofloxacin	570	7	60	97	99	97	60	97	92
Clarithromycin	80	100	250	33	150	100	80	100	80
Clindamycin	100	0	1000	0	292	0	100	0	-
Erythromycin	500	0	1000	0	731	0	500	0	-
Levofloxacin	1000 ^a	0	250	63	375	53	250	63	64
Metronidazole	NA	NA	130	40	83	70	83	70	62
Moxifloxacin	500 ^b	0	130	0	552	0	130	0	-
Norfloxacin	120000	0	500	0	64	77	64	77	75
Sulfamethoxazole	600	0	16000	0	59110	0	600	0	-
Trimethoprim	100000	0	500	0	1187	0	500	0	-

^aBased on the toxicity value for *Microcystis flos-aquae* provided by (Wan et al., 2014).

^bBased on the toxicity value for *Microcystis aeruginosa* provided by (Wan et al., 2021).

Table 2. Metabolites of antibiotics selected found in IWW and EWW samples after a LC-IMS-HRMS screening

Metabolite	Ion	<i>m/z</i>	Elemental composition	Mass error (ppm)	Mass error (mDa)	Observed for parent compound
3-desmethyl Trimethoprim	[M+H] ⁺	277.12826	C ₁₃ H ₁₇ N ₄ O ₃ ⁺	-4.5	-1.3	
	Fragment	261.09872	C ₁₂ H ₁₃ N ₄ O ₃ ⁺	1.4	0.4	√
	Fragment	123.06649	C ₅ H ₇ N ₄ ⁺	6.6	0.8	√
Clindamycin sulfoxide	[M+H] ⁺	441.18208	C ₁₈ H ₃₃ ClN ₂ O ₆ S ⁺	0.1	0.0	
	Fragment	126.12765	C ₁₈ H ₃₃ ClN ₂ O ₆ S ⁺	-0.6	-0.1	√
	Fragment	377.18452	C ₁₈ H ₃₃ ClN ₂ O ₆ S ⁺	2.0	0.7	√
<i>N</i> -acetylCiprofloxacin	[M+H] ⁺	374.15168	C ₁₉ H ₂₁ FN ₃ O ₄ ⁺	1.7	0.6	
	Fragment	231.05823	C ₁₂ H ₈ FN ₂ O ₂ ⁺	7.8	1.8	√
Oxociprofloxacin	[M+H] ⁺	346.12042	C ₁₇ H ₁₇ FN ₃ O ₄ ⁺	1.9	0.7	
	Fragment	328.10916	C ₁₇ H ₁₇ FN ₃ O ₄ ⁺	-0.1	0.0	x
	Fragment	287.07105	C ₁₇ H ₁₇ FN ₃ O ₄ ⁺	3.4	1.0	x
	Fragment	217.04074	C ₁₇ H ₁₇ FN ₃ O ₄ ⁺	-0.2	0.0	x