

Supplementary material

Antibiotic pollution and risk assessment under different cultivation modes in aquaculture ponds of the Taihu Lake Basin, China

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Table S1. Cultivation modes of sample location

Sample location	Cultivation mode	Location	Label
Changzhou City	Fish	31°38'27.53"N, 119°30'46.93"E	S9
Changzhou City	Fish	31°36'40.04"N, 119°52'36.11"E	S6
Changzhou City	Crab and shrimp	31°42'27.83"N, 119°48'59.54"E	S5
Wuxi City	Fish	31°40'6.17"N, 120°38'48.01"E	S4
Wuxi City	Crab and shrimp	31°41'11.18"N, 120°38'16.56"E	S7
Wuxi City	Crab	31°29'47.99"N, 119°44'5.51"E	S1
Gaochun City	Crab	31°21'55.24"N, 118°50'25.10"E	S2
Gaochun City	Crab and shrimp	31°24'29.77"N, 118°54'14.29"E	S8
Suzhou City	Crab	31° 2'32.82"N, 120°23'19.48"E	S3
Suzhou City	Crab and shrimp	31°12'56.72"N, 120°47'30.16"E	S10

Table S2. Information of the samples in aquaculture ponds

Chl-*a*, chlorophyll-*a*; DO, dissolved oxygen; NH₄⁺-N, ammonia-N; TN, total nitrogen; TOC, total organic carbon; TP, total phosphorus

Label	Sample area	Temperature (°C)	pH	DO (mg L ⁻¹)	TOC (mg L ⁻¹)	TN (mg L ⁻¹)	TP (mg L ⁻¹)	NH ₄ ⁺ -N (mg L ⁻¹)	Chl- <i>a</i> (mg m ⁻³)
S1	Wuxi	35.90	9.18	9.69	23.04	3.34	0.27	0.14	16.04
S2	Gaochun	31.90	8.02	4.09	15.28	1.62	0.13	0.04	6.46
S3	Suzhou	33.33	7.90	5.65	21.43	2.92	0.17	0.13	3.58
S4	Wuxi	33.73	7.92	6.70	17.53	2.65	0.59	0.14	149.26
S5	Changzhou	35.63	8.48	9.17	19.05	1.90	0.51	0.13	11.48
S6	Changzhou	33.43	7.84	5.62	23.88	3.88	0.44	0.12	33.20
S7	Wuxi	32.50	8.36	5.84	15.47	1.50	0.11	0.12	4.92
S8	Gaochun	31.76	7.81	5.16	15.02	2.71	0.84	0.53	9.81
S9	Changzhou	32.26	7.89	4.74	17.32	2.05	0.20	0.13	7.39
S10	Suzhou	33.35	7.03	6.83	12.04	1.33	0.11	0.97	4.51

Table S3. Optimised liquid chromatography–tandem mass spectrometry (LC→MS/MS) parameters for the antibiotics

AZY, azithromycin; CIP, ciprofloxacin; CLR, clarithromycin; ENR, enrofloxacin; OFL, ofloxacin; OTC, oxytetracycline; RTM, roxythromycin; SDZ, sulfadiazine; SMZ, sulfamethoxazole; TC, tetracycline

Compound	Retention time (min)	MRM →transitions	Fragmentor (V)	Collision energy (eV)
SDZ	2.45	250.9→155.7 ^A	40	20
		250.9→92	40	32
SMZ	3.72	279→185.9 ^A	75	23
		279→155.9	75	25
ENR	2.98	360.0→342 ^A	100	28
		365.1→321.1	70	36
OFL	1.97	362.2→318.1 ^A	124	26
		334→290	120	26
CIP	2.79	331.9→288.1 ^A	95	24
		340.1→332	95	30
RTM	7.63	837.5→158.1 ^A	102	47
		837.5→679.8	102	29
AZY	7.59	749.5→158.2 ^A	64	40
		749.5→590.6	64	30
CLR	7.59	748.9→158.2 ^A	95	37
		748.9→590.6	95	29
TC	5.22	445.1→410.0 ^A	80	26
		445.1→426.8	80	17
OTC	4.18	461.1→426.1 ^A	80	25
		461.1→443.1	80	17

^AMRM transition was used for quantification.

Table S4. Ecotoxicological information and estimated predicted no effect concentrations (PNECs) of antibiotics for aquatic organisms

LC₅₀ or EC₅₀ is the lowest median effective concentration value obtained from the literature.

References cited are: ECOSAR, Ecological Structure Activity Relationships (see <https://cfub.epa.gov/ecotox/>); 1, Lützhøft *et al.* (1999); 2, Wollenberger *et al.* (2000); 3, Ferrari *et al.* (2004); 4, Isidori *et al.* (2005); 5, Kim *et al.* (2007); 6, Robinson *et al.* (2005); 7, Brain *et al.* (2004); 8, Halling-Sorensen *et al.* (2000); 9, Park and Choi (2008); 10, Cunningham *et al.* (2006); 11, Choi *et al.* (2008); 12, Food and Drug Administration, Center for Drug Evaluation and Research (1996); 13, Yang *et al.* (2008); 14, Wollenberger *et al.* (2000). Compound abbreviations are: AZY, azithromycin; CIP, ciprofloxacin; CLR, clarithromycin; ENR, enrofloxacin; OFL, ofloxacin; OTC, oxytetracycline; RTM, roxythromycin; SDZ, sulfadiazine; SMZ, sulfamethoxazole; TC, tetracycline

Compound	Taxonomic group	Species	LC ₅₀ or EC ₅₀ values (mg L ⁻¹)	PNEC (ng L ⁻¹)	Reference
SDZ	Algae	<i>M. aeruginosa</i>	0.135 (72 h)	135	1
	Invertebrates	<i>D. magna</i>	221 (48 h)	2.21 × 10 ⁵	2
SMZ	Algae	<i>leopoliensis</i>	0.027 (96 h)	27	3
	Invertebrates	<i>C. dubia</i>	0.21 (7 days)	210	4
	Fish	<i>O. latipes</i>	562.5 (4 days)	5.63 × 10 ⁵	5
CIP	Algae	<i>M. aeruginosa</i>	0.017 (24 h)	17	6
	Algae	<i>P. subcapitata</i>	18.7 (24 h)	18.7 × 10 ³	6
	Plants	<i>L. minor</i>	0.203 (24 h)	203	6
	Plants	<i>L. gibba</i>	0.698 (7 days)	698	7
	Fish	<i>B. rerio</i>	100 (7 h)	1 × 10 ⁵	8
ENR	Algae	<i>M. aeruginosa</i>	0.049 (24 h)	49	6
	Algae	<i>P. subcapitata</i>	3.10 (24 h)	3.1 × 10 ³	6
	Plants	<i>L. minor</i>	0.114 (24 h)	114	6
	Invertebrates	<i>D. magna</i>	56.7 (48 h)	5.67 × 10 ⁴	9
	Invertebrates	<i>M. macrocopa</i>	>200 (48 h)	2 × 10 ⁵	9
	Fish	<i>O. latipes</i>	>100 (48 h)	1 × 10 ⁵	9
OFL	Algae	<i>M. aeruginosa</i>	0.021 (24 h)	21	6
	Algae	<i>P. subcapitata</i>	12.10 (24 h)	1.21 × 10 ⁴	6
	Algae	<i>P. subcapitata</i>	1.44 (72 h)	1440	10
	Plants	<i>L. minor</i>	0.126 (24 h)	126	6
	Plants	<i>L. gibba</i>	0.532 (7 days)	532	7
	Invertebrates	<i>C. dubia</i>	17.41 (48 h)	17410	10
	Fish	<i>D. rerio</i>	1000 (96 h)	1 × 10 ⁶	4
	RTM	Algae	<i>P. subcapitata</i>	4.663 (96 h)	4663
Invertebrates		<i>D. magna</i>	9.1 (96 h)	9100	11

Compound	Taxonomic group	Species	LC ₅₀ or EC ₅₀ values (mg L ⁻¹)	PNEC (ng L ⁻¹)	Reference
	Fish	<i>O. latipes</i>	288.3 (96 h)	2.88 × 10 ⁵	11
AZY	Algae	<i>P.subcapitata</i>	1.874 (96 h)	1874	ECOSAR
	Invertebrates	<i>Daphnia</i> sp.	>120 (acute)	1.2 × 10 ⁵	12
	Fish	<i>D. rerio</i>	18.822 (96 h)	18822	ECOSAR
CLR	Algae	<i>P.subcapitata</i>	0.002 (72 h)	2	4
	Invertebrates	<i>C. dubia</i>	8.16 (7 days)	8160	4
	Fish	<i>D. rerio</i>	>1000 (72 h)	1 × 10 ⁶	4
OTC	Algae	<i>P. subcapitata</i>	0.17 (72 h)	170	4
	Invertebrates	<i>C. dubia</i>	0.18 (7 days)	180	4
	Fish	<i>D. rerio</i>	>1000 (96 h)	1 × 10 ⁶	4
TC	Algae	<i>P.subcapitata</i>	0.5 (72 h)	500	13
	Invertebrates	<i>D. magna</i>	44.8 (21 days)	44800	14

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