

Supporting Information

Supplemental Text

Text S1 Study area overview and sampling procedures

1.1 Study area overview

The Chaohu basin is located in the middle of two water systems, the Yangtze River and the Huai River, in the central part of Anhui Province. It covers an area of 13350 km² and spans several counties and cities under the jurisdiction of Hefei and Lu'an in Anhui Province. The center of the basin, Chaohu Lake, is situated between 31°25'~31°43'N and 117°16'~117°51'E, shaped like a bird's nest, from which it was named. As fifth-largest freshwater lake in China, it serves as an urban drinking water source for 9 million residents in Hefei and Chaohu Cities and is a typical large shallow and important lake. The dense river system in the basin, formed by its characteristic topography, converges radially into Chaohu Lake. The lake is divided into western and eastern lakes by Mushan Island. The western lake is surrounded by Hefei, the capital of Anhui Province, and a large discharge of domestic and industrial sewage flows into this region with Nanfei, Shiwuli, and Pai Rivers. The eastern lake is surrounded by Chaohu City, with water mainly derives from the Zhegao, Tongyang, and Zhao Rivers. Yuxi River is not only a tributary of the Yangtze River but also the only outflow of Chaohu Lake.

The agricultural economy of Chaohu basin has been developing rapidly, with plantation as the main industry and aquaculture as a supplement, and it is famous as the homeland of fish and rice. With the improvement of urbanization and industrialization and the rapid growth of population, the traditional agriculture-based economy of the Chaohu basin is gradually transforming, and the industrial economy has become the main force and has a certain scale of development, especially in the urban areas of Hefei and Chaohu Cities. At present, there are more than 2500 industrial enterprises in the basin, especially Hefei, the largest and fastest growing city in the basin, with a total urban area of 840 km² and a built-up area of 360 km², has a complete industrial system (including metallurgy, machinery, food processing and chemical industry, etc). Its number of factories and enterprises accounts for more than 52% of the whole basin.

1.2 Sampling procedures

Sample collection was conducted in July 2021 (Summer wet season) and December 2021 (winter dry season). During this period (from July 2021 to December 2021), the basic weather information in the watershed is detailed in Table S2 (data information from monitoring stations). In this study, water and sediment samples were collected from 20 sampling points from L1 to L20 in lakes (western lake: L1-L8; eastern lake; L9-L20) and 19 sampling points from R1 to R19 in rivers ((western river: R1-R9; eastern river: R10-R19). Sediment samples were collected using gravity sediment samplers, and three parallel aliquots were taken and mixed at each point, and then stored in acid-treated brown wide-mouth bottles and immediately stored in a cryostat. The water quality parameters (temperature (Temp), pH, dissolved oxygen (DO), oxidation reduction potential (ORP), and electrical conductivity (Ec)) were monitored in situ online using the multi-parameter water quality monitor. The sediment conventional indicators (e.g., ORP) were measured on-site using portable measuring instruments. The use of the standard solution to calibrate the multi-parameter detector before each usage. After each on-site sample collection, the samples will be immediately returned to the laboratory and the corresponding follow-up procedures will be completed within one week.

Text S2 Samples Analysis

2.1 Sample pretreatment

The antibiotics in the samples were extracted by solid phase extraction (SPE) according to previously studies (Chen et al., 2020b). Briefly, three parallel water samples (1 L) were filtered using 0.45 µm GF/F. The filtered samples were adjusted to pH = 3 with HCL solution and then fortified with 200 mg Na₂EDTA and 50 ng of internal standards, followed by SPE using PolySery HLB cartridges (Shanghai ANPEL Corp., China). After SPE, 12 mL of methanol was used for elution and further concentrated to dryness while being gently streamed with nitrogen. Immediately afterwards, these compounds were redissolved in 500 µL of methanol (containing 50 ng NOR-d5) and preserved in a refrigerator at -40°C for the following analysis.

For sediment samples, three sieved parallel samples (2 g dry weight) were weighed into 30 mL centrifugal tubes, along with 20 ng of internal standard was added, respectively. The samples were then combined, placed at 4°C overnight, and shielded from light. Phosphate-citric acid (10 mL, pH = 3.0) was added to each glass tube together with acetonitrile (10 mL), agitated on a vortex shaker for 10 minutes, sonicated for 15 minutes, then centrifuged for 10 minutes to collect the supernatant. After repeating the extraction process twice, the supernatants of the three extracts were combined. Then, in order to remove the organic solvent, the acquired supernatant was transferred to a 200 mL round bottom flask and evaporated on a rotary evaporator. The concentrated residue in the flask was diluted to 200 mL with the use of ultrapure water, guaranteeing that the organic solvent content of solution was less than 5%. The following processes are equivalent to those that were previously detailed for water SPE. The supernatant was analyzed by high performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS).

2.2 Analysis of antibiotics

PerkinElmer LX-50 liquid chromatography equipped with QSight 420 electrospray-tandem triple quadrupole mass spectrometry (MS/MS; PerkinElmer, Canada) were used to analyze the target antibiotics. The analytes were separated at 40 °C with a flow rate of 0.4 mL/min on the ZORBAX SB-C18 column (2.1mm x 150mm, 3.5 µm; Agilent, USA). The final solution was injected into the instrument at a volume of 5 µL, and positive ion mode analysis was performed on it. The MS/MS was operated in the predetermined multiple reaction monitoring (S-MRM) mode for 20 ms of dwell time. Additionally, Table S4 provides the gradient elution program, and Table S5 includes a list of the optimized MS/MS parameters for each analyte and the matching internal standard. Additional MS settings are as follows: source temperature, 250 °C; ion source temperature, 450 °C; ionization voltage, 4500 V; HSID temperature, 200 °C; nebulizer gas, 150 °C; electrospray v1pos, 5000 °C. Standard operating procedures were used to define the limit of detection (LOD) and limit of quantitation (LOQ) for each target analyte of the approach (EPA, 1986).

Text S3 Ecological and human health risk assessment

3.1 Ecological risk assessment-risk quotient (RQ) method

Risk quotient (RQ) method was conducted to evaluated ecological risk of antibiotics according to the European technical guidance document on risk assessment (European, 2003). To avoid the uncertainty produced by data selection, toxicity data of no observed effect concentrations (NOECs), lowest observed effect concentration (LOEC), effect/lethal concentration for 10 percent of the population affected (EC/LC10), and the median effect/lethal concentration (EC/LC50) were all included. For each effect measurement of each species with multiple data, the most sensitive endpoints were selected (Wang et al., 2022). RQs was calculated through the measured environmental concentration (\overline{MEC} , the average concentration calculated from observed values for single antibiotic) divided by the predicted no-effect concentration (PNEC) (Chen et al., 2020b).

$$RQ = \overline{MEC}/PNEC \quad (S1)$$

PNEC is the predicted no-effect concentration derived by the most sensitive toxicity data with assessment factors (AF) of 10, 50, 100, or 1000 depending on test endpoints of NOEC, LOEC, EC/LC10, or EC/LC50.

$$PNEC = \frac{EC_{50}(LC_{50})}{AF}, \frac{EC_{10}(LC_{10})}{AF}, \frac{LOEC}{AF}, \text{ or } \frac{NOEC}{AF} \quad (S2)$$

Detailed toxicity data of antibiotics for aquatic species were collected from ECOTOX database (<https://cfpub.epa.gov/ecotox/>) and available literature. The RQ values were classified into the following levels: minimal risk (< 0.01), low risk (0.01–0.1), medium risk (0.1–1), as well as high risk (≥ 1) (Wu et al., 2022a).

3.2 Ecological risk assessment-species sensitivity distribution (SSD) method

Species sensitivity distribution (SSD) curves were constructed based on acute toxicity data of 7 antibiotics with varying risk levels, which represents the sensitivity of aquatic species to certain compound. The construction and application of SSD mainly include the following steps:

- (1) acquisition of antibiotic toxicology data;
- (2) species distribution and data processing;
- (3) SSD curve fitting;
- (4) 5% hazardous concentration (HC₅) and potential affected fraction (PAF) calculation.

The SSD fitting curve was constructed using the Burrlioz (version 2.0) calculation software provided by the Australian Commonwealth Scientific and Industrial Research Organization (CSIRO). Detailed toxicity data of antibiotics for aquatic species were collected from ECOTOX database (<https://cfpub.epa.gov/ecotox/>) and available literature.

Among them, the parametric equation of Burr III function is:

$$F(X) = 1/[1 + (b/X)^c]^k \quad (S3)$$

Where X is the environmental concentration ($\mu\text{g}\cdot\text{L}^{-1}$), b , c and k are three different parameters of the function (the same below). When k tends to infinity, the Burr III distribution will change into the Reweibull type distribution:

$$F(X) = \exp(-\frac{a}{x^b}) \quad (S4)$$

The formula for calculating HC(q) using Burr III distribution is:

$$HC(q) = \frac{b}{\left[\left(\frac{1}{q}\right)^{\frac{1}{k}} - 1\right]^{\frac{1}{c}}} \quad (S5)$$

The numerical value of HC₅ indicates the degree of impact of antibiotics on aquatic organisms. That is, under this ecological risk threshold represented by HC₅, 95% of organisms in the environment can be protected from harmful effect. PAF represents the proportion of species affected when the environmental concentration exceeds the biotoxicological endpoint value, which corresponds to the cumulative probability of the SSD curve under a given pollutant concentration condition (Besseling et al., 2019). The formula for calculating PAF from Burr III distribution is:

$$PAF(x) = \frac{1}{\left[1 + \left(\frac{b}{x}\right)^c\right]^k} \quad (S6)$$

Under the determined SSD curve, HC(q) (HC₅ in this study) and PAF can be calculated based on the correlation function value of the SSD curve and Rurrioz analysis software (version 2.0).

3.3 Human health risk assessment

The RQ-based human health risk assessment of antibiotic exposure through drinking water was evaluated at different life stages (eq. (S7)). It was estimated by dividing the concentration of each antibiotic in finished drinking water (DWC) from the drinking water treatment plant (DWTP) by a corresponding drinking water equivalent level (DWEL).

$$RQ = \frac{DWC}{DWEL} \quad (S7)$$

Considering the removal efficiencies (R) of antibiotics in DWTP, DWC was calculated by eq. (S8), where R was assumed to be 46.8% in this study based on the results of previous studies (Li et al., 2019).

$$DWC = MEC \times (1 - R) \quad (S8)$$

DWEL was calculated using the following equation:

$$DWEL = \frac{ADI \times BW \times HQ}{DWI \times AB \times FOE} \quad (S9)$$

where ADI is the acceptable daily intake ($\mu\text{g}/\text{kg}/\text{day}$) for each antibiotic (Table S18); BW represents the median body weight (kg) at the different life stages selected (Table S19) (de Jesus Gaffney et al., 2015); HQ indicates the hazard quotient assumed to be 1; DWI is the age specific drinking water intake (L/day) (Table S19) (de Jesus Gaffney et al., 2015); AB is the gastrointestinal absorption rate assumed to be 1, and FOE is frequency of exposure (350 days/365 days = 0.96). RQ values ≥ 1 was considered as a potential risk to the exposed population.

Text S4 Fluorescence composition of dissolved organic matter (DOM)

Five DOM fluorescence fractions were derived from EEM-PARAFAC analysis in the Chaohu basin (Fig. S4), including terrestrial humic fluorescence fraction (C1), microbial source humic fluorescence fraction (C2), tryptophan-like fluorescence fraction (C3), protein-like fluorescence fraction (C4), and tyrosine-like fluorescence fraction (C5). These fluorescence peaks are present in river DOM (Ryan et al., 2022), lake DOM (Caldero-Pascual et al., 2022), and marine DOM (Chen et al., 2018b). Strikingly, river and lake DOM components are more strongly influenced by human activities and anthropogenic pollutants (Xia et al., 2022). Pollution causes an increase in the fluorescence intensity of protein-like components in the aquatic environment. Researchers have studied DOM river characteristics using 3D-EEM and reported that DOM fluorescence consists of flavic acid-like fluorescence peaks and protein-like fluorescence peaks (Su et al., 2023). In general, DOM fluorescence spectra from rivers contaminated by human activities will contain strong protein-like fluorophores (Hudson et al., 2007). Overall, the new analytical approach using fluorescence DOM as an indicator to explore sources of antibiotic-like contaminants is a groundbreaking step in establishing a qualitative and quantitative source allocation method in aquatic environments.

Supplemental Tables

Table S1 Basic information for each sampling site.

Sampling sites	Geographic location (E, N)		City/County	Site characteristics	
L1	117.3893	31.6812	Feixi	Western lake	
L2	117.3567	31.6849	Feixi	Western lake	
L3	117.3356	31.6752	Feixi	Western lake	
L4	117.32	31.6566	Feixi	Western lake	
L5	117.3826	31.5695	Feixi	Western lake	
L6	117.3712	31.6546	Feixi	Western lake	
L7	117.4203	31.6454	Feidong	Western lake	
Lake	L8	117.3615	31.6115	Feixi	western lake
	L9	117.5388	31.5569	Juchao	Eastern lake
	L10	117.4693	31.5658	Juchao	Eastern lake
	L11	117.5204	31.5047	Juchao	Eastern lake
	L12	117.5586	31.4713	Juchao	Eastern lake
	L13	117.6204	31.5221	Juchao	Eastern lake
	L14	117.6702	31.5382	Juchao	Eastern lake
	L15	117.6335	31.5778	Juchao	Eastern lake

	L16	117.7538	31.6128	Juchao	Eastern lake
	L17	117.6654	31.6318	Juchao	Eastern lake
	L18	117.6909	31.5569	Juchao	Eastern lake
	L19	117.7556	31.6014	Juchao	Eastern lake
	L20	117.8314	31.5934	Juchao	Eastern lake
River	R1	117.4602	31.8759	Feidong	Western river
	R2	117.3022	31.8524	Baohe	Western river
	R3	117.4062	31.7098	Feidong	Western river
	R4	117.312	31.721	Baohe	Western river
	R5	117.2888	31.6658	Feixi	Western river
	R6	117.3988	31.5296	Lujiang	Western river
	R7	117.2521	31.5053	Lujiang	Western river
	R8	117.3568	31.5482	Lujiang	Western river
	R9	117.2430	31.5236	Lujiang	Western river
	R10	117.6340	31.6831	Juchao	Eastern river
	R11	117.6290	31.6799	Juchao	Eastern river
	R12	117.6365	31.6578	Juchao	Eastern river
	R13	117.6804	31.6621	Juchao	Eastern river
	R14	117.7498	31.7716	Juchao	Eastern river
	R15	117.7911	31.6212	Juchao	Eastern river
	R16	117.8289	31.6086	Juchao	Eastern river
	R17	117.8733	31.5737	Juchao	Eastern river
	R18	117.8407	31.5945	Juchao	Eastern river
	R19	117.5501	31.4242	Lujiang	Eastern river

Table S2 Basic meteorological information of the Chaohu basin.

	Air Temperature (°C)	Water Temperature (°C)	Rainfall (mm)	Relative humidity
Summer wet season	23~36	25.6~31.8	389	70~84
Winter dry season	-10~16	4.3~11.5	94.5	63~71

Table S3 Relevant information and properties of antibiotics.

Category	Antibiotics	Abbr. ^a	CAS No.	Molecular formula	Molecular weight (g/mol)	Log _{kw} ^b	pK _a ^c
SAs	Sulfadiazine	SDZ	68-35-9	C10H10N4O2S	250.3	-0.09	2.00, 6.48
	Sulfathiazole	STZ	72-14-0	C9H9N3O2S2	255.3	0.05	2.20, 7.24
	Trimethoprim	TMP	738-70-5	C14H18N4O3	290.3	0.91	3.23, 6.76
	Sulfapyridine	SPD	144-83-2	C11H11N3O2S	249.3	0.35	2.90, 8.54
	Sulfadimidine	SDD	57-68-1	C12H14N4O2S	278.33	0.89	2.65, 7.65
	Sulfamethoxypyridazine	SMP	80-35-3	C11H12N4O3S	280.3	0.32	2.09, 6.95
	Sulfamonomethoxine	SMM	1220-83-3	C11H12N4O3S	280.3	0.70	1.98, 5.96
	Sulfachloropyridazine	SCP	80-32-0	C10H9ClN4O2S	284.7	0.31	1.87, 5.45
	Sulfamethoxazole	SMX	723-46-6	C10H11N3O3S	253.3	0.89	1.85, 5.60
FQs	Enoxacin	ENO	74011-58-8	C15H17FN4O3	320.3	-0.20	5.50, 8.59
	Floxacin	FLE	79660-72-3	C17H18F3N3O3	369.3	0.24	NA ^d
	Norfloxacin	NOR	70458-96-7	C16H18FN3O3	319.3	-1.03	3.11, 6.10, 8.60, 10.56
	Levofloxacin	LEV	100986-85-4	C18H20FN3O4	361.4	-0.39	5.19, 7.07
	Pazufloxacin	PAZ	127045-41-4	C16H15FN2O4	318.3	-	NA
	Pefloxacin	PEF	70458-92-3	C17H20FN3O3	333.4	0.27	5.66, 6.47
	Ciprofloxacin	CIP	85721-33-1	C17H18FN3O3	331.3	0.28	3.10, 6.14, 8.70, 10.58
	Antofloxacin	ANT	119354-43-7	C ₁₈ H ₂₁ FN ₄ O ₄	376.38	-	NA
	Lomefloxacin	LOM	98079-51-7	C17H19F2N3O3	351.3	-0.30	5.00, 5.87, 9.23
	Danofloxacin	DAN	112398-08-0	C19H20FN3O3	357.4	0.44	6.07, 8.56
	Enrofloxacin	ENR	93106-60-6	C19H22FN3O3	359.4	0.70	3.86, 6.19, 7.59, 9.86
	Sparfloxacin	SPA	110871-86-8	C19H22F2N4O3	392.4	2.50	5.75, 8.79
	Nadifloxacin	NAD	124858-35-1	C ₁₉ H ₂₁ FN ₂ O ₄	360.38	-	NA
Flumequine	FLU	42835-25-6	C14H12FN3O3	261.3	1.60	6.50	
TCs	Oxytetracycline	OTC	79-57-2	C22H24N2O9	460.4	-0.90	3.27, 7.32, 9.11
	Tetracycline	TC	60-54-8	C22H24N2O8	444.4	-1.30	3.30, 7.68, 9.69
	Chlorotetracycline	CTC	57-62-5	C22H23ClN2O8	478.9	-0.62	3.30, 7.55, 9.15

	Doxycycline	DC	564-25-0	C ₂₂ H ₂₄ N ₂ O ₈	444.4	-0.02	7.75
MLs	Clarithromycin	CTM	81103-11-9	C ₃₈ H ₆₉ N ₃ O ₁₃	747.9	3.16	8.99
	Roxithromycin	ROX	80214-83-1	C ₄₁ H ₇₆ N ₂ O ₁₅	837.05	2.75	9.17
	Tylosin	TYL	1401-69-0	C ₄₆ H ₇₇ N ₃ O ₁₇	916.1	1.63	7.73
LAs	Lincomycin	LIN	154-21-2	C ₁₈ H ₃₄ N ₂ O ₆ S	406.5	0.56	7.60
	Clindamycin	CLIN	18323-44-9	C ₁₈ H ₃₃ ClN ₂ O ₅ S	425.0	2.16	7.55, 12.16

^a Abbr.: Abbreviation.

^b K_{ow}: octanol/water partition coefficient.

^c pK_a: acid dissociation constant.

^d NA: Not available.

Table S4 The gradient elution programs in a positive ion mode.

Time (min)	Pump A (%)	Pump B (%)
0	90	10
2	90	10
6	80	20
7	70	30
10	40	60
12	5	95
15	5	95
15.1	90	10
17	90	10

Notes: Pump A: water containing 0.1% formic acid; Pump B: acetonitrile containing 0.1% formic acid.

Table S5 Retention Times (RT) and mass spectrometry parameters of the antibiotics monitored in the present study.

Antibiotics	Retention Time (min)	Precursor ion (m/z)	Product ion (m/z)	CE	EV	CCL2
Sulfonamides						
Sulfamonomethoxine	6.93	281	92.3, 156	-45, -24	6, 8	-84, -80
Sulfamethoxazole	7.87	254	156.1, 92.2	-21, -40	21, 13	-76, -72
Trimethoprim	4.04	291.1	230.1, 123.1	-27, -41	46, 37	-92, -100
Sulfadiazine-13C6	3.04	257.1	162.1	-20	15	-72
Sulfamethoxazole-D4	7.88	258.1	160.1	-21	28	-72
Trimethoprim-D3	3.95	294.2	230.2	-29	20	-100
Fluoroquinolones						
Norfloxacin	4.88	320.1	276.2, 233.1	-21, -31	26, 28	-92, -104
Ciprofloxacin	5.21	332.1	231.1, 314.2	-47, -26	15, 15	-148, -120
Enrofloxacin	5.99	360.2	316.3, 245.1	-24, -35	44, 40	-92, -120
Ciprofloxacin-D8	5.20	340.1	322.3	-26	39	-128
Tetracyclines						
Tetracycline	5.38	445.1	410.3, 427.3	-24, -17	17, 15	-116, -116
Doxycycline	7.95	445.2	428.3, 321.2	-22, -37	23, 30	-128, -120
Oxytetracycline	4.71	461.2	426.2, 443.3	-23, -16	25, 24	-152, -116
Tetracycline-D6	5.36	451.2	416.3	-24	27	-132
Lincosamides						
Lincomycin	2.69	407.2	126.2, 359.4	-32, -8	41, 14	-108, -116
Lincomycin-D3	2.65	410.2	129.4	-39	37	-108

Table S6 The most sensitive PNECs for antibiotics in the water phase.

Antibiotics	PNEC (ng/L)	Reference
SDZ	135	
STZ	1000	
TMP	5.8	
SDD	8700	(Yang et al., 2008)
SMP	3820	(Białk-Bielińska et al., 2011)
SMM	90	(Wu et al., 2022b)
SCP	32250	(Białk-Bielińska et al., 2011)
SMX	0.01	
FLE	1294650	(Wu et al., 2022b)
NOR	53	
PEF	1423040	(Wu et al., 2022b)
LEV	19928	
CIP	697	
LOM	80	
ENR	49	
FLU	159	
OTC	100	
TC	0.1	
CTC	360	
DC	5380	(Wu et al., 2022b)
CTM	2	
ROX	47	
LIN	70	(Tran et al., 2019)
CLIN	56	

Notes: Other PNECs are derived from the most sensitive toxicity data from ECTOX database.

Table S7 Concentrations and detection frequencies of antibiotics in the water phase and sediment phase.

Category	Antibiotics	Water (ng/L)				Sediment (ng/g)			
		DF ^a (%)	Mean±SD ^b	median	Range	DF	Mean±SD	Median	Range
SAs	SDZ	47.44	0.03±0.05	-	nd ^c -0.2	100.00	0.09±0.12	0.05	nd-0.76
	STZ	20.51	0.01±0.02	-	nd-0.10	10.26	-	-	nd-0.02
	TMP	53.85	0.25±0.32	0.11	nd-1.57	93.59	0.04±0.07	0.02	nd-0.45
	SPD	12.82	0.04±0.16	-	nd-1.52	28.21	0.01±0.03	-	nd-0.22
	SDD	94.87	0.16±0.09	0.14	nd-0.57	2.56	-	-	nd-0.03
	SMP	20.51	0.01±0.03	-	nd-0.18	0.00	-	-	nd
	SMM	67.95	0.09±0.17	0.04	nd-1.12	46.15	0.01±0.01	-	nd-0.06
	SCP	44.87	0.02±0.04	-	nd-0.29	10.26	0.00±0.01	-	nd-0.03
	SMX	94.87	0.16±0.25	0.11	nd-2.14	100.00	0.13±0.14	0.10	0.02-1.05
FQs	ENO	73.08	1.65±1.60	1.34	nd-6.58	17.95	0.16±0.61	-	nd-3.75
	FLE	0.00	-	-	--	30.77	0.31±2.05	-	nd-18.20
	NOR	51.28	0.55±0.92	0.01	nd-5.07	84.62	17.16±79.62	1.16	nd-672.42
	LEV	80.77	2.09±3.21	0.89	nd-17.01	96.15	22.00±78.68	1.69	nd-574.03
	PAZ	5.13	0.01±0.06	-	nd-0.35	3.85	0.03±0.17	-	nd-1.33
	PEF	21.79	0.21±0.43	-	nd-1.88	21.79	0.66±4.20	-	nd-36.89
	CIP	21.79	0.05±0.14	-	nd-0.81	71.79	1.72±8.27	0.14	nd-70.54
	ANT	17.95	0.13±0.34	-	nd-1.60	14.10	0.04±0.11	-	nd-0.64
	LOM	24.36	0.04±0.08	-	nd-0.35	53.85	1.09±6.71	0.04	nd-58.94
	DAN	15.38	0.02±0.06	-	nd-0.24	3.85	0.01±0.06	-	nd-0.52
	ENR	30.77	0.49±1.66	-	nd-13.40	66.67	0.72±2.18	0.15	nd-14.82
	SPA	14.10	0.03±0.10	-	nd-0.74	5.13	0.05±0.28	-	nd-2.23
	NAD	0.00	-	-	-	8.97	0.02±0.07	-	nd-0.42
	FLU	57.69	0.16±0.23	0.13	nd-1.60	66.67	0.07±0.11	0.05	nd-0.79
TCs	OTC	16.67	0.05±0.14	-	nd-0.81	100.00	4.62±11.24	1.11	0.14-75.99
	TC	64.10	1.66±6.95	0.50	nd-61.06	71.79	13.91±111.01	0.30	nd-987.50
	CTC	35.90	0.81±1.42	-	nd-8.44	50.00	1.31±3.27	0.13	nd-24.38
	DC	30.77	0.24±0.60	-	nd-3.00	98.72	0.95±1.56	0.47	nd-9.79
	CTM	19.23	0.01±0.01	-	nd-0.06	1.28	-	-	nd-0.04

MLS	ROX	1.28	0.01±0.02	-	nd-0.15	2.56	0.03±0.18	-	nd-1.16
	TYL	0.00	-	-	-	0.00	-	-	nd
LAs	LIN	87.18	12.12±31.82	2.53	nd-200.21	0.00	-	-	nd
	CLIN	100.00	33.59±188.47	4.79	0.42-1676.87	0.00	-	-	nd

^a. DF: detection frequency.

^b. Mean ± SD: arithmetic mean ± standard deviation.

^c. nd: not detected; i.e., lower than the method detection limits.

Table S8 Concentrations and detection frequency of antibiotics in the waters and sediments of river and lake.

Sample	Water (ng/L)						Sediment (ng/g)					
	River			Lake			River			Lake		
	DF (%)	^a Mean	Range	DF (%)	Mean	Range	DF (%)	Mean	Range	DF (%)	Mean	Range
SDZ	51	0.037	nd ^b -0.20	43	0.025	nd-0.18	100	0.075	0.01-0.76	100	0.103	0.01-0.64
STZ	31	0.014	nd-0.10	10	0.001	nd-0.02	13	0.001	nd-0.02	8	0.000	nd-0.01
TMP	62	0.320	nd-1.12	45	0.176	nd-1.57	97	0.063	nd-0.45	90	0.013	nd-0.07
SPD	13	0.047	nd-1.12	13	0.036	nd-0.64	34	0.017	nd-0.22	23	0.004	nd-0.04
SDD	87	0.153	nd-0.57	100	0.160	0.05-0.33	3	0.000	nd-0.01	3	0.001	nd-0.03
SMP	15	0.008	nd-0.18	25	0.009	nd-0.09	0	-	n-	0	-	-
SMM	69	0.070	nd-0.46	65	0.106	nd-1.12	39	0.007	nd-0.04	53	0.014	nd-0.06
SCP	59	0.029	nd-0.29	30	0.015	nd-0.14	13	0.002	nd-0.03	8	0.001	nd-0.02
SMX	87	0.150	nd-0.46	100	0.170	0.03-2.14	100	0.126	0.02-1.05	100	0.134	0.04-0.75
ENO	67	1.785	nd-6.00	78	1.528	nd-6.58	21	0.298	nd-3.75	15	0.029	nd-0.43
FLE	0	-	-	0	-	-	37	0.595	nd-18.20	25	0.041	nd-0.77
NOR	59	0.535	nd-3.59	43	0.409	nd-5.07	89	33.411	nd-672.42	80	1.713	nd-22.75
LEV	87	3.057	nd-17.01	73	1.167	nd-7.55	95	42.861	nd-574.03	98	2.179	nd-26.57
PAZ	8	0.023	nd-0.35	3	0.002	nd-0.08	8	0.063	nd-1.33	0	0.000	-
PEF	28	0.277	nd-1.88	15	0.142	nd-1.50	32	1.274	nd-36.89	13	0.080	nd-1.54
CIP	21	0.064	nd-0.81	23	0.040	nd-0.53	82	3.297	nd-70.54	63	0.227	nd-3.26
ANT	23	0.143	nd-1.20	13	0.113	nd-1.60	11	0.034	nd-0.64	18	0.040	nd-0.42
LOM	21	0.040	nd-0.30	28	0.041	nd-0.35	66	2.103	nd-58.94	43	0.131	nd-2.11
DAN	28	0.039	nd-0.23	3	0.006	nd-0.24	3	0.014	nd-0.52	5	0.001	nd-0.02
ENR	31	0.335	nd-4.19	30	0.506	nd-13.40	79	1.374	nd-14.82	55	0.108	nd-0.70
SPA	15	0.037	nd-0.7364	13	0.025	nd-0.29	11	0.104	nd-2.23	0	0.000	-
NAD	0	-	-	0	-	-	11	0.026	nd-0.42	8	0.012	nd-0.27
FLU	56	0.202	nd-1.5979	58	0.116	nd-0.84	63	0.093	nd-0.79	70	0.054	nd-0.22
OTC	10	0.051	nd-0.8118	23	0.055	nd-0.44	100	6.366	014-75.99	100	2.955	0.14-35.01

TC	69	0.930	nd-10.74	58	2.353	nd-61.06	74	27.236	nd-987.50	70	1.255	nd-22.18
CTC	28	0.624	nd-4.6152	43	0.987	nd-8.4383	61	2.148	nd-24.38	40	0.514	nd-4.14
DC	36	0.343	nd-2.93	25	0.139	nd-3.00	100	1.452	0.12-9.79	98	0.474	nd-1.84
CTM	21	0.006	nd-0.06	18	0.003	nd-0.03	3	0.001	nd-0.04	0	-	-
ROX	3	0.004	nd-0.15	0	-	-	5	0.060	nd-1.16	0	-	-
TYL	0	-	-	0	-	-	0	-	-	0	-	-
LIN	85	18.301	nd-200.21	88	6.241	nd-134.37	0	-	-	0	-	-
CLIN	97	58.566	0.41-1676.87	100	9.863	1.21-63.41	0	-	-	0	-	-

^a. DF: detection frequency.

^b. nd: not detected; i.e., lower than the method detection limits.

Table S9 Concentrations of the antibiotic groups in the water phase and sediment phase.

Sample	Water (ng/L)					Sediment (ng/g)				
	SAs	FQs	TCs	MLs	LAs	SAs	FQs	TCs	MLs	LAs
L1	1.14	2.57	1.17	nd ^a	41.59	0.33	2.30	2.84	nd	nd
L2	0.81	9.11	3.43	nd	41.00	0.10	3.66	4.75	nd	nd
L3	0.55	4.35	0.92	0.01	13.87	0.27	2.48	7.11	nd	nd
L4	0.74	3.36	0.80	nd	23.26	0.23	5.50	6.66	nd	nd
L5	0.38	2.80	5.35	nd	23.50	0.22	3.45	4.10	nd	nd
L6	0.89	3.63	1.61	0.01	13.27	0.52	3.50	2.27	nd	nd
L7	0.60	3.50	2.07	nd	12.98	0.18	1.99	4.93	nd	nd
L8	0.34	2.11	30.67	nd	6.82	0.31	2.44	1.67	nd	nd
L9	0.66	4.54	2.05	nd	3.89	0.18	0.33	0.82	nd	nd
L10	0.39	3.69	2.65	0.01	4.88	0.23	2.60	2.07	nd	nd
L11	0.28	3.08	nd	0.01	11.86	0.27	0.20	6.17	nd	nd
L12	0.63	6.11	0.56	nd	4.67	0.27	1.03	4.18	nd	nd
L13	1.10	10.28	7.46	0.01	2.68	0.16	0.35	7.94	nd	nd
L14	0.30	8.04	2.45	nd	7.66	0.22	1.45	3.93	nd	nd
L15	1.27	3.82	5.05	nd	79.80	0.39	0.83	19.80	nd	nd
L16	0.81	2.65	0.30	0.01	6.30	0.61	0.31	4.29	nd	nd
L17	2.02	2.09	0.38	nd	9.97	0.21	0.58	4.14	nd	nd
L18	0.29	2.83	0.77	0.01	3.90	0.26	28.53	12.82	nd	nd
L19	0.25	0.67	2.51	nd	5.81	0.18	28.37	2.30	nd	nd
L20	0.53	2.68	0.50	nd	4.40	0.28	2.39	1.164	nd	nd
R1	0.80	15.83	9.73	nd	29.06	0.23	58.09	16.02	nd	nd
R2	1.29	20.95	3.38	nd	25.46	0.56	996.56	71.44	0.58	nd
R3	1.99	6.00	0.34	0.01	38.94	0.73	6.91	4.85	nd	nd
R4	1.66	5.23	1.37	0.04	1030.66	0.46	29.08	10.43	nd	nd
R5	0.85	1.91	1.69	nd	64.25	0.77	6.222	2.19	nd	nd

R6	0.24	4.22	1.13	nd	15.83	0.16	5.86	508.16	nd	nd
R7	0.36	7.07	0.94	nd	12.97	0.16	4.91	2.06	nd	nd
R8	0.70	6.30	0.74	nd	68.27	0.11	10.31	8.30	nd	nd
R9	0.41	6.65	0.87	nd	62.64	0.14	15.17	4.97	nd	nd
R10	0.79	3.98	1.03	0.09	24.03	0.11	103.84	10.47	nd	nd
R11	0.79	6.08	1.75	0.01	3.50	0.23	6.30	2.86	nd	nd
R12	1.21	2.57	0.73	nd	6.96	0.15	3.34	0.75	nd	nd
R13	0.79	2.81	3.80	nd	2.35	0.08	28.96	0.63	nd	nd
R14	0.54	5.35	2.71	nd	16.93	0.21	14.37	5.67	nd	nd
R15	0.54	5.49=	2.48	nd	4.93	0.25	252.44	45.43	nd	nd
R16	0.62	14.01	2.09	0.01	12.39	0.13	44.44	3.66	nd	nd
R17	0.84	5.80	0.47	0.02	25.67	0.40	25.95	0.97	0.58	nd
R18	0.30	1.95	0.45	0.01	10.17	0.11	10.44	7.26	nd	nd
R19	0.97	2.06	1.28	nd	5.46	0.58	2.14	0.73	nd	nd

^a nd: not detected; i.e., lower than the method detection limits.

Table S10 Proportions of the antibiotic groups in the water phase and sediment phase.

Sample	Water					Sediment				
	SAs	FQs	TCs	MLs	LAs	SAs	FQs	TCs	MLs	LAs
L1	2.44	5.53	2.52	0.00	89.51	6.03	42.02	51.95	0.00	0.00
L2	1.48	16.76	6.31	0.00	75.44	1.21	42.95	55.83	0.00	0.00
L3	2.78	22.08	4.68	0.04	70.42	2.71	25.13	72.16	0.00	0.00
L4	2.63	11.93	2.86	0.00	82.58	1.84	44.41	53.75	0.00	0.00
L5	1.18	8.74	16.71	0.00	73.36	2.81	44.43	52.76	0.00	0.00
L6	4.58	18.70	8.31	0.03	68.38	8.31	55.58	36.10	0.00	0.00
L7	3.14	18.26	10.79	0.00	67.80	2.48	28.04	69.49	0.00	0.00
L8	0.84	5.28	76.80	0.00	17.08	7.03	55.13	37.84	0.00	0.00
L9	5.92	40.79	18.37	0.00	34.92	13.52	24.53	61.95	0.00	0.00
L10	3.35	31.76	22.81	0.09	41.98	4.67	52.99	42.34	0.00	0.00
L11	1.85	20.22	0.00	0.07	77.86	4.09	2.97	92.94	0.00	0.00
L12	5.27	51.05	4.64	0.00	39.04	4.90	18.78	76.33	0.00	0.00
L13	5.13	47.73	34.61	0.06	12.46	1.93	4.15	93.92	0.00	0.00
L14	1.65	43.58	13.27	0.00	41.49	3.96	25.92	70.12	0.00	0.00
L15	1.42	4.24	5.62	0.00	88.72	1.85	3.96	94.19	0.00	0.00
L16	8.06	26.32	2.94	0.07	62.61	11.63	5.98	82.39	0.00	0.00
L17	13.96	14.43	2.65	0.00	68.96	4.33	11.81	83.86	0.00	0.00
L18	3.73	36.31	9.89	0.09	49.98	0.64	68.56	30.80	0.00	0.00
L19	2.71	7.27	27.19	0.00	62.82	0.58	91.96	7.46	0.00	0.00
L20	6.59	33.07	6.12	0.00	54.22	7.26	62.40	30.34	0.00	0.00
R1	1.43	28.56	17.56	0.00	52.44	0.31	78.15	21.55	0.00	0.00
R2	2.53	41.00	6.62	0.00	49.85	0.05	93.21	6.68	0.05	0.00
R3	4.21	12.69	0.72	0.04	82.35	5.85	55.33	38.82	0.00	0.00
R4	0.16	0.50	0.13	0.00	99.20	1.15	72.75	26.10	0.00	0.00
R5	1.24	2.78	2.46	0.00	93.52	8.43	67.74	23.84	0.00	0.00

R6	1.12	19.69	5.30	0.00	73.89	0.03	1.14	98.83	0.00	0.00
R7	1.70	33.11	4.42	0.00	60.76	2.27	68.82	28.91	0.00	0.00
R8	0.93	8.28	0.98	0.00	89.81	0.59	55.09	44.32	0.00	0.00
R9	0.59	9.43	1.23	0.00	88.75	0.71	74.79	24.50	0.00	0.00
R10	2.63	13.30	3.47	0.30	80.30	0.10	90.75	9.15	0.00	0.00
R11	6.55	50.07	14.46	0.04	28.88	2.48	67.06	30.46	0.00	0.00
R12	10.56	22.40	6.33	0.00	60.71	3.48	78.92	17.60	0.00	0.00
R13	8.14	28.82	38.97	0.00	24.07	0.26	97.61	2.13	0.00	0.00
R14	2.12	20.94	10.63	0.00	66.31	1.02	70.98	28.00	0.00	0.00
R15	4.04	40.86	18.44	0.00	36.66	0.08	84.68	15.24	0.00	0.00
R16	2.13	48.12	7.16	0.04	42.55	0.28	92.14	7.58	0.00	0.00
R17	2.57	17.68	1.42	0.05	78.28	1.41	93.04	3.47	2.08	0.00
R18	2.32	15.12	3.48	0.06	79.02	0.60	58.62	40.77	0.00	0.00
R19	9.96	21.05	13.12	0.00	55.87	16.76	62.19	21.05	0.00	0.00

Notes: unit: %.

Table S11 Structural differences in antibiotic composition were tested using the one-way PERMANOVA test. P.value ≤ 0.05 represents statistically significant.

	Water		Sediment	
	F ^a	P-values ^b	F	P-values
River vs Lake	2.78	0.011	8.33	0.001
Summer vs Winter	2.86	0.007	3.68	0.003
Western vs Eastern (River)	4.32	0.001	1.91	0.037
Western vs Eastern (Lake)	5.79	0.001	2.59	0.016

^a F: represents the test value (F.model).

^b P-values: represents significance.

Table S12 The basic physicochemical properties of the water samples.

Sample site	T (°C)	Ec ($\mu\text{s}/\text{cm}$)	DO (mg/L)	ORP	pH	TN (mg/L)	TP (mg/L)
L1	19.50	401.00	7.63	148.50	7.81	3.24	0.31
L2	19.45	331.00	8.14	146.50	8.08	2.52	0.17
L3	19.60	337.50	8.21	148.50	8.16	1.91	0.11
L4	19.50	338.00	7.65	162.50	7.87	2.39	0.13
L5	19.35	285.00	7.83	172.50	7.59	2.36	0.22
L6	19.30	429.00	7.88	163.50	7.88	2.97	0.43
L7	19.50	313.00	9.43	152.50	8.31	1.86	0.31
L8	19.35	331.00	8.88	160.50	8.05	1.63	0.29
L9	19.75	302.00	8.56	143.50	8.19	1.27	0.20
L10	19.70	333.50	8.84	150.50	8.24	2.17	0.36
L11	19.95	382.00	8.73	152.00	8.35	1.92	0.20
L12	19.95	359.50	7.85	163.50	8.10	2.47	0.18
L13	19.70	351.00	8.39	154.50	8.25	0.98	0.30
L14	19.85	318.00	8.83	159.00	8.12	1.02	0.28
L15	19.95	296.50	8.78	146.00	8.24	2.12	0.26
L16	18.90	305.50	8.01	137.00	8.01	7.64	0.27
L17	20.20	312.00	8.83	136.00	8.31	1.86	0.18
L18	19.35	300.00	8.73	145.50	8.15	1.16	0.17
L19	18.30	320.00	8.38	137.50	8.03	0.61	0.15
L20	18.75	315.50	7.65	142.00	7.72	1.43	0.38
R1	20.65	389.50	8.60	123.50	7.95	3.82	0.21
R2	18.90	386.00	7.50	127.00	6.37	5.91	0.26
R3	22.00	370.00	7.70	143.00	7.57	4.90	0.30
R4	22.40	508.00	9.75	129.00	7.75	5.77	0.21
R5	20.30	503.00	7.35	144.00	7.53	4.82	0.25
R6	20.00	244.50	8.50	133.50	7.87	3.21	0.37
R7	21.75	179.40	9.20	142.00	7.95	3.20	0.08

R8	21.95	193.60	8.05	141.00	7.71	1.89	0.10
R9	21.95	236.95	8.60	144.50	7.52	2.90	0.11
R10	21.55	412.50	8.25	142.00	7.88	2.52	0.11
R11	21.65	321.50	7.95	87.90	7.77	1.58	0.14
R12	23.75	368.00	10.40	133.50	8.25	2.92	0.11
R13	21.85	270.00	9.00	114.50	8.16	3.07	0.07
R14	22.90	377.00	8.55	135.50	8.18	4.54	0.11
R15	20.10	413.00	8.40	132.50	8.22	3.34	0.16
R16	21.65	393.00	8.70	148.50	7.98	1.88	0.07
R17	21.15	419.50	7.60	140.50	7.91	4.99	0.16
R18	22.20	307.50	7.55	143.00	8.21	1.88	0.16
R19	21.90	280.00	8.10	125.00	8.17	1.62	0.16

Table S13 The basic physicochemical properties of the sediment samples.

Sample site	Ec ($\mu\text{s}/\text{cm}$)	DO (mg/L)	ORP	PH	TN (mg/kg)	TP (mg/kg)	SOC (g/kg)
L1	161.15	7.58	220.50	6.75	540.00	686.20	11.825
L2	293.00	7.55	226.50	6.51	825.10	1289.46	15.865
L3	265.50	7.30	231.50	6.55	761.67	1121.88	14.45
L4	172.50	7.74	222.00	6.62	848.78	879.66	11.92
L5	230.10	7.27	238.50	6.67	554.27	598.64	7.915
L6	222.00	7.80	245.50	6.22	772.23	874.98	9.47
L7	217.85	7.33	256.00	5.41	810.55	740.95	12.17
L8	172.25	7.32	261.00	6.37	787.09	745.59	12.7
L9	212.40	7.51	263.00	6.77	464.60	432.11	6.8
L10	105.45	7.68	238.50	6.98	618.99	588.08	10.33
L11	260.70	7.48	275.50	5.18	703.31	513.25	9.5
L12	231.70	7.47	242.00	6.79	545.24	524.55	10.66
L13	179.75	7.72	240.00	6.71	886.87	583.56	10.23
L14	133.15	7.30	237.00	6.97	541.36	561.43	10
L15	192.85	7.58	235.50	6.98	738.95	598.67	10.345
L16	212.50	7.16	234.50	7.01	678.73	680.05	8.49
L17	124.15	7.40	240.50	6.83	678.98	626.73	11.59
L18	227.80	7.49	249.50	6.66	736.19	599.17	11.795
L19	292.50	7.42	233.00	7.04	679.55	800.85	11.91
L20	177.35	7.26	237.50	6.99	406.19	474.08	8.185
R1	455.50	7.33	231.00	7.44	646.00	628.55	9.745
R2	729.00	7.32	236.00	7.61	951.40	1238.07	20.005
R3	183.10	7.21	231.00	7.42	361.07	417.47	6.73
R4	311.00	7.24	236.00	7.35	259.28	370.39	3.53
R5	512.70	7.19	214.00	7.45	501.32	548.29	5.47
R6	315.00	7.15	217.00	7.56	522.14	827.90	10.195

R7	320.00	7.27	200.50	7.51	776.62	1526.51	29.06
R8	290.00	7.20	213.50	7.54	422.00	832.54	9.605
R9	193.15	7.01	206.00	7.54	572.71	802.94	13.02
R10	420.50	7.14	225.00	7.74	1015.60	1024.62	17.39
R11	405.00	7.40	228.50	7.54	699.52	559.29	6.8
R12	234.50	7.01	228.50	7.61	388.26	435.04	7.225
R13	183.85	7.69	225.00	7.45	626.12	291.90	7.545
R14	204.50	7.23	195.00	7.55	625.91	730.02	11.485
R15	375.00	7.25	225.50	7.57	584.47	1336.35	15.465
R16	532.00	7.23	222.50	7.49	690.36	921.63	20.315
R17	201.05	7.35	204.50	7.70	546.25	1130.00	11.755
R18	409.50	7.60	213.00	7.66	557.92	842.39	11.55
R19	167.55	7.19	211.00	7.47	296.39	335.36	5.425

Table S14 Relationship between P-PC values of antibiotics and physicochemical properties of the water phase and sediment phase in the river system.

Environmental factors	SDZ-P-PC	TMP-P-PC	SMM-P-PC	SMX-P-PC	NOR-P-PC	LEV-P-PC	FLU-P-PC	TC-P-PC	DC-P-PC	SUM-P-PC	
Water	pH	0.097	-0.675**	0.054	0.132	0.048	0.076	0.234	0.019	-0.407	-0.309
	ORP	-0.061	0.275	0.06	0.247	0.207	0.008	0.056	0.012	0.179	-0.074
	DO	-0.241	-0.514*	-0.043	-0.261	-0.072	-0.067	-0.17	0.061	-0.159	-0.144
	Ec	-0.116	0.529*	0.084	0.363	0.126	0.263	-0.187	-0.265	-0.231	-0.003
	T	0.124	-0.62**	-0.57*	-0.352	-0.001	-0.403	-0.205	-0.36	-0.225	-0.725***
	DOC	-0.03	-0.309	0.481*	0.447	0.142	0.72***	0.125	-0.049	-0.443	0.37
	NO ₂ -N	-0.182	0.21	-0.049	-0.198	-0.198	-0.066	-0.091	-0.256	0.569*	-0.088
	NO ₃ -N	0.21	0.629**	-0.115	-0.054	-0.222	0.008	-0.305	-0.021	0.608*	0.154
	NH ₄ -N	0.11	0.128	0.121	0.007	-0.421	0.034	0.025	-0.149	-0.231	0.104
	DIN	0.212	0.631**	-0.062	-0.054	-0.345	0.016	-0.266	-0.078	0.498	0.169
	TN	-0.072	0.602*	0.076	0.02	-0.186	0.061	0.057	-0.011	0.357	0.186
TP	0.482*	0.66**	0.232	0.029	-0.25	-0.012	0.016	0.611**	0.511*	0.502*	
COD _{Mn}	0.238	-0.3	0.075	0.196	-0.219	0.517*	-0.231	-0.202	-0.26	0.145	
Sediment	pH	-0.226	-0.027	0.162	-0.059	0.485*	0.196	0.344	0.052	-0.359	0.239
	ORP	0.065	0.025	0.022	-0.196	-0.061	0.213	-0.432	-0.019	0.139	0.264
	DO	-0.221	-0.021	0.053	-0.076	-0.173	-0.008	0.238	-0.213	-0.114	-0.03
	Ec	-0.435	0.597*	0.241	0.345	-0.006	0.203	-0.196	-0.045	0.053	0.388
	DOC	-0.173	0.228	0.062	0.128	-0.209	-0.107	0.233	-0.035	0.641**	-0.107
	TN	-0.468	0.125	0.161	0.089	0.547*	0.182	0.028	-0.103	0	0.288
	TP	-0.447	0.278	0.523*	0.307	0.118	0.440	0.481*	0.071	0.289	0.438
	SOC	-0.401	0.119	0.338	0.182	0.203	0.211	0.205	-0.057	0.293	0.255

Notes, ***: Significant correlation at the 0.001 level. **: Significant correlation at the 0.01 level. *: Significant correlation at the 0.05 level.

Table S15 Relationship between P-PC values of antibiotics and physicochemical properties of the water phase and sediment phase in the lake system.

Environmental factors	SDZ-P-PC	TMP-P-PC	SMM-P-PC	SMX-P-PC	NOR-P-PC	LEV-P-PC	FLU-P-PC	TC-P-PC	DC-P-PC	SUM-P-PC	
Water	pH	-0.046	0.053	0.052	-0.031	-0.023	-0.409	-0.162	0.093	-0.132	0.064
	ORP	0.206	-0.125	0.204	-0.172	-0.026	0.055	-0.196	-0.095	0.477	-0.292
	DO	-0.108	0.157	0.322	-0.027	0.023	-0.201	0.211	-0.017	-0.027	0.138
	EC	0.671**	-0.381	-0.246	-0.066	-0.163	-0.243	-0.382	-0.104	-0.347	-0.227
	T	0.049	-0.048	0.033	-0.257	-0.157	-0.612**	-0.312	0.005	0.154	-0.404
	DOC	-0.075	0.04	0.033	0.126	0.004	-0.038	0.037	-0.116	-0.438	0.212
	NO ₂ -N	0.592*	-0.521*	-0.147	-0.012	-0.079	-0.042	-0.198	-0.076	-0.29	-0.191
	NO ₃ -N	0.075	-0.511*	-0.243	-0.068	0.013	0.096	-0.302	0.159	0.034	-0.216
	NH ₄ -N	-0.105	0.152	-0.198	0.155	-0.157	-0.244	-0.26	0.152	-0.27	-0.13
	DIN	0.045	-0.406	-0.309	0.038	-0.085	-0.072	-0.399	0.165	-0.137	-0.253
	TN	0.088	-0.757**	-0.305	0.691***	-0.213	-0.202	-0.489*	-0.112	0.11	-0.252
	TP	0.692***	0.155	-0.05	0.13	-0.429	-0.384	0.313	-0.491*	-0.353	-0.32
COD _{Mn}	0.244	-0.447	-0.289	-0.382	-0.117	0.18	0.099	-0.09	0.479*	-0.303	
Sediment	pH	-0.305	0.446	0.109	0.036	-0.032	0.202	0.092	-0.055	-0.259	0.129
	ORP	0.419	0.233	0.125	0.153	0.028	-0.229	0.226	-0.096	-0.11	0.037
	DO	0.399	-0.574*	-0.223	-0.369	0.139	-0.022	-0.236	-0.151	0.127	-0.022
	Ec	-0.01	-0.458*	-0.116	0.084	0.253	0.33	-0.284	0.308	-0.286	0.304
	DOC	-0.025	0.221	-0.026	0.344	-0.036	-0.126	-0.416	-0.214	0.536*	-0.109
	TN	-0.246	-0.692**	-0.076	0.002	0.302	0.058	-0.532*	0.182	0.395	0.096
	TP	-0.265	-0.515*	-0.174	-0.125	0.098	0.118	-0.448*	0.295	0.064	-0.039
	SOC	-0.504*	-0.434*	0.09	-0.211	0.339	0.043	-0.376	0.387	0.044	0.144

Notes, ***: Significant correlation at the 0.001 level. **: Significant correlation at the 0.01 level. *: Significant correlation at the 0.05 level.

Table S16 Concentrations and spectral parameters of DOM in the water phase.

Sample	DOC (mg/L)	a (350)	Sr	SUVA ₂₅₄	BIX	HIX	FI	C1	C2	C3	C4	C5
L1	8.83	4.26	0.47	4.67	0.10	3.88	1.98	0.244	0.315	0.146	0.134	0.004
L2	7.95	2.99	0.50	4.40	0.10	3.61	1.97	0.185	0.239	0.266	0.167	0.117
L3	8.51	3.68	0.59	4.22	0.09	3.54	1.99	0.183	0.200	0.093	0.091	0.124
L4	6.46	3.68	0.50	5.25	0.13	3.39	1.97	0.239	0.274	0.262	0.107	0.102
L5	8.44	5.30	0.46	5.06	0.10	4.30	1.94	0.261	0.367	0.326	0.161	0.200
L6	6.31	3.57	0.50	5.45	0.07	3.32	1.98	0.344	0.370	0.288	0.092	0.007
L7	10.09	3.45	0.55	3.59	0.14	3.88	2.09	0.263	0.310	0.175	0.268	0.315
L8	11.46	3.11	0.52	3.10	0.10	3.58	1.94	0.392	0.485	0.573	0.091	0.347
L9	12.36	2.07	0.61	3.75	0.11	3.31	1.98	0.265	0.317	0.286	0.175	0.017
L10	12.08	3.45	0.54	2.71	0.11	3.50	2.00	0.285	0.325	0.378	0.090	0.126
L11	9.19	4.03	1.24	3.70	0.13	3.69	2.00	0.339	0.358	0.153	0.130	0.423
L12	13.71	4.03	0.51	3.87	0.09	3.84	1.96	0.305	0.283	0.168	0.122	0.175
L13	13.08	3.68	0.64	2.44	0.11	3.42	1.95	0.327	0.331	0.168	0.209	0.006
L14	7.11	2.76	0.57	4.51	0.18	3.76	1.97	0.354	0.341	0.190	0.119	0.036
L15	13.91	2.42	0.56	2.29	0.12	3.61	2.09	0.303	0.332	0.238	0.107	0.108
L16	10.29	3.22	0.69	3.19	0.13	3.62	1.98	0.427	0.382	0.115	0.142	0.322
L17	9.09	20.04	0.14	5.06	0.10	3.42	1.96	0.313	0.323	0.294	0.193	0.355
L18	11.36	2.42	0.64	3.42	0.14	3.18	1.91	0.352	0.346	0.141	0.134	0.048
L19	12.01	2.53	0.53	3.53	0.07	3.53	2.03	0.245	0.264	0.292	0.211	0.422
L20	8.55	3.92	0.69	4.16	0.07	3.27	1.96	0.404	0.459	0.428	0.184	0.231
R1	10.89	5.30	0.59	3.57	0.26	3.15	1.94	0.334	0.322	0.136	0.074	0.011
R2	9.15	3.45	0.50	3.80	0.21	2.96	2.11	0.296	0.314	0.150	0.092	0.059
R3	10.74	4.03	0.47	3.29	0.33	2.35	2.07	0.395	0.378	0.143	0.144	0.136
R4	5.80	3.68	0.51	5.60	0.42	2.25	2.16	0.306	0.337	0.316	0.132	0.348
R5	9.16	5.07	0.82	4.14	0.15	2.70	2.05	0.329	0.318	0.107	0.156	1.106
R6	9.75	4.72	0.53	4.18	0.10	4.99	1.95	0.364	0.308	0.219	0.236	0.217
R7	9.65	4.03	0.49	3.60	0.15	4.68	1.93	0.453	0.359	0.242	0.289	0.061
R8	8.76	5.76	0.48	4.84	0.03	4.57	1.93	0.189	0.237	0.394	0.062	0.111
R9	6.29	6.10	0.49	6.21	0.13	4.60	1.91	0.466	0.354	0.301	0.198	0.158
R10	12.41	5.64	0.47	3.36	0.22	4.62	1.95	0.316	0.339	0.220	0.102	0.408

R11	10.78	5.07	0.46	3.64	0.18	5.02	1.94	0.338	0.318	0.217	0.186	0.037
R12	10.29	4.61	0.50	4.37	0.18	5.00	1.97	0.205	0.269	0.309	0.090	0.272
R13	14.99	4.72	0.54	3.85	0.15	5.65	1.98	0.386	0.370	0.291	0.141	0.166
R14	12.17	5.53	0.47	4.02	0.19	4.65	1.90	0.613	0.494	0.359	0.364	0.292
R15	19.77	4.61	0.50	1.88	0.10	5.55	2.06	0.353	0.340	0.370	0.305	0.140
R16	12.03	2.30	0.63	2.63	0.15	3.24	2.12	0.334	0.313	0.210	0.522	0.007
R17	10.59	2.30	0.47	3.50	0.13	3.62	1.97	0.440	0.369	0.360	0.206	0.123
R18	10.22	2.42	0.54	3.97	0.06	3.82	1.99	0.359	0.361	0.428	0.095	0.024
R19	10.85	2.76	0.50	4.15	0.08	3.91	1.96	1.807	1.523	0.877	1.595	1.593

Table S17 Concentrations and spectral parameters of DOM in the sediment phase.

Sample	DOC (mg/L)	a (350)	Sr	SUVA ₂₅₄	BIX	HIX	FI	C1	C2	C3	C4	C5
L1	6.95	14.16	0.40	14.50	0.03	2.45	1.85	0.304	0.355	0.144	0.133	0.006
L2	13.45	12.32	0.29	6.95	0.13	1.82	1.95	0.298	0.359	0.114	0.184	0.000
L3	7.78	5.76	0.35	7.87	0.11	2.23	1.95	0.319	0.382	0.110	0.058	0.002
L4	16.95	4.38	0.38	3.60	0.05	1.96	2.04	0.313	0.351	0.199	0.059	0.005
L5	18.63	2.07	0.37	2.76	0.07	1.64	1.97	0.363	0.377	0.162	0.036	0.006
L6	9.38	3.45	0.35	5.82	0.09	2.05	1.88	0.397	0.397	0.087	0.043	0.006
L7	10.13	21.07	0.71	10.93	0.02	1.60	1.88	0.306	0.334	0.182	0.080	0.006
L8	13.83	15.20	0.48	7.62	0.01	1.27	1.96	0.304	0.347	0.181	0.059	0.008
L9	18.40	12.32	0.50	4.88	0.01	1.14	1.91	0.348	0.328	0.066	0.046	0.013
L10	15.38	24.76	0.52	9.57	0.00	1.87	1.80	0.339	0.355	0.192	0.047	0.006
L11	28.20	1.61	0.39	2.61	0.06	1.06	2.01	0.350	0.375	0.144	0.044	0.008
L12	18.73	2.99	0.40	2.59	0.09	1.49	2.03	0.332	0.357	0.137	0.043	0.008
L13	15.73	2.76	0.60	3.63	0.06	1.65	1.95	0.267	0.312	0.138	0.059	0.006
L14	20.63	2.42	0.26	2.41	0.08	2.00	1.99	0.252	0.290	0.175	0.058	0.008
L15	12.80	3.22	0.32	3.97	0.13	2.12	2.00	0.330	0.370	0.102	0.045	0.004
L16	26.98	3.92	0.34	3.12	0.10	2.29	2.03	0.302	0.337	0.162	0.052	0.005
L17	20.85	4.03	0.37	2.49	0.03	2.52	1.97	0.366	0.349	0.075	0.051	0.014
L18	14.93	2.99	0.34	3.21	0.09	2.36	2.05	0.385	0.359	0.071	0.049	0.014
L19	8.98	3.22	0.28	6.86	0.16	2.76	1.96	0.261	0.345	0.334	0.074	0.000
L20	4.03	5.53	0.41	14.20	0.04	2.83	1.77	0.342	0.359	0.130	0.045	0.003
R1	16.25	5.99	0.31	3.63	0.19	3.07	1.83	0.327	0.338	0.111	0.106	0.013
R2	10.23	7.14	0.34	8.96	0.64	2.49	1.95	0.291	0.302	0.092	0.144	0.111
R3	16.38	53.08	0.53	26.39	0.08	2.99	1.67	0.293	0.300	0.081	0.062	0.097
R4	9.93	4.61	0.30	5.45	0.44	2.21	1.92	0.296	0.304	0.072	0.070	0.017
R5	15.28	144.51	0.49	30.36	0.03	3.27	1.64	0.265	0.268	0.066	0.065	0.032
R6	12.80	10.02	0.40	11.07	0.20	3.44	1.81	0.153	0.242	0.187	0.073	0.105
R7	32.85	7.25	0.28	2.24	0.48	5.36	1.90	0.250	0.253	0.090	0.047	0.057
R8	15.31	20.73	0.41	17.34	0.14	2.84	1.68	0.296	0.307	0.243	0.093	0.247
R9	9.05	7.48	0.34	13.45	0.07	4.39	1.72	0.257	0.280	0.092	0.173	0.023
R10	10.45	10.48	0.32	17.70	0.29	4.84	1.83	0.264	0.315	0.138	0.051	0.051

R11	9.00	4.84	0.29	8.38	0.21	3.82	1.78	0.284	0.292	0.061	0.061	0.053
R12	3.72	5.41	0.35	15.20	0.20	3.15	1.81	0.288	0.289	0.059	0.051	0.121
R13	13.54	5.64	0.35	6.59	0.07	2.92	1.86	0.315	0.308	0.057	0.049	0.035
R14	6.27	5.41	0.21	10.89	0.16	3.42	1.82	0.273	0.307	0.315	0.057	0.016
R15	10.83	5.53	0.35	8.26	0.20	4.69	1.85	0.289	0.282	0.060	0.051	0.130
R16	15.50	9.21	0.31	6.37	0.23	4.23	1.89	0.249	0.253	0.069	0.046	0.048
R17	9.34	4.49	0.34	8.55	0.18	4.49	1.80	0.258	0.261	0.071	0.050	0.071
R18	23.33	7.14	0.32	7.36	0.24	2.63	1.86	0.263	0.258	0.072	0.059	0.045
R19	6.17	17.27	0.49	16.58	0.09	2.47	1.62	0.252	0.254	0.051	0.039	0.053

Table S18 List of accepted daily intake (ADI, $\mu\text{g}/\text{kg}$ bw/day) values for antibiotics.

Antibiotic	ADI ^a	Reference
SDZ	20	(Leung et al., 2013)
STZ	50	(Schwab et al., 2005)
TMP	4.2	(Schwab et al., 2005)
SPD	50	(de Jesus Gaffney et al., 2015)
SDD	1.6	(Leung et al., 2013)
SCP	50	(Li et al., 2018a)
SMX	130	(Schwab et al., 2005)
NOR	190	(Schwab et al., 2005)
CIP	1.6	(Schwab et al., 2005)
OTC	30	(Schwab et al., 2005)
TC	30	(Schwab et al., 2005)
CTM	0.2	(Leung et al., 2013)
ROX	0.4	(Leung et al., 2013)
TYL	0.85	(Leung et al., 2013)
LIN	25	(Schwab et al., 2005)

of antibiotics were assumed to be identical. Values of isomers were assumed to be identical.

^a Values of hydrous and anhydrous forms

Table S19 Selected age groups and respective median body weights and drinking water intakes (DWI, L/day).

Age groups	Body weight (kg)	DWI (L/day)
0-3 months	5.6	1.15
3-6 months	7.2	1.14
6-12 months	9.4	1.18
1-2 years	12	0.85
2-3 years	13.8	0.83
3-6 years	19	1.16
6-11 years	36	1.55
11-16 years	56	1.90
16-18 years	57	1.77
Adult (≥ 18 years)	60	2.04

Supplemental Figures

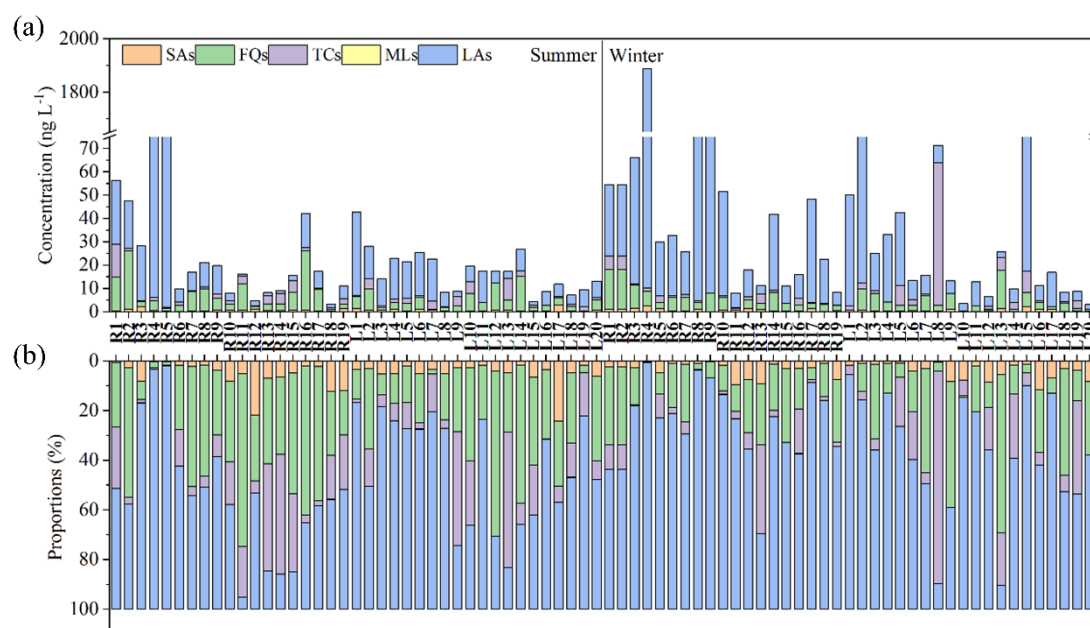


Fig. S1 Occurrence and structural composition of antibiotics in the water phase from various sampling sites.

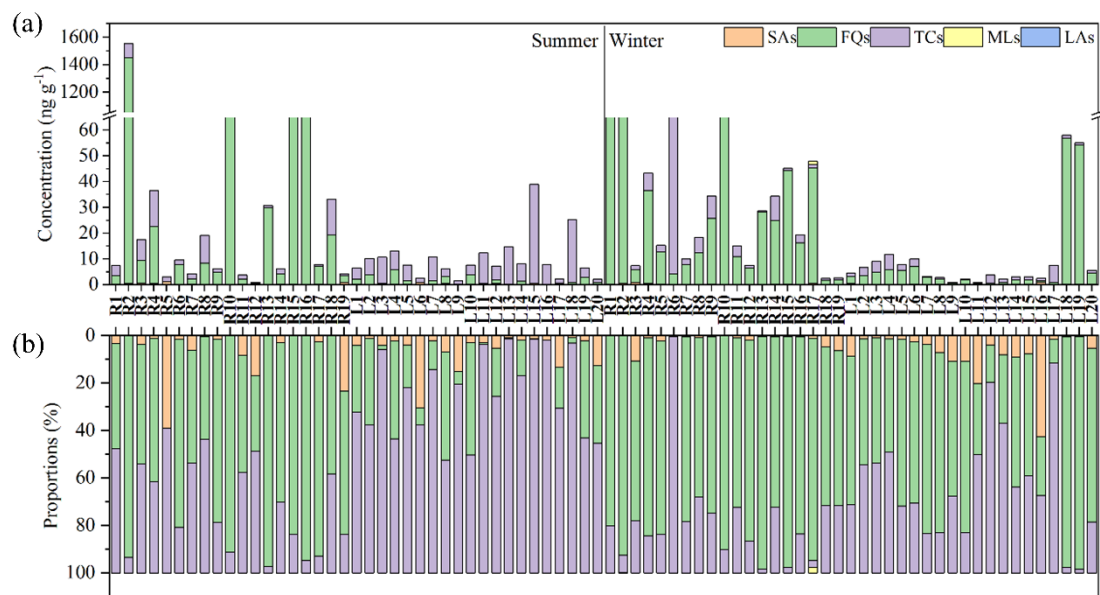


Fig. S2 Occurrence and structural composition of antibiotics in the sediment phase from various sampling sites.

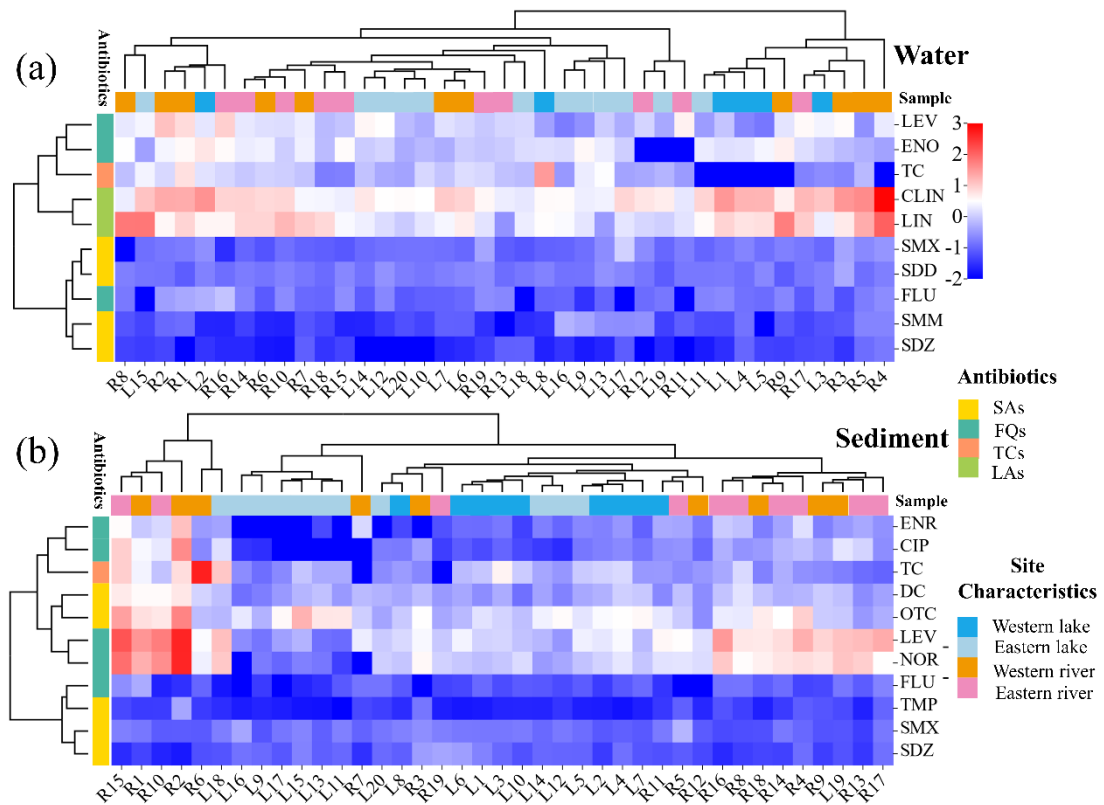


Fig. S3 Heatmap of antibiotics clustered by concentration profiles in the water phase (a) and sediment phase (b). Among the 32 antibiotics, only high-frequency detected antibiotics (detection frequency >80.0%) were included in the heat map analysis. (Abbreviations: SAs: sulfonamides; FQs: fluoroquinolones; TCs: tetracyclines; LAs: lincosamides).

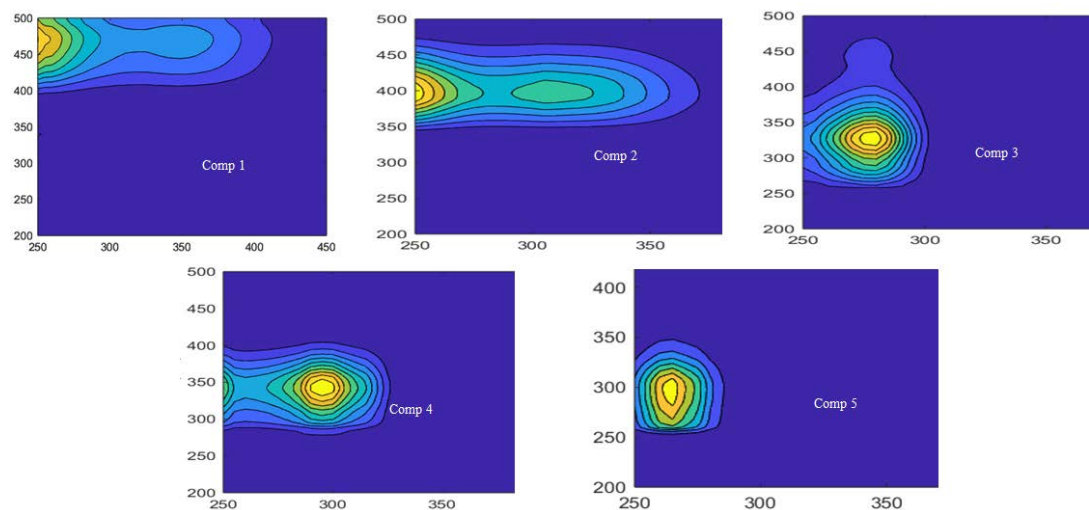


Fig. S4 Five DOM fluorescence fractions were derived from EEM-PARAFAC analysis in the Chaohu basin, including terrestrial humic fluorescence fraction (C1), microbial source humic fluorescence fraction (C2), tryptophan-like fluorescence fraction (C3), protein-like fluorescence fraction (C4), and tyrosine-like fluorescence fraction (C5).

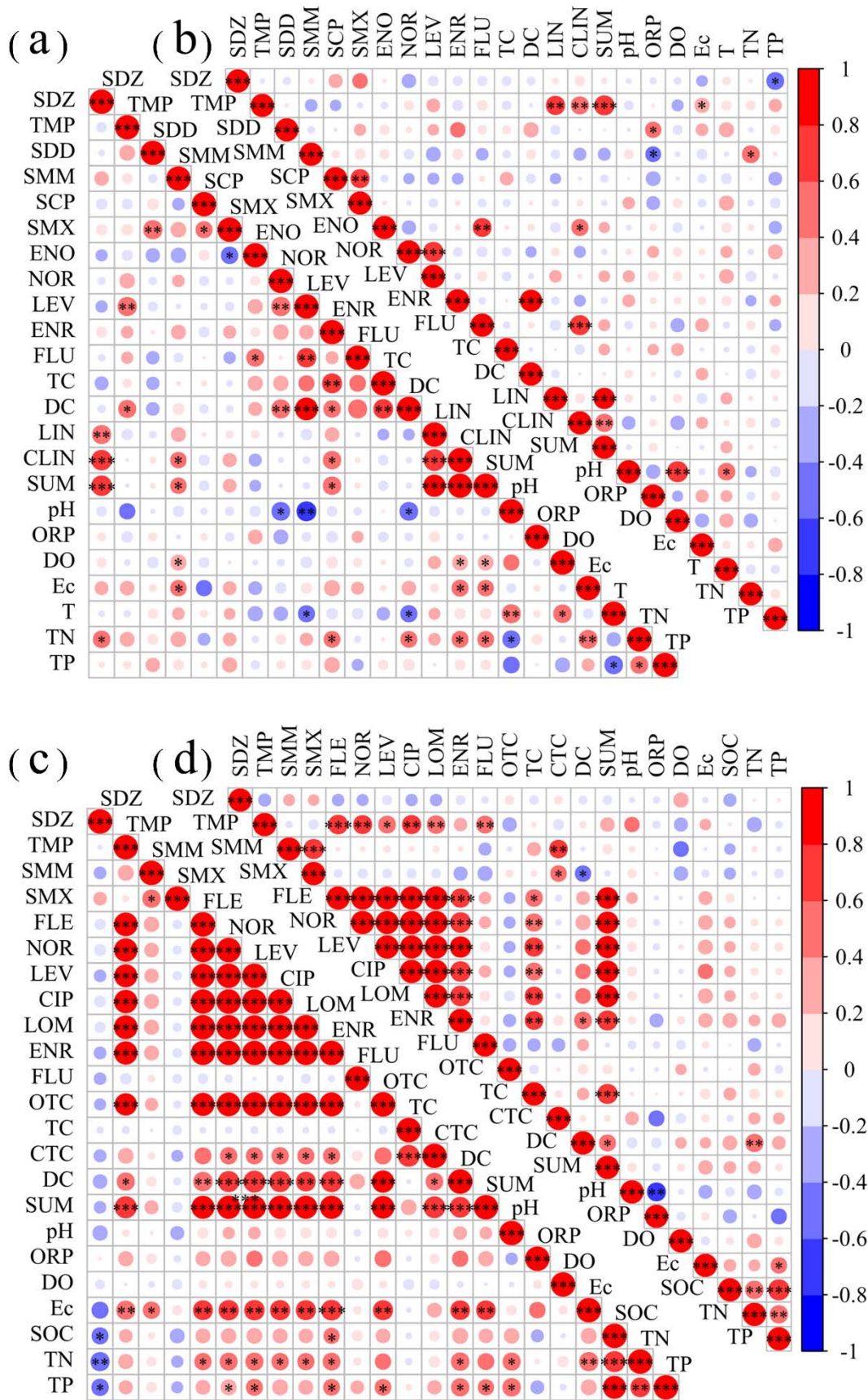


Fig. S5 Correlation analysis of antibiotic concentrations and environmental factors in the waters ((a) river system; (b) lake system) and sediments ((c) river system; (d) lake system) of the Chaohu basin. Antibiotics with low detection (<50.0%) were excluded. *: $P < 0.05$; **: $P < 0.01$; ***: $P < 0.001$.

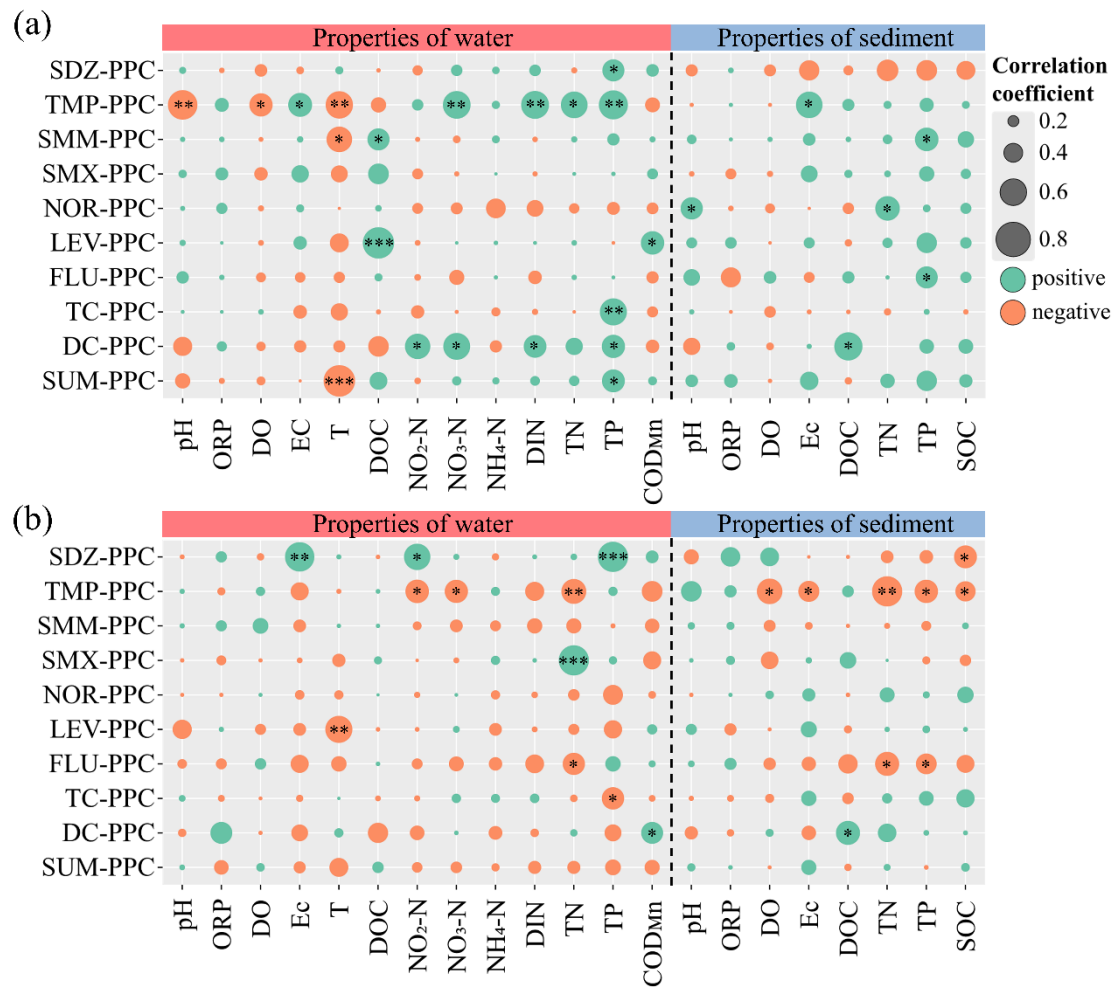


Fig. S6 Correlation of P-PC values with environment indicators of the water phase and sediment phase in the river system (a) and lake system (b). The large circle represents the large correlation and vice versa. *: $P < 0.05$; **: $P < 0.01$; ***: $P < 0.001$.

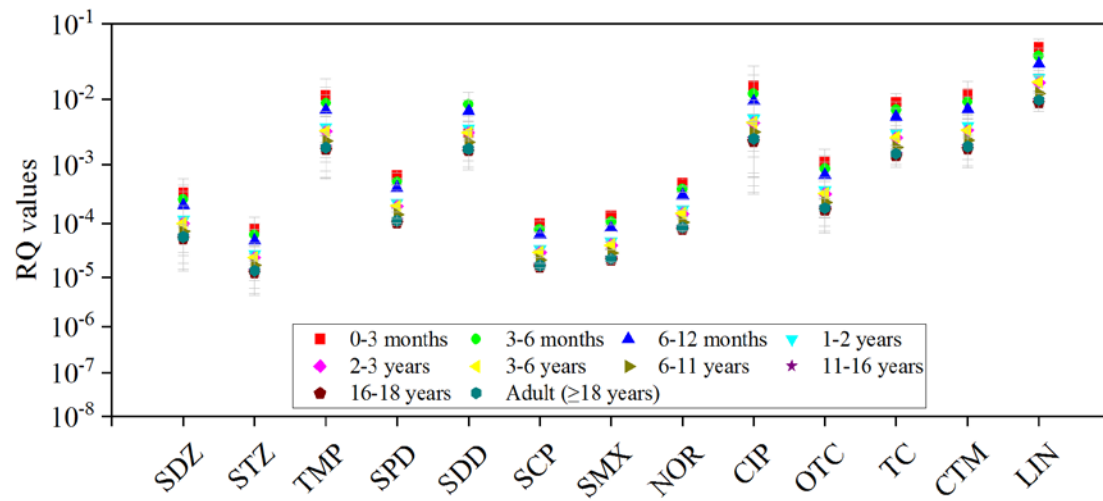


Fig. S7 Risk quotients (RQs) of selected antibiotics for human health in the water phase.

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