Supporting Information:

A comprehensive evaluation of antibiotics emission and fate in the river basins of China: Source analysis, multimedia modelling, and linkage to bacterial resistance

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Number of pages: 60

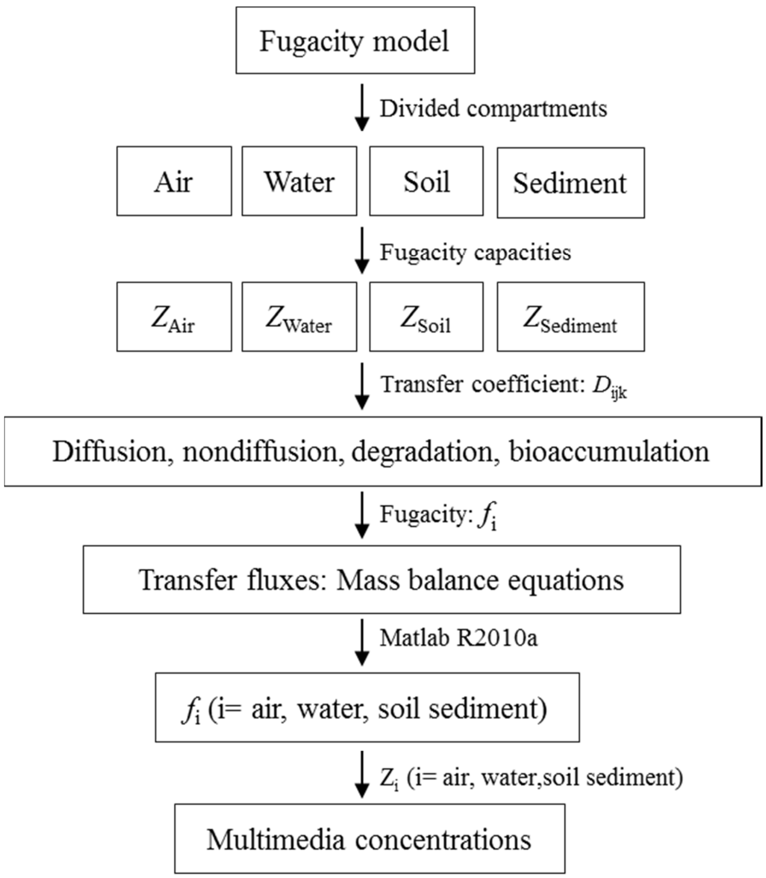
Number of texts: 5

Number of figures: 5

Number of tables: 10

Multimedia model description

Flow chart of the multimedia model



Mass balance equations for Level III fugacity model

For steady-state conditions the total input fluxes from the individual compartment equal to the output flux, and the equation is a simple algebraic expression. The mass balance equations were established in terms of transfer fluxes for the 4 bulk compartments of air, water, soil and sediment, respectively:

$$T_{01t} + T_{21d} + T_{31d} = T_{10t} + T_{12d} + T_{12p} + T_{12w} + T_{13d} + T_{13p} + T_{13w} + T_{10m},$$

$$T_{02t} + T_{02h} + T_{02p} + T_{12d} + T_{12p} + T_{12w} + T_{32e} + T_{32l} + T_{42d} + T_{42r} = T_{20t} + T_{21d} + T_{24d} + T_{24s} + T_{20m} + T_{2f},$$

$T_{13d} + T_{13p} + T_{13w} + T_{23h} + T_{03p} + T_{03c} + T_{03o} = T_{30m} + T_{31d} + T_{32e} + T_{321}$,

$T_{24d} + T_{24s} = T_{40m} + T_{42d} + T_{42r}$,

The definition of the transfer processes and their relationship between various parameters are listed in Table S3. The model was performed by using Matlab R2010a.

Parameters

(1). A nonequilibrium and steady-state model and expressions used in the study are described for emissions, advective flows, degrading reactions, and interphase transport by diffusive and nondiffusive processes. The input parameters to the model consist of a description of the environment (such as area of the water, soil and sediment), the physical-chemical (such as organic carbon normalized partition coefficients, *K*oc) and reaction properties (such as coefficients of degradation rate in water, soil and sediment) of the chemical and emission rates (such as antibiotic emissions by human and animal, T_{02h}, T_{02p}, T_{23h}, T_{03p}, T_{03c}, T_{03o}).

(2). The parameters collected used for modelling are listed in Table S4-S6. Some of the environmental parameters were taken from the default value of Mackay and Paterson [1], and applied to all 58 Basins. Parameters about physical and chemical properties of those target chemicals were also applied to all the Basins. The rest of parameters, such as water area, depth and organic carbon content of each media, were the site-specific data from the published papers or reports. When there were more than one value available (n > 1), arithmetic or geometric mean and standard deviations were computed. For the log-normal distribution, geometric means were used as input; for the normal distribution, arithmetic mean values were selected.

For the advective flows in the area through water (T_{02t}), we have made the following assumptions: 1). Since we have chosen the independent secondary basins in China, it is assumed that there will be no advective flows for each basin. 2). For some first level basins in China, including Heilongjiang

(ID: 1), Yellow River (ID: 18), Yangtze River Upstream (ID: 25), Yangtze River Downstream (ID: 26), the Pearl River Delta (ID: 43), they receive chemicals from output flux of their corresponding secondary basins. In details, ID 1 receives the input flux from Basins ID 2 and 3; ID 18 receives the input flux from Basins ID 19 and 20; ID 25 receives the input flux from Basins ID 27, 28, 29 and 30; ID 26 receives the input flux from Basins ID 31, 32 and 33; ID 43 receives the input flux from Basins ID 40, 41 and 42.

Mass inventory

The mass inventories in air, water, soil and sediment were calculated based on the collected river basin data sets and the corresponding predicted concentrations, by using the following equations:

$I_a = C_1 \times A_1 \times h_1 \times 10^{-9}$, $I_w = C_2 \times A_2 \times h_2 \times 10^{-9}$, $I_{so} = C_3 \times A_3 \times h_3 \times \rho_{33} \times 10^{-6}$, $I_{se} = C_4 \times A_4 \times h_4 \times \rho_{43} \times 10^{-6}$,

Where I_a, I_w, I_{so} and I_{se} are the mass inventories of TCS in the compartments of air, water, soil and sediment, with the unit of kg, respectively; C_1 and C_2 are the predicted concentration of a chemical in air and water, with the unit of ng/L, respectively; C_{so} and C_{se} are the predicted concentrations in soil and sediment with the unit of ng/g, respectively; A_1, A_2, A_3, and A_4 is the area of air, water, soil and sediment respectively, with the unit of m^2. In reality, the area of sediment is equal to the area of water (A_2), and the area of air equal to the sum of the area of water (A_2) and soil (A_3); h_1, h_2, h_3 and h_4 are the average depth of air, water, soil and sediment, respectively, with the unit of m; ρ_{33} is the soil density and ρ_{43} is sediment density, and both with the unit of t/m^3. All the parameters used to solving the equations can be found in Table S4-S6.

Uncertainty analysis

Pori to the uncertainty analysis, a sensitivity analysis was performed firstly. The sensitivity of various input parameters in the model are tested by comparing predicted results without any changed variable with those having only one variable changed by ±10%, expressed as sensitivity coefficient (C_S). Those sensitive parameters were subject to uncertainty analysis. Uncertainty analysis is concerned with propagation of the various sources of uncertainty to the model output. Monte Carlo simulation was used in quantitative predictions. In the analysis, probability distributions for input parameters were used to replace discrete values, by randomly selecting values from each input parameter distribution. The simulation was run for 500 times using a build-in function of "randn" in Matlab. Difference between the third and the first quartiles (Abbreviated as SQR), based on statistics from the repeated output, was used to quantify the uncertainties.

Standard deviations (SDs) are an important part of uncertainty analysis as they were used in the function of "randn". Table S10 displayed all the standard deviations used in the model. If only a single value was found (n = 1) for a certain parameter, a standard deviation was derived from an artificially assigned coefficient of variation (CV) as follows:

1) There was no available value about densities of solids in water, soil and sediment and fish, the CV was same as the corresponding values of Dongjiang River watershed. ρ_{12} was 58%, ρ_{22} was 47%, ρ_{32} was 58%, ρ_{f} was 20%;
2) For the physical and chemical properties of the target chemicals, 100% was adopted if only a value was calculated using EPI;
3) B_4 is associated with surface sediment porosity. As the investigated data for the all Basin sediment porosity was 55-75% and an average level was 65%. And the corresponding result for the B_4 was 16%. And 16% was also adopted for CV of K_{24};
4) As the CVs for advection water flow (Q_{20t}) of Chaobaihe (73%), Dongjiang (54%), Pearl River Delta (79%), Hainan (26%), Yueguiqiong (13%), Yuanjiang (97%) and Irtysh River (18%) were available, the average CVs for all the other Basins are 51%.
5) As the water area (A_2) is affected by both advection water flow and water depth, the CV

was a larger value among them. And the same for the soil area (A_3).

6) 84% was selected for CVs of K_r based on the observed CV of K_S (84%) in Dongjiang River. And all the other basins are with the same value.
7) Without relevant information, 100% was used conservatively for A_{32}, Y_f, L_4, and X_{2f} and antibiotics emissions from human, pig, chicken and other animals.

The uncertainty analysis result (Figure S4) was discussed in terms of the uncertainty of predicted concentration in water compartment as an example.

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Figure captions:

Figure S1 Flow chart of market survey for antibiotics usage.

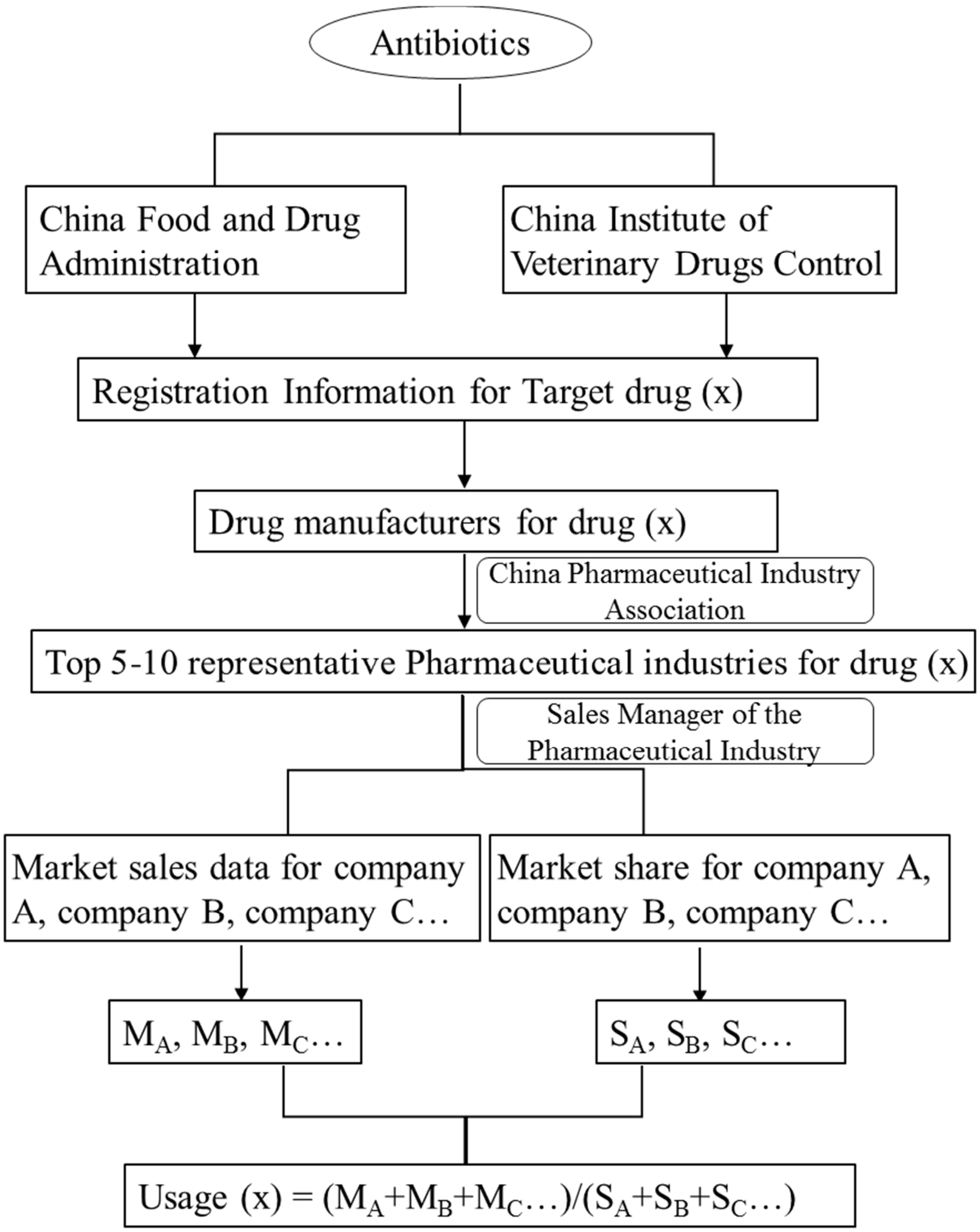
Figure S2 Average contribution of each transport flux to the total input or output fluxes in air, water, soil and sediment compartments. The left bar of each chemical category represents the input fluxes and the right bar denotes the output fluxes. The transfer processes defined in the model are listed in Table S3.

Figure S3 Distribution of the seven categories of antibiotics in the environmental compartments in terms of mass inventory.

Figure S4 Uncertainty analysis for modelling concentrations in water compartment for 36 target chemicals in all the 58 basins. The SQR was result of the difference between the log-transfer first and the third quartiles. The horizontal lines represent 10^{th} and 90^{th} percentiles, and the boxes represent 25^{th} and 75^{th} percentiles, while outliers are shown as individual points. Median concentrations are shown as solid horizontal lines.

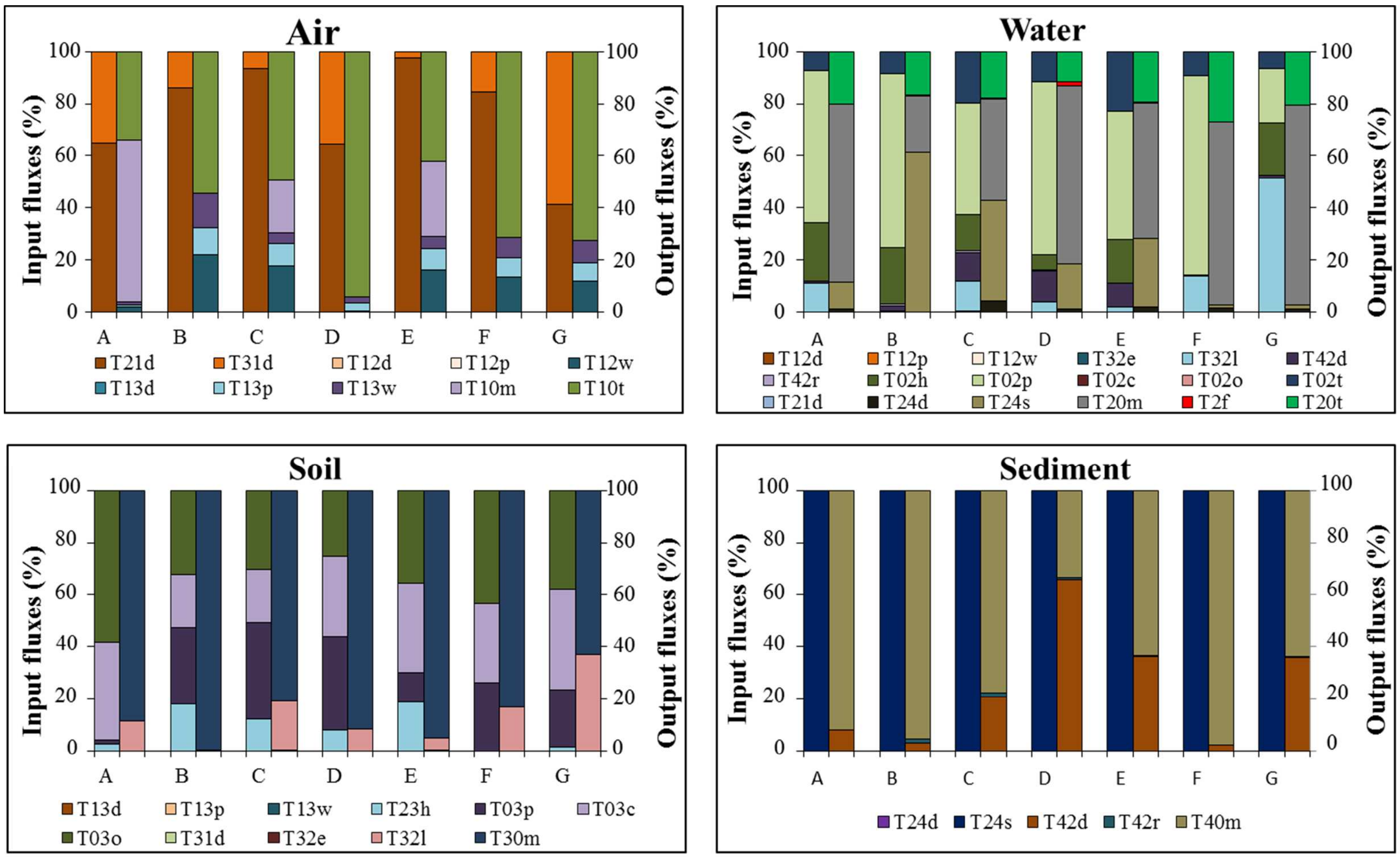
Figure S5 Redundancy analysis (RDA) ordination plots showing relations of bacterial resistance to seven respective antibiotics in hospitals and rivers (A), and the relations between hospital bacterial resistance rates and antibiotic usages (B). Those hospital bacterial resistance rates were in the year of 2011 (A) and 2008 (B). In the graph A, the blue lines and red lines represent the resistance to *Escherichia coli* in the hospitals and rivers; empty circle symbols 1, 2, 3, 4 and 5 represent the Pear River, Dongjiang River, Haihe River, Liaohe River and Yellow River, respectively. Accordingly, the bacterial resistance data in the hospitals are selected from the city hospitals where these rivers flow through. The RDA 1 and RDA 2 explained 60.8% and 36.5% of the total variance, respectively. In the graph B, the bacterial resistance data for three bacterial species in the hospitals (blue line), antibiotics usage data including DIDs (defined daily doses per 1000 inhabitants per day) and regional total usages, and environmental concentrations (PECs) (red line) are available for two respective antibiotics (CFX: ciprofloxacin, SMX: sulfamethoxazole/trimethoprim). Empty circle symbols represent the six regions of China. The RDA 1and RDA 2 explained 83.6% and 8.7% of the total variance, respectively. Abbreviations: CFX: ciprofloxacin; SMX: sulfamethoxazole/trimethoprim; CAZ: ceftazidime; AMP: ampicillin; PRL: piperacillin; CN: gentamicin; KZ: cephazolin.

Figure S1



Antibiotics
China Food and Drug Administration
China Institute of Veterinary Drugs Control
Registration Information for Target drug (x)
Drug manufacturers for drug (x)
China Pharmaceutical Industry Association
Top 5-10 representative Pharmaceutical industries for drug (x)
Sales Manager of the Pharmaceutical Industry
Market sales data for company A, company B, company C…
Market share for company A, company B, company C…
M_A, M_B, M_C…
S_A, S_B, S_C…
Usage (x) = (M_A+M_B+M_C…)/(S_A+S_B+S_C…)

Figure S2



A: Sulfonamides B:Tetracyclines C: Fluoroquinolones D: Macrolides E: β-Lactams F: Chloramphenicols G: Lincomycin

Figure S3

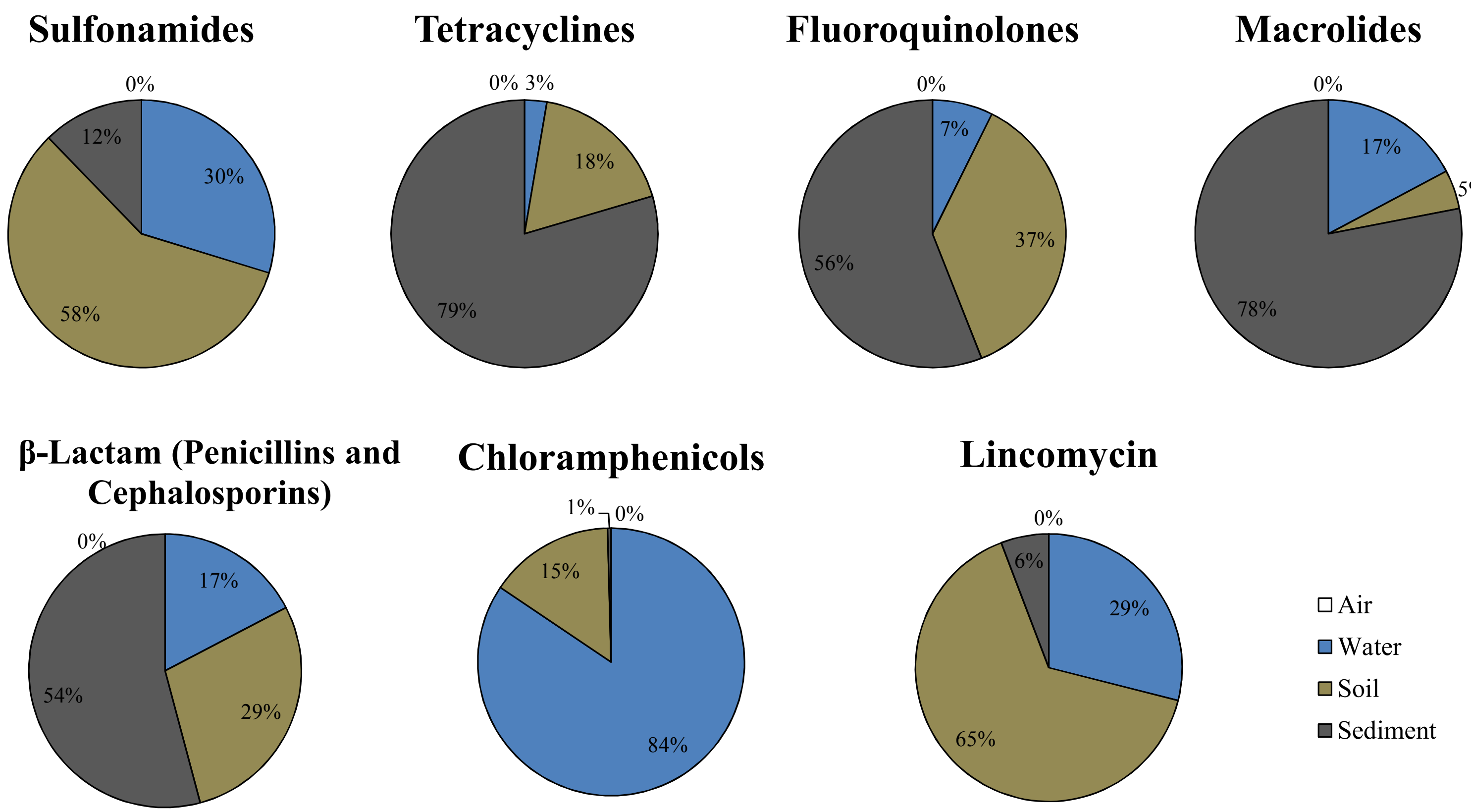
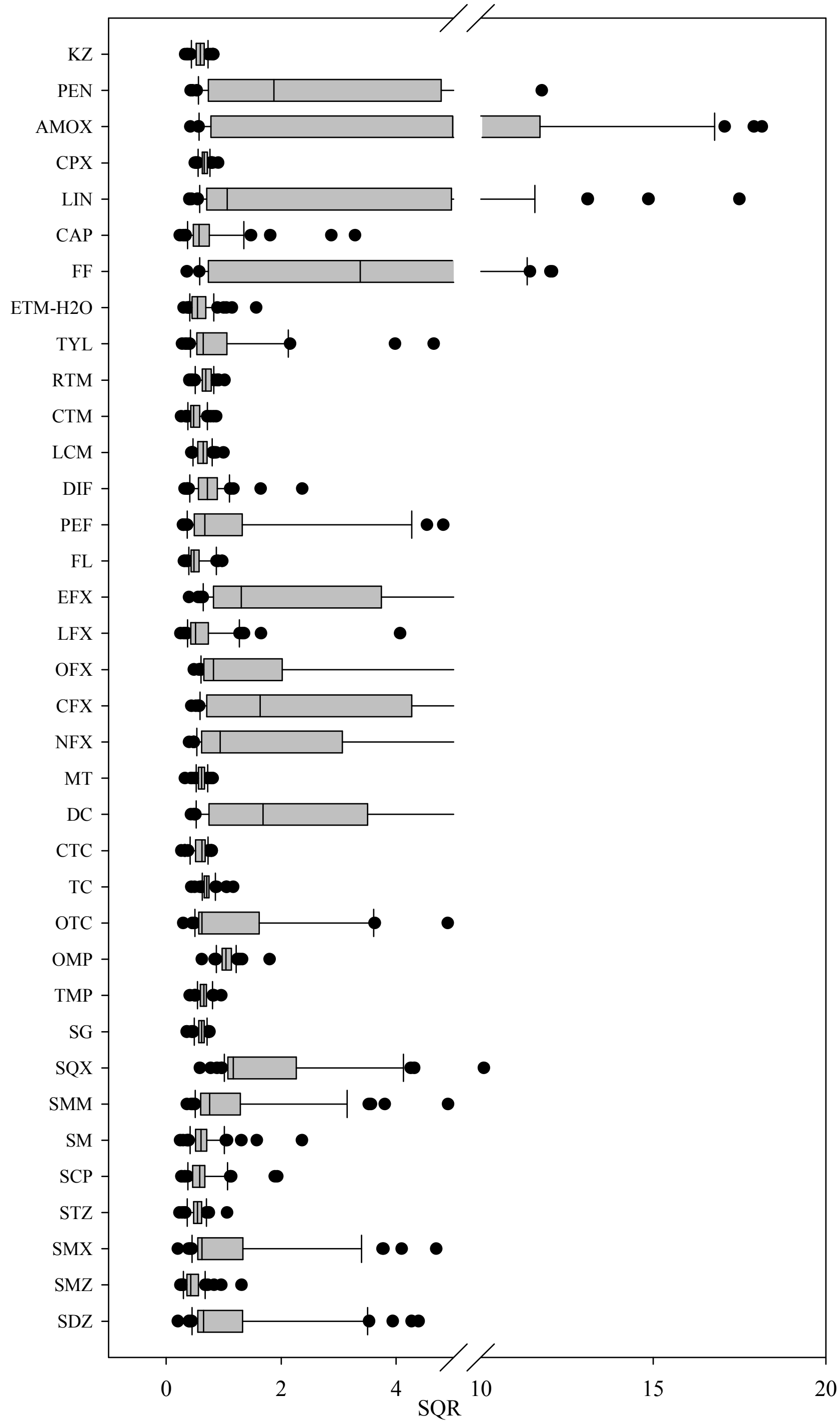

Sulfonamides
0%
12%
30%
58%
Tetracyclines
0% 3%
18%
79%
Fluoroquinolones
0%
7%
37%
56%
Macrolides
0%
17%
5%
78%
β-Lactam (Penicillins and Cephalosporins)
0%
17%
29%
54%
Chloramphenicols
1%
0%
15%
84%
Lincomycin
0%
6%
29%
65%
Air
Water
Soil
Sediment

Figure S4


KZ
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AMOX
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OFX
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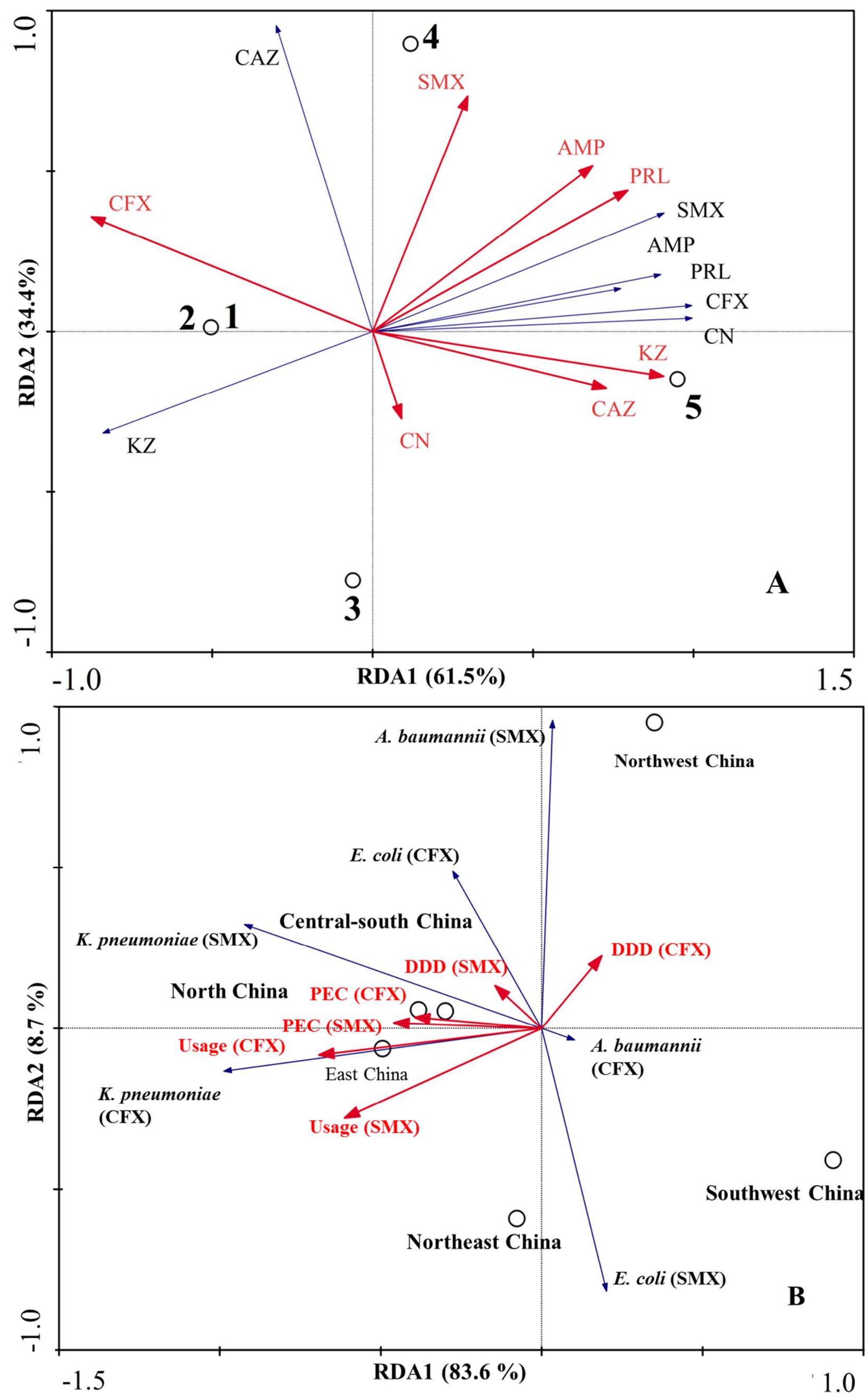
Figure S5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2
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KZ
CAZ
5
CN
KZ
3
A
1.0
-1.0
-1.0
1.5
RDA1 (61.5%)
RDA2 (34.4%)
A. baumannii (SMX)
Northwest China
E. coli (CFX)
Central-south China
K. pneumoniae (SMX)
DDD (CFX)
DDD (SMX)
North China
PEC (CFX)
PEC (SMX)
Usage (CFX)
A. baumannii
(CFX)
East China
K. pneumoniae
(CFX)
Usage (SMX)
Southwest China
Northeast China
E. coli (SMX)
B
1.0
-1.0
-1.5
1.0
RDA1 (83.6 %)
RDA2 (8.7 %)

Table S1 Basin information and populations for seven regions of China. [1]

Region	Province	Area (km^2)	GDP (billion yuan)	Populations (×10000)			
				Human	pig	Chicken	Others [a]
East China	Shanghai	8239	2018	2380	179	3650	17
	Jiangsu	106742	5406	7920	1787	12265	356
	Zhejiang	105397	3467	5477	1405	10348	111
	Anhui	140126	1721	5988	1812	33319	240
	Fujian	124016	1970	3748	1296	9938	86
	Jiangxi	166894	1295	4504	1912	20002	250
	Shandong	157126	5001	9685	3757	74667	256
	Total	808540	20878	39702	12149	164190	1318
Central China	Henan	165536	2960	9406	4777	67744	177
	Hubei	185888	2225	5779	4174	72936	416
	Hunan	211855	2215	6639	4872	41650	249
	Total	1819856	36545	79463	32937	451127	2752
South China	Guangdong	179813	5707	10594	2257	35605	365
	Guangxi	237558	1304	4682	2467	45333	156
	Hainan	35354	286	887	439	9944	44
	Total	2835860	51241	117450	51921	724340	4158
North China	Beijing	16411	1788	2069	187	2596	9
	Tianjin	11917	1289	1413	194	8896	37
	Hebei	188434	2658	7288	2651	58520	137
	Shanxi	156711	1211	3611	664	9391	15
	Inner Mongolia	1145121	1588	2490	694	4305	153
	Total	4389808	60061	135207	56749	817992	4552
Northwest China	Shaanxi	205795	1445	3753	1442	8319	25
	Gansu	404091	565	2578	591	4129	34
	Qinghai	717481	189	573	117	342	20
	Ningxia	51954	234	647	52	918	29
	Xinjiang	1664897	751	2233	361	2000	96
	Total	8579147	64833	147480	60006	838005	4909
Northeast China	Liaoning	148064	2485	4389	1593	27500	140
	Jilin	191124	1193.924	2750	1001	15000	67
	Heilongjiang	452645	1369.158	3834	1382	15000	97
	Total	11805311	71055	161907	64511	898765	5360
Southwest China	Chongqing	82269	1141	2945	1524	6850	43
	Sichuan	484056	2387	8076	5132	25007	172
	Guizhou	176152	685	3484	1604	9632	30
	Yunnan	383194	1031	4659	2709	3775	86
	Xizang	1202072	70.1	308	34	68	24
	Total	14585699	77739	185213	76896	959097	5811

a: the total weight for meat of sheep, cow and fish, with the unit of 10000 tons.

1. NBSC (National Bureau of Statistics of China), The sixth nationwide population census bulletin in 2010 in China. In National Bureau of Statistics of China, 2011; http://www.stats.gov.cn/tjsj/pcsj/rkpc/6rp/indexch.htm.

Table S2 Reported fraction data of the unchanged form and glucuronide conjugates for each antibiotic excreted by human (A), pig (B) and chicken (C).

A. Human

Substance	Excretion rate via urine/feces/bile (%)			References
	Unchanged	Glucuronide	Total	
SDZ	52.3 (30-78) [a]	-	52.3 (30-78)	2-4
SMZ	65.9 (41.7-77.5)	-	65.9 (41.7-77.5)	4-6
SMX	15.2 (9.7-20)	12.3 (9.66-15)	15.2 (9.7-20)	7-12
STZ	51.34 [b]	-	51.34	
SCP	-	-	-	
SM	51.34	-	51.34	
SMM	10 (8-12)	40.5 (12-69)	10 (8-12)	13, 14
SQX	-	-	-	
SG	51.34	-	51.34	
TMP	60.5 (40-80)	-	60.5 (40-80)	7-9, 15-19
OMP	-	-	-	
OTC	66.7 (50-80)	-	66.7 (50-80)	9, 20, 21
TC	57.9 (36.9-90)	-	57.9 (36.9-90)	9, 20, 22, 23
CTC	46 (18-70)	-	46 (18-70)	9, 20, 21
DC	47	24	47	7, 9, 23
MT	36.5 (20.2-47.3)	-	36.5 (20.2-47.3)	4, 20, 22, 24, 25
NFX	61.5	-	61.5	10, 15, 24, 25
CFX	53.8 (29.5-83.7)	-	53.8 (29.5-83.7)	7, 10, 15, 26-34
OFX	75.8 (70-82)	24.2	75.8 (70-82)	7, 30, 32, 35
LFX	71 (60-80)	-	71 (60-80)	4, 36
EFX	-	-	-	
FL	76.0 (67.1-86)	-	76.0 (67.1-86)	4, 37, 38
PEF	10.6 (9.3-13.2)	-	10.6 (9.3-13.2)	25, 31, 37
DIF	75	-	75	39
LCM	7.64-11.54		7.64-11.54	40
CTM	33.7 (14.4-60)	-	33.7 (14.4-60)	4, 7, 9, 15, 41-44
RTM	66.7 (57-74.5)	-	66.7 (57-74.5)	4, 9, 15, 18, 45
TYL	-	-	-	
ETM-H_2O	35 (3.5-98)	-	35 (3.5-98)	4, 9, 10, 15, 41, 46
FF	-	-	-	
CAP	10.1 (8-15)	83.3	10.1 (8-15)	4, 9, 47
LIN	51 (49-53)	-	51 (49-53)	4
CPX	91	-	91	4
AMOX	70 (60-85)	-	70 (60-85)	4, 9, 10, 15
PEN	50 (40-70)	-	50 (40-70)	4, 9
KZ	91	-	91	4

B. Pig

Substance	Excretion rate via urine/feces/bile (%)					Ref.
	Unchanged		Glucuronide	Total		
	Urine	feces	-	Urine	feces	
SDZ	42.4	1.6	-	42.4	1.6	3
SMZ	24.5	0.9	-	24.5	0.9	48
SMX	19.9	0.9	81.5	99.0	0.9	49
STZ	88.1	3.4	-	88.1	3.4	50

Substance	Excretion rate via urine/feces/bile (%)					Ref.
	Unchanged		Glucuronide	Total		
	Urine	feces	-	Urine	feces	
SCP	35.3	1.4	-	35.3	1.4	
SM	35.3	1.4	-	35.3	1.4	
SMM	4.6	0.2	-	4.6	0.2	51
SQX	35.6	1.4	-	35.6	1.4	
SG	35.6	1.4	-	35.6	1.4	
TMP	32.3 (13.1-70)	1.2	-	32.3 (13.1-70)	1.2	49
OMP	34.7	1.3	-	34.7	1.3	
OTC	59 (42-75)	28.1	-	59 (42-75)	28.1	52, 53
TC	~52.5	25.0	-	~52.5	25.0	54
CTC	55.8	26.5	-	55.8	26.5	
DC	55.8	26.5	-	55.8	26.5	
MT	55.8	26.5	-	55.8	26.5	
NFX	30.0	27.5	-	30.0	27.5	55
CFX	36.8 (26.2-53.1)	33.7	-	36.8 (26.2-53.1)	33.7	56
OFX	27.8	25.5	-	27.8	25.5	
LFX	27.8	25.5	-	27.8	25.5	
EFX	21.0	19.2	-	21.0	19.2	57
FL	27.8	25.5	-	27.8	25.5	
PEF	27.8	25.5	-	27.8	25.5	
DIF	23.6	67.4	-	23.6	67.4	58
LCM	3.5	5.0	-	3.5	5.0	
CTM	12.1	17.5	-	12.1	17.5	
RTM	24.0	34.7	-	24.0	34.7	
TYL	0.4	38.6	-	0.4	38.6	59
ETM-H_2O	12.6	18.2	-	12.6	18.2	
FF	47.5	15.0	-	47.5	15.0	60
CAP	26.5	40.6	-	26.5	40.6	
LIN	5.5	15.1	0.9	5.5	16.0	61
CPX	91.0 [c]		-	91.0	0.0	
AMOX	65.0	10.0	-	65.0	10.0	10
PEN	50.0	7.7	-	50.0	7.7	
KZ	91.0		-	91.0	0.0	

C. Chicken

Substance	Excretion rate via urine/feces/bile (%)			Ref.
	Unchanged	Glucuronide	Total	
SDZ	28.8	-	28.8	
SMZ	13.9	-	13.9	62
SMX	28.8	-	28.8	
STZ	28.8	-	28.8	
SCP	28.8	-	28.8	
SM	28.8	-	28.8	
SMM	20	-	20	62
SQX	28.8	-	28.8	
SG	28.8	-	28.8	
TMP	28.8	-	28.8	
OMP	28.8	-	28.8	
OTC	52.5	-	52.5	

Substance	Excretion rate via urine/feces/bile (%)			Ref.
	Unchanged	Glucuronide	Total	
TC	52.5	-	52.5	54
CTC	52.5	-	52.5	
DC	52.5	-	52.5	
MT	52.5	-	52.5	
NFX	53	-	53	
CFX	53	-	53	
OFX	53	-	53	
LFX	53	-	53	
EFX	53	-	53	63
FL	53	-	53	
PEF	53	-	53	
DIF	53	-	53	
LCM	67	-	67	
CTM	67	-	67	
RTM	67	-	67	
TYL	67	-	67	54
ETM-H_2O	67	-	67	
FF	42	-	42	64
CAP	54.1	-	54.1	
LIN	66.2	-	66.2	61
CPX	91	-	91	
AMOX	70	-	70	
PEN	50	-	50	
KZ	91	-	91	

a. Average (Minimum-Maximum);
b. The numbers in purple color are reported average values of each antibiotic category used for those without available exertion values in published reports;
c. The numbers in blue color are those values of β-lactams (only 4 antibiotics CPX, AMOX, PEN and KZ) used for animals based on the respective data for human.

Table S3 Transfer processes and corresponding D value calculating method.

Symbol [a]	Transfer process	Related D value	Fugacity multiplied
T_{10t}	Advective flows out of the area through air	$Q_{10t}\times Z_1$ [b]	f_1
T_{01t}	Advective flows in the area through air	---	---
T_{20t}	Advective flows out of the area through water	$Q_{20t}\times Z_2$ [b]	f_2
T_{02t}	Advective flows in the area through water	---	---
T_{02h}	Rate of antibiotic entering water by human	---	---
T_{02p}	Rate of antibiotic entering water by pig	---	---
T_{23h}	Rate of antibiotic entering soil during wastewater irrigation	---	---
T_{03p}	Rate of antibiotic entering soil by pig	---	---
T_{03c}	Rate of antibiotic entering soil by chicken	---	---
T_{03o}	Rate of antibiotic entering soil by other animals	---	---
T_{12d}	Diffusion from air to water	$A_2/(1/(K_{12}\times Z_{11})+1/(K_{21}\times Z_{22}))$	f_1
T_{21d}	Diffusion from water to air	$A_2/(1/(K_{12}\times Z_{11})+1/(K_{21}\times Z_{22}))$	f_2
T_{13d}	Diffusion from air to soil	$A_3/(1/(K_{13}\times Z_{11})+L_3/(B_1\times Z_{11}+B_2\times Z_{22}))$	f_1
T_{31d}	Diffusion from soil to air	$A_3/(1/(K_{13}\times Z_{11})+L_3/(B_1\times Z_{11}+B_2\times Z_{22}))$	f_3
T_{24d}	Diffusion from water to sediment	$A_4/(1/(K_{24}\times Z_{22})+L_4/(B_4\times Z_{22}))$	f_2
T_{42d}	Resuspension from sediment to water	$A_4/(1/(K_{24}\times Z_{22})+L_4/(B_4\times Z_{22}))$	f_4
T_{12p}	Dry precipitations from air to water	$A_2\times K_p\times X_{13}\times Z_{13}$	f_1
T_{12w}	Wet precipitations from air to water	$A_2\times K_w\times S_c\times X_{13}\times Z_{13}$	f_1
T_{13p}	Dry precipitations from air to soil	$A_3\times K_p\times X_{13}\times Z_{13}$	f_1
T_{13w}	Wet precipitations from air to soil	$A_3\times K_w\times S_c\times X_{13}\times Z_{13}$	f_1

Symbol [a]	Transfer process	Related D value	Fugacity multiplied
T_{24s}	Sedimentation	$A_4 \times K_s \times Z_{23}$	f_2
T_{42r}	Resuspension	$A_4 \times K_r \times Z_{43}$	f_4
T_{32e}	Erosion from soil to water in suspended solids	$A_3 \times K_e \times Z_{33}$	f_3
T_{32l}	Erosion from soil to water in liquid phase	$A_3 \times K_l \times Z_{22}$	f_3
T_{2f}	Bioaccumulation in fish	$Y_f \times Z_{2f} / \rho_f$	f_2
T_{10m}	Degradation in air	$K_{m1} \times A_1 \times h_1 \times Z_1$	f_1
T_{20m}	Degradation in water	$K_{m2} \times A_2 \times h_2 \times (Z_2 - X_{2f} \times Z_{2f})$	f_2
T_{30m}	Degradation in soil	$K_{m3} \times A_3 \times h_3 \times Z_3$	f_3
T_{40m}	Degradation in sediment	$K_{m4} \times A_4 \times h_4 \times Z_4$	f_4

a. Subscripts 1,2,3 and 4 refer to four bulk compartments: air, water, soil and sediment, respectively. Subscript 0 refers to no specific compartment. Subscripts t, h, d, p, w, s, r, e, l, m and f for advective flow, human activities, diffusive, dry and wet precipitation, sedimentation, resuspension, erosion as solid and water, degradation and fish accumulation, respectively.

b. Z refers to the fugacity capacity. For the air compartment, Z is $1/RT$ for all compounds where R is the gas constant (8.314 $Pa \cdot m^3/mol \cdot K$) and T is the absolute temperature (K). For compounds in water, Z_{water} is $1/H$ where H is the Henry's Law constant ($Pa \cdot m^3/mol$). In solid phase, Z_{solid} equals $K_{OC} f_{oc} \rho_s / H$, where K_{OC} is organic carbon partition coefficient of the solid phase (L/kg); f_{oc} is organic carbon fraction of the solid phase and ρ_s is density of the solid phase (kg/L). Z_1 equals to "$Z_{11}+Z_{13} \times X_{13}$"; and Z_2 equals to "$Z_{22}+Z_{23} \times X_{23}+ Z_{2f} \times X_{2f}$"; Z_3 equals to "$Z_{31} \times X_{31}+ Z_{32} \times X_{32}+ Z_{33} \times X_{33}$"; Z_4 equals to "$Z_{42} \times X_{42}+ Z_{43} \times X_{43}$".

Table S4 Definition of model parameters

Symbol	Unit	Definition	Symbol	Unit	Definition	Symbol	Unit	Definition	Symbol	Unit	Definition
A_2	m^2	Area of water phase	O_{23}	w/w	Contents of organic carbon in solids in water	R	$Pa \cdot m^3/mol \cdot K$	Universal gas constant	K_{13}	m/h	Air-side mass transfer coefficient over soil
A_3	m^2	Area of soil phase	O_{33}	w/w	Contents of organic carbon in solids in soil	H	$Pa \cdot m^3/mol$	Henry's constant	K_{21}	m/h	Water-side mass transfer coefficient over air
h_1	m	Thickness of air	O_{43}	w/w	Contents of organic carbon in solids in sediment	Ps	Pa	Vapor pressure	K_{24}	m/h	Water-side mass transfer coefficient over sediment
h_2	m	Depth of water	ρ_{23}	kg/L	Densities of solids in water	K_{OC}	L/kg	Organic carbon normalized partition coefficients	L_3	m	Diffusion path lengths in soil
h_3	m	Thickness of soil	ρ_{33}	kg/L	Densities of solids in soil	t_1	h	Half-life of the chemical in air	L_4	m	Diffusion path lengths in sediment
h_4	m	Thickness of sediment	ρ_{43}	kg/L	Densities of solids in sediment	t_2	h	Half-life of the chemical in water	K_p	m/h	Dry deposition velocity
X_{13}	v/v	Volume fractions of solids in air	ρ_f	kg/L	Densities of fish	t_3	h	Half-life of the chemical in soil	K_w	m/h	Rain rate

Symbol	Unit	Definition	Symbol	Unit	Definition	Symbol	Unit	Definition	Symbol	Unit	Definition
X_{23}	v/v	Volume fractions of solids in water	Y_f	t/h	Production of fish	t_4	h	Half-life of the chemical in sediment	S_c	m/h	Rain scavenging rate
X_{31}	v/v	Volume fractions of air in soil	Q_{01t}	m3/h	Advection air flow in area	BCF_f		Bioconcentration factors for fish in water	K_s	m/h	Sedimentation rate in water
X_{32}	v/v	Volume fractions of water in soil	Q_{02t}	m^3/h	Advection water flow in area	B_1	m^2/h	Molecular diffusivity in air	K_l	m/h	runoff rates of dissolved components
X_{33}	v/v	Volume fractions of solids in soil	Q_{20t}	m^3/h	Advection water flow out of area	B_2	m^2/h	Molecular diffusivity in water	K_e	m/h	runoff rates of solid in soil
X_{42}	v/v	Volume fractions of water in sediment	Q_{02h}	m^3/h	Wastewater discharge rate	B_4	m^2/h	Molecular diffusivity in sediment	K_r^e	m/h	Resuspension rate in sedimentation
X_{43}	v/v	Volume fractions of solids in sediment	T	K	Local absolute temperature	K_{12}	m/h	Air-side mass transfer coefficient over water	f	%	Removal efficiency of target compounds in STP
X_{2f}	v/v	Volume fractions of fish in water									

Table S5. Physical and chemical properties of 36 antibiotics

Symbol	Unit	SDZ		SMZ		SMX		STZ		SCP		SM	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
H	Pa·m^3/mol	2.11E-08	65	1.96E-05	65	9.69E-08	65	5.93E-09	65	2.08E-07	65	9.48E-07	66
Ps	Pa	2.29E-04	65	9.09E-07	65	1.73E-05	65	4.32E-06	65	1.77E-07	65	1.11E-06	66
K_{OC}	m^3/t	1.25E+02	67	1.17E+02	67-69	1.53E+03	65	2.00E+02	69	1.29E+02	70	1.35E+02	65
BCF_f	g/L	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65
t_1	h	8.20E+00	65	4.46E+00	65	1.28E+00	65	4.79E+00	65	1.05E+01	65	9.17E+00	65
t_2	h	9.00E+02	68	8.72E+02	16, 71	5.29E+02	16, 71-74	9.12E+02	16	1.44E+03	65	9.00E+02	65
t_3	h	6.55E+02	75	1.80E+03	65	4.80E+01	76	1.80E+03	65	4.87E+02	67, 77	1.80E+03	65
t_4	h	1.25E+03	68, 78	1.25E+03	71	5.68E+02	71, 73	8.10E+03	65	1.30E+04	65	8.10E+03	65
B_2	m^2/h	5.44E-07	79	4.91E-07	79	5.40E-07	79	5.59E-07	79	5.24E-07	79	5.09E-07	79
B_4	m^2/h	1.10E-07	79	9.96E-08	79	1.10E-07	79	1.13E-07	79	1.06E-07	79	1.03E-07	79
f	%	7.20E+01	80-88	4.93E+01	80, 84-91	5.35E+01		9.10E+01	88, 92	6.79E+01	93	7.08E+01	93
M	°C	2.55E+02	65	2.00E+02	65	1.70E+02	65	2.01E+02	65	1.87E+02	65	2.15E+02	65
ρ	g/cm^3	1.50E+00	94	1.40E+00	94	1.60E+00	94	1.60E+00	94	1.60E+00	94	1.50E+00	94

Symbol	Unit	SMM		SQX		SG		TMP		OMP		OTC	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
H	Pa·m^3/mol	2.44E-09	65	4.41E-10	65	1.02E-10	65	4.51E-08	65	2.42E-09	65	4.79E-22	65
Ps	Pa	1.11E-06	65	1.49E-08	65	5.31E-05	65	3.04E-06	65	1.00E-06	65	4.60E-21	65
K_{OC}	m^3/t	1.35E+02	65	2.10E+03	65	1.29E+02	65	2.84E+03	67	9.05E+02	65	2.33E+02	95
BCF_f	g/L	3.16E+00	65	3.92E+00	65	3.16E+00	65	1.77E+00	65	3.16E+00	65	3.16E+00	65
t_1	h	3.24E+00	65	3.84E+00	65	3.95E+00	65	4.05E+00	65	1.26E+00	65	1.34E-01	65
t_2	h	9.00E+02	65	9.00E+02	65	9.00E+02	65	1.44E+03	16	1.44E+03	65	2.16E+02	68

Symbol	Unit	SMM		SQX		SG		TMP		OMP		OTC	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
t_3	h	1.80E+03	65	1.80E+03	65	1.80E+03	65	2.64E+03	16, 67, 97	2.88E+03	65	6.65E+02	67, 77, 97, 100, 101
t_4	h	8.10E+03	65	8.10E+03	65	8.10E+03	65	2.08E+03	68, 78	2.40E+03	65	1.75E+03	68, 78, 97, 104
B_2	m^2/h	5.09E-07	79	4.89E-07	79	6.19E-07	79	4.52E-07	79	4.58E-07	79	4.09E-07	79
B_4	m^2/h	1.03E-07	79	9.92E-08	79	1.26E-07	79	9.18E-08	79	9.30E-08	79	8.30E-08	79
f	%	7.61E+01	87	5.16E+01	88, 93	1.85E+00	65	5.28E+01	82, 87, 89-92, 105-110	-	-	7.64E+01	87, 93
M	°C	2.04E+02	65	2.48E+02	65	1.90E+02	65	1.83E+02	65	2.01E+02	65	3.27E+02	65
ρ	g/cm^3	1.50E+00	94	1.50E+00	94	1.60E+00	94	1.20E+00	94	1.30E+00	94	1.70E+00	94

Symbol	Unit	TC		CTC		DC		MT		NFX		CFX	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
H	$Pa \cdot m^3/mol$	4.72E-19	65	3.50E-19	65	1.31E-20	65	5.42E-21	65	8.82E-14	65	5.16E-14	65
Ps	Pa	2.77E-19	65	7.79E-20	65	6.61E-20	65	6.32E-20	65	1.11E-09	65	3.80E-11	65
K_{OC}	m^3/t	1.96E+04	68, 69, 96	5.62E+04	96	1.55E+02	65	3.14E+02	65	9.21E+01	65	6.62E+04	97, 98
BCF_f	g/L	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65
t_1	h	9.26E-01	65	1.12E+00	65	1.34E-01	65	3.98E-01	65	7.94E-01	65	8.15E-01	65
t_2	h	7.20E+01	68	4.32E+03	65	1.44E+03	65	1.44E+03	65	1.44E+03	65	1.44E+03	99
t_3	h	4.32E+03	70	6.49E+02	68, 102, 103	2.88E+03	65	2.88E+03	65	1.15E+03	75	1.56E+03	97
t_4	h	1.30E+04	65	3.89E+03	65	1.30E+04	65	1.30E+04	65	1.30E+04	65	1.30E+04	65
B_2	m^2/h	4.03E-07	79	4.00E-07	79	4.03E-07	79	4.19E-07	79	4.33E-07	79	4.61E-07	79
B_4	m^2/h	8.18E-08	79	8.12E-08	79	8.18E-08	79	8.50E-08	79	8.80E-08	79	9.36E-08	79

Symbol	Unit	TC		CTC		DC		MT		NFX		CFX	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
f	%	7.48E+01	82, 83, 87, 89, 90, 93, 106, 110	8.83E+01	87	8.88E+01	87, 111	6.60E+01	87	7.19E+01	81-84, 86, 87, 90-93, 109, 110, 112, 113	6.88E+01	16, 82-84, 86, 87, 89, 90, 92, 93, 106, 112
M	°C	1.65E+02	65	1.69E+02	65	3.14E+02	65	3.14E+02	65	2.24E+02	65	2.59E+02	65
ρ	g/cm^3	1.60E+00	94	1.70E+00	94	1.60E+00	94	1.70E+00	94	1.30E+00	94	1.50E+00	94

Symbol	Unit	OFX		LFX		EFX		FL		PEF		DIF	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
H	$Pa{\cdot}m^3/mol$	1.18E-16	65	1.37E-13	65	1.50E-13	65	4.50E-13	65	1.94E-13	65	4.28E-14	65
Ps	Pa	2.43E-11	65	5.71E-10	65	4.08E-10	65	4.91E-10	65	4.35E-10	65	3.00E-12	65
K_{OC}	m^3/t	4.41E+04	98	2.52E+02	65	7.00E+04	98	3.49E+02	65	1.12E+02	65	2.91E+03	65
BCF_f	g/L	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65
t_1	h	7.48E-01	65	1.89E+00	65	7.86E-01	65	2.05E+00	65	7.84E-01	65	8.06E-01	65
t_2	h	1.20E+02	72	4.32E+03	65	4.32E+03	16	4.32E+04	65	4.32E+03	65	4.32E+04	99
t_3	h	2.88E+03	65	8.64E+03	65	5.78E+03	97, 114	8.64E+03	65	8.64E+03	65	8.64E+04	65
t_4	h	1.30E+04	65	3.89E+04	65	3.89E+04	65	3.89E+04	65	3.89E+04	65	3.89E+04	65
B_2	m^2/h	4.10E-07	79	4.10E-07	79	4.22E-07	79	4.15E-07	79	4.22E-07	79	3.97E-07	79
B_4	m^2/h	8.31E-08	79	8.31E-08	79	8.57E-08	79	8.43E-08	79	8.57E-08	79	8.05E-08	79
f	%	5.21E+01	80, 81, 83, 85-87, 91, 93, 105, 109, 113	6.80E+01	84-87, 93, 113	6.99E+01	86, 93, 113	4.98E+01	85-87, 113	7.37E+01	93	8.89E+01	86
M	°C	2.40E+02	65	2.40E+02	65	2.21E+02	65	2.64E+02	65	2.71E+02	65	3.22E+02	65

Symbol	Unit	OFX		LFX		EFX		FL		PEF		DIF	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
ρ	g/cm^3	1.50E+00	94	1.30E+00	94	1.40E+00	94	1.40E+00	94	1.30E+00	94	1.40E+00	94

Symbol	Unit	LCM		CTM		RTM		TYL		ETM-H_2O		FF	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
H	$Pa\cdot m^3/mol$	4.09E-25	65	1.76E-24	65	5.03E-26	65	5.85E-33	65	5.49E-24	65	7.40E-13	65
Ps	Pa	7.85E-23	65	3.09E-23	65	1.39E-27	65	2.65E-32	65	2.83E-23	65	1.83E-10	65
K_{OC}	m^3/t	1.06E+02	65	1.49E+02	65	9.63E+03	65	2.22E+03	95, 96	5.67E+02	65	3.86E+01	97
BCF_f	g/L	2.36E+01	65	1.53E+01	65	1.05E+01	65	2.77E+00	65	4.85E+01	65	3.16E+00	65
t_1	h	3.51E-01	65	6.45E-01	65	7.51E-01	65	3.00E-02	65	6.37E-01	65	1.53E+01	65
t_2	h	1.44E+03	65	4.32E+03	65	4.32E+03	16	2.42E+03	115	8.76E+03	116	1.44E+03	65
t_3	h	2.88E+03	65	8.64E+03	65	8.64E+03	65	5.42E+02	67, 68, 76, 102, 103, 117	4.80E+02	117	1.52E+02	97
t_4	h	1.30E+04	65	3.89E+04	65	3.89E+04	65	2.24E+02	104	3.89E+04	65	1.75E+02	68, 78
B_2	m^2/h	2.72E-07	79	2.50E-07	79	2.46E-07	79	2.22E-07	79	2.57E-07	79	4.41E-07	79
B_4	m^2/h	5.53E-08	79	5.08E-08	79	4.99E-08	79	4.51E-08	79	5.22E-08	79	8.94E-08	79
f	%	3.38E+00	65	5.21E+01	87, 90, 107	4.28E+01	81, 82, 85-87, 90, 107	5.96E+01	84-86, 91, 93	4.95E+01	81, 82, 84-87, 89-91, 93, 107, 110	1.85E+00	65
M	°C	3.50E+02	65	3.50E+02	65	3.50E+02	65	3.50E+02	65	3.50E+02	65	1.55E+02	65
ρ	g/cm^3	1.30E+00	94	1.20E+00	94	1.30E+00	94	1.20E+00	94	1.20E+00	94	1.50E+00	94

Symbol	Unit	CAP		LIN		CPX		AMOX		PEN		KZ	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
H	$Pa\cdot m^3/mol$	2.32E-13	65	3.04E-18	65	2.81E-12	66	2.52E-16	66	1.18E-09	65	2.04E-18	66

Symbol	Unit	CAP		LIN		CPX		AMOX		PEN		KZ	
		Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.	Values	Ref.
Ps	Pa	2.33E-10	65	1.79E-15	65	4.32E-13	66	6.25E-15	66	1.20E-08	65	2.00E-16	66
K_{OC}	m^3/t	1.00E+01	65	5.90E+01	97	6.63E+02	65	8.66E+02	97	4.21E+02	65	2.10E+03	65
BCF_f	g/L	3.37E-01	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65	3.16E+00	65
t_1	h	8.29E+00	65	9.03E-01	65	1.16E+00	65	1.85E+00	65	3.68E+00	65	1.34E+00	65
t_2	h	1.44E+03	65	9.00E+02	65	9.00E+02	65	9.00E+02	65	9.00E+02	65	9.00E+02	65
t_3	h	2.88E+03	65	1.80E+03	65	1.80E+03	65	1.80E+03	65	7.20E+02	70	1.80E+03	65
t_4	h	3.46E+02	68	8.10E+03	65	8.10E+03	65	8.10E+03	97	8.10E+03	65	8.10E+03	65
B_2	m^2/h	4.68E-07	79	3.76E-07	79	4.49E-07	79	4.35E-07	79	4.40E-07	79	4.54E-07	79
B_4	m^2/h	9.50E-08	79	7.63E-08	79	9.11E-08	79	8.84E-08	79	8.94E-08	79	9.21E-08	79
f	%	5.24E+01	81, 87, 93	5.22E+01	84, 87, 92	9.02E+01	87, 92, 109, 110	9.00E+01	92, 118	6.32E+01	92, 109	6.73E+01	109
M	°C	1.50E+02	65	2.62E+02	65	3.63E+02	65	1.94E+02	65	2.16E+02	65	1.90E+02	65
ρ	g/cm^3	1.50E+00	94	1.30E+00	94	1.50E+00	94	1.50E+00	94	1.40E+00	94	2.00E+00	94

Table S6 Default values of environmental parameters [119].

Symbol	Unit	Definition	Values
h_1	m	Thickness of air	1000
h_3	m	Thickness of soil	0.1
h_4	m	Thickness of sediment	0.05
X_{13}	v/v	Volume fractions of solids in air	7.2×10^{-12}
X_{31}	v/v	Volume fractions of air in soil	0.25
X_{32}	v/v	Volume fractions of water in soil	0.25
X_{33}	v/v	Volume fractions of solids in soil	0.5
X_{42}	v/v	Volume fractions of water in sediment	0.7
X_{43}	v/v	Volume fractions of solids in sediment	0.3
X_{2f}	v/v	Volume fractions of fish in water	1×10^{-6}
ρ_{23}	kg/L	Densities of solids in water	2.4
ρ_{33}	kg/L	Densities of solids in soil	2.65
ρ_{43}	kg/L	Densities of solids in sediment	2.4
ρ_f	kg/L	Densities of fish	1.45
R	$Pa\cdot m^3/ mol\cdot K$	Universal gas constant	8.314
B_1	m^2/h	Molecular diffusivity in air	0.04
K_{12}	m/h	Air-side mass transfer coefficient over water	3
K_{13}	m/h	Air-side mass transfer coefficient over soil	1
K_{21}	m/h	Water-side mass transfer coefficient over air	0.03
K_{24}	m/h	Water-side mass transfer coefficient over sediment	0.01
L_3	m	Diffusion path lengths in soil	0.05
L_4	m	Diffusion path lengths in sediment	0.025
K_p	m/h	Dry deposition velocity	10.8
S_c	m/h	Rain scavenging rate	2×10^{5}
K_s	m/h	Sedimentation rate in water	4.6×10^{-6}
K_r	m/h	Resuspension rate in sedimentation	1.14×10^{-8}
K_l	m/h	runoff rates of dissolved components	3.9×10^{-5}
K_e	m/h	runoff rates of solid in soil	2.3×10^{-8}

Table S7 Environmental parameters for all of the basins

Basin ID	A_2	A_3	h_2	X_{23}	O_{23}	O_{33}	O_{43}	Y_f	Q_{20t}	T	K_w
1	1.28E+10	1.85E+10	1.12E+00	4.17E-05	1.46E-02	3.83E-02	6.13E-03	7.94E+02	8.37E+05	2.75E+02	6.58E-07
2	2.16E+10	1.74E+11	1.65E+00	4.21E-05	2.54E-02	4.25E-02	6.13E-03	4.06E+01	1.04E+07	2.77E+02	7.30E-05
3	1.39E+09	1.98E+10	3.50E+00	4.21E-05	2.58E-02	2.74E-02	6.00E-02	4.40E+00	6.12E+06	2.75E+02	7.21E-05
4	1.85E+09	1.67E+09	8.00E-01	4.21E-05	2.58E-02	2.25E-02	6.00E-02	4.64E-01	8.37E+05	2.77E+02	5.74E-05
5	1.54E+09	3.66E+09	2.00E+00	4.21E-05	2.58E-02	2.90E-02	7.64E-03	1.01E+00	8.93E+05	2.77E+02	5.74E-05
6	3.34E+09	1.48E+08	3.00E+00	2.33E-02	2.88E-02	3.83E-02	3.46E-02	0.00E+00	1.21E+06	2.72E+02	3.32E-05
7	3.40E+10	4.99E+10	6.02E-01	7.57E-04	8.80E-03	1.55E-02	6.60E-03	6.92E+01	3.08E+06	2.80E+02	9.66E-05
8	3.90E+09	1.20E+10	4.98E-01	2.38E-02	2.42E-02	1.38E-02	1.50E-02	9.16E+00	7.49E+05	2.81E+02	7.03E-05
9	8.64E+09	1.27E+10	4.00E-01	7.57E-04	5.55E-03	1.55E-02	6.47E-01	1.38E+01	1.17E+06	2.83E+02	1.05E-04
10	5.04E+09	3.17E+09	2.17E+00	7.57E-04	5.55E-03	1.55E-02	3.59E-02	4.03E+00	3.62E+06	2.80E+02	1.41E-04
11	1.32E+10	4.56E+09	2.50E-01	1.97E-03	6.00E-03	1.38E-02	2.50E-02	1.11E+01	2.02E+05	2.81E+02	3.63E-05
12	1.79E+10	2.13E+10	3.00E-01	3.10E-03	7.80E-03	1.07E-02	2.50E-02	1.07E+01	4.44E+05	2.85E+02	2.26E-05
13	2.13E+08	1.64E+10	1.60E+00	1.80E-03	1.10E-02	1.66E-02	1.36E-02	9.99E+00	2.99E+06	2.84E+02	6.23E-05
14	2.15E+09	1.60E+10	3.20E-01	3.10E-03	7.80E-03	1.66E-02	1.50E-02	1.24E+01	5.23E+05	2.84E+02	4.21E-05
15	9.55E+08	1.40E+10	2.70E+00	3.10E-03	7.80E-03	1.66E-02	3.59E-02	6.66E+00	3.07E+04	2.83E+02	4.01E-05
16	3.53E+09	1.69E+10	1.30E+00	3.10E-03	7.80E-03	8.20E-03	5.42E-04	3.74E+01	2.51E+03	2.87E+02	7.53E-05
17	3.41E+09	3.77E+09	3.00E-01	1.30E-03	3.03E-02	3.03E-02	3.63E-02	2.18E+01	9.74E+05	2.83E+02	4.21E-05
18	4.79E+11	1.11E+11	7.70E-02	2.00E-03	5.10E-03	1.70E-02	1.20E-03	2.44E+01	2.15E+06	2.82E+02	2.63E-05
19	1.03E+09	8.10E+09	2.00E+00	8.40E-03	1.44E-02	2.00E-02	7.49E-02	1.15E-02	1.35E+06	2.46E+02	5.71E-05
20	7.81E+09	2.46E+10	5.86E-01	2.70E-02	2.76E-02	1.15E-02	1.60E-02	5.06E+00	1.19E+06	2.83E+02	2.71E-05
21	7.35E+09	2.21E+10	1.50E+00	9.58E-05	1.86E-02	8.20E-03	1.41E-02	5.91E+01	8.49E+05	2.86E+02	7.79E-05
22	7.49E+10	8.49E+10	2.31E-01	2.05E-04	1.00E-02	1.70E-02	2.90E-03	1.80E+02	3.59E+06	2.88E+02	8.14E-05
23	2.03E+10	3.46E+10	4.67E-01	4.79E-04	5.98E-03	1.70E-02	2.90E-03	1.73E+00	2.31E+05	2.87E+02	8.87E-05
24	1.35E+10	1.22E+10	1.40E+00	2.00E-06	1.00E-06	1.90E-02	4.53E-02	5.28E+01	9.18E+04	2.84E+02	1.25E-04
25	1.93E+11	5.63E+10	6.96E-01	3.61E-04	6.62E-03	3.46E-02	1.41E-01	2.89E+01	2.12E+07	2.87E+02	9.44E-05
26	4.48E+10	3.17E+10	1.80E+00	1.67E-04	1.72E-02	1.87E-02	1.98E-02	2.26E+02	1.22E+07	2.89E+02	1.52E-04
27	7.39E+10	3.04E+09	6.91E-01	9.44E-05	1.88E-02	3.46E-02	1.41E-01	0.00E+00	6.89E+06	2.93E+02	1.01E-04
28	3.28E+10	7.08E+09	3.00E+00	1.52E-04	1.27E-02	3.46E-02	1.41E-01	0.00E+00	1.03E+07	2.87E+02	1.80E-06
29	1.80E+10	2.33E+10	4.00E+00	3.47E-04	6.48E-03	3.46E-02	1.41E-01	7.94E+03	7.63E+06	2.87E+02	1.13E-04
30	2.23E+10	1.18E+10	1.90E+00	8.96E-05	1.39E-02	3.68E-02	7.07E-02	9.12E+00	5.94E+06	2.88E+02	1.02E-04

Basin ID	A_2	A_3	h_2	X_{23}	O_{23}	O_{33}	O_{43}	Y_f	Q_{20t}	T	K_w
31	7.34E+10	5.64E+10	1.75E+00	6.94E-05	1.11E-02	2.65E-02	1.76E-02	3.71E+03	1.94E+07	2.89E+02	1.02E-04
32	7.24E+10	1.67E+10	7.73E-01	1.98E-04	8.28E-03	1.15E-02	1.91E-02	6.21E+01	5.42E+06	2.89E+02	1.21E-04
33	1.32E+11	3.81E+10	1.01E+00	2.75E-05	3.74E-02	2.26E-02	1.76E-02	3.25E+02	1.71E+07	2.90E+02	2.43E-04
34	6.05E+09	8.83E+09	3.10E+00	2.34E-05	3.72E-02	1.90E-02	1.18E-02	6.91E+01	2.47E+06	2.86E+02	1.20E-04
35	2.78E+09	1.03E+10	2.93E+00	1.02E-04	1.75E-02	2.41E-02	6.55E-02	6.90E-01	4.26E+06	2.90E+02	1.72E-04
36	1.40E+10	4.49E+09	1.23E+00	6.20E-05	2.44E-02	2.41E-02	6.55E-02	7.82E+00	1.69E+06	2.91E+02	1.49E-04
37	3.05E+10	6.98E+09	1.66E+00	4.17E-05	3.14E-02	3.39E-02	6.55E-02	3.24E+02	7.12E+06	2.92E+02	8.08E-05
38	5.60E+09	3.78E+09	1.56E+00	1.16E-04	1.63E-02	3.39E-02	6.55E-02	3.41E+02	7.62E+06	2.92E+02	8.08E-05
39	1.17E+10	5.30E+09	1.00E+00	1.25E-04	1.57E-02	2.28E-02	6.55E-02	6.29E-01	2.55E+06	2.91E+02	1.54E-04
40	2.44E+10	4.23E+10	2.03E+00	8.48E-05	1.69E-02	3.78E-02	1.14E-02	1.49E+05	2.53E+07	2.92E+02	4.00E-05
41	4.23E+10	6.18E+09	1.10E+00	5.42E-05	2.69E-02	3.78E-02	1.42E-02	4.39E+01	7.71E+06	2.93E+02	1.95E-04
42	2.08E+08	3.27E+00	4.80E+00	9.50E-06	3.48E-02	9.80E-03	1.42E-02	5.77E+01	3.94E+06	2.95E+02	2.25E-04
43	3.91E+09	3.91E+09	1.11E+00	1.13E-04	3.05E-02	3.78E-02	2.20E-02	3.45E+00	2.99E+06	2.96E+02	2.62E-04
44	1.93E+09	4.19E+09	1.15E+00	4.79E-05	2.89E-02	3.78E-02	1.55E-02	1.39E+02	3.09E+07	2.98E+02	1.87E-04
45	2.42E+10	1.25E+10	1.57E+00	1.13E-04	1.66E-02	2.88E-02	1.14E-02	9.54E+02	5.46E+06	2.96E+02	6.00E-05
46	2.74E+10	1.24E+10	1.35E+00	1.63E-03	5.47E-03	3.60E-02	7.49E-02	1.93E-01	5.47E+06	2.91E+02	9.14E-05
47	2.36E+10	1.08E+10	1.75E+00	3.28E-04	7.63E-03	3.60E-02	7.49E-02	1.25E+01	8.68E+06	2.84E+02	6.86E-05
48	1.89E+10	9.27E+09	2.88E+00	1.58E-04	1.30E-02	3.60E-02	7.49E-02	1.33E-01	8.02E+06	2.85E+02	7.32E-05
49	8.03E+10	1.27E+09	1.61E+00	2.05E-04	1.08E-02	3.24E-02	7.49E-02	0.00E+00	1.20E+06	2.78E+02	4.27E-05
50	5.65E+09	5.77E+06	5.00E-01	1.25E-03	4.84E-03	3.24E-02	7.49E-02	0.00E+00	7.88E+04	2.73E+02	1.71E-05
51	2.54E+09	5.95E+08	4.00E+00	3.17E-05	3.67E-02	2.43E-02	7.49E-02	0.00E+00	8.37E+05	2.76E+02	3.86E-05
52	5.08E+10	7.13E+09	8.00E-03	3.08E-03	7.77E-03	1.92E-02	1.74E-02	4.45E-03	0.00E+00	2.80E+02	2.97E-05
53	6.35E+10	7.23E+09	1.00E-01	4.04E-04	6.40E-03	1.63E-02	7.49E-02	0.00E+00	0.00E+00	2.79E+02	6.27E-06
54	7.28E+09	5.21E+08	7.00E-01	7.40E-04	4.87E-03	2.42E-02	7.49E-02	0.00E+00	0.00E+00	2.79E+02	2.11E-05
55	5.82E+10	1.31E+10	2.94E-01	2.15E-04	9.93E-03	2.11E-02	7.49E-02	0.00E+00	0.00E+00	2.78E+02	2.55E-05
56	5.99E+10	1.31E+08	2.94E-01	2.46E-04	9.40E-03	2.11E-02	7.49E-02	0.00E+00	0.00E+00	2.83E+02	5.31E-05
57	4.07E+10	9.83E+09	1.00E+00	1.60E-03	5.49E-03	2.11E-02	3.65E-01	0.00E+00	0.00E+00	2.86E+02	8.60E-06
58	6.19E+10	2.80E+08	2.19E-01	2.05E-04	1.08E-02	3.24E-02	7.49E-02	0.00E+00	0.00E+00	2.79E+02	2.37E-05

References: 1.Local Statistical Yearbook in 2011; 2.Water Resources and Sediment Bulletin for Huaihe River Basin, Huanghe River Basin, Haihe River Basin, Yangtze River Basin, Taihu Basin, Songhuajiang and Liaohe River Basin, Pearl River Basin in 2011; 3.Water Resources Bulletin and Environmental Bulletin for each Province in China in 2011; 4.Hydropower knowledge network, http://www.waterpub.com.cn; 5.Thematic Database for Human-Earth System, http://www.data.ac.cn/zrzy/ntBA82.asp?p=N301&g=%3D&z=&query=+%C8%B7%C8%CF+&m=BA82&k=1&r=33&name=&pass=&danwei; 6.China Soil Scientific Database, http://www.soil.csdb.cn/myweb/page/8.vpage.

Table S8 Comparison between the reported measured environmental concentrations (MECs) and the predicted environmental concentrations (PECs) from this study in water (A) and sediment (B) compartments at the river basin level.

A. Water

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
SDZ	30.5	0.97		14.0	85.9	0.79	120
	4.04	3.60	3.82	3.82	167	1.64	121
	192	nd	24.5		270	1.04	122, 123
	1600	0.86	258	160	788	0.48	124, 125
	66.0	nd			666		123
	10.0	nd			290		123
	6.60	0.24	2.38	1.71	101	1.63	126
			< 5		19.8	0.60	84
	37.4	0.45	6.19	1.50	44.4	0.86	127, 128
			< 5		18.5	0.57	84
	113	1.39	26.2		42.5	0.21	129, 130
	60.5		13.0	7.80	28.1	0.33	131, 132
	379	0.62	49.7	3.45	30.6	-0.21	133
	301	0.25	19.0	4.05	60.7	0.51	134
	18.0	1.26	4.58	2.72	229	1.70	135, 136
	4.80	nd			25.6		137
SMZ	26.4	nd			33.6		120
	85.1	nd		13.4	106	0.90	122, 123
	16.0	nd			113		123
	108	0.29	17.8	4.65	35.4	0.30	126
	6.00	<5			8.74		84
	33.8	nd	4.97	1.70	16.7	0.53	127, 128
	10.0	7.00			8.19		84
	654	nd	149		17.1	-0.94	129, 130, 138

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
SMZ	776	0.14	34.8	18.1	9.76	-0.55	131, 132
	720	0.09	58.9	18.1	32.2	-0.26	134
	751	1.31	65.1	8.35	111	0.23	135, 139
	6.60	nd			11.4		137
SMX	173	6.70		66.6	35.1	-0.28	120
	1.71	1.32	1.52	1.52	48.0	1.50	121
	171	nd			144		122, 123
	6800	3.00	466	83.0	265	-0.25	124, 125
	108	33.0			239		123
	148	12.0			78.9		123
	527	0.68	100.0	39.1	23.3	-0.63	126
	23.0	<5			7.06		84
	13.4	0.30	2.96	2.10	8.55	0.46	127
	21.0	18.0			7.36		84
	260	4.79	23.4	11.3	8.09	-0.46	129, 130, 138, 140
	93.4	1.20	11.6	7.00	8.66	-0.13	126, 131
	135	0.48	12.4	2.75	19.6	0.20	134
	279	1.99	20.7	8.40	51.9	0.40	135, 136, 139
	15.9	nd			7.85		137
STZ	8.50	nd		3.90	12.7	0.51	120
	1.38	nd	0.08		49.3	2.79	124
	3.70	0.40	1.23	0.55	3.71	0.48	127
	135	nd	40.0	40.0	3.31	-1.08	129, 138
	2.70	0.12	0.89	0.64	3.88	0.64	133
	0.76	nd			3.49		137
SCP	8.10	nd		2.10	51.0	1.39	120
	2.50	0.74	1.62	1.62	86.9	1.73	121

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
SCP	47000	0.75	6385	270	286	-1.35	125
	27.1	3.25	13.1	8.85	17.4	0.12	130, 138
SM	6.70	1.00	2.82	1.50	8.62	0.49	126, 131
SMM	35.1	1.50		8.40	19.6	0.37	120
	1.42	1.04	1.23	1.23	80.0	1.81	121
	23.1	nd	6.92		260	1.57	124
	49.0	0.40	17.2	14.7	9.03	-0.28	131
SQX	13.6	nd		2.90	1.13	-0.41	120
	0.78	0.21	0.43	0.37	1.53	0.55	128
	64.2	nd	21.5		1.11	-1.29	129
SG	8.00	nd		3.60	12.1	0.53	120
	4.85	1.47	3.16	3.16	17.5	0.74	121
TMP	121	5.30		29.0	51.8	0.25	120
	1126	nd	242		248	0.01	122, 123
	540	24.0	168	150	700	0.62	125
	120	nd			149		123
	3558	0.82	825	31.5	45.1	-1.26	126
	8.00	6.00			15.7		84
	19.0	0.10	3.08	1.50	21.0	0.83	127
	7.00	5.00			22.0		84
	14.2	0.20	3.96	0.37	33.7	0.93	130, 138, 140
	68.3	0.77	8.40	2.85	28.5	0.53	133
	106	0.41	23.8	13.0	100	0.63	134
	169	47.1	115	139	200	0.24	139
	4.10	nd			19.7		137
OTC	4.64	1.34	2.99	2.99	21.5	0.86	121
	361107	4.64	48730		253	-2.28	122, 141

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
OTC	11000	2.50	582	55.0	211	-0.44	125
	72.0	nd			197		123
	<5				4.11		84
	61.8	4.20	14.4	4.50	4.98	-0.46	127, 128
	<5				7.62		84
	78.3	15.3	41.0	35.1	5.07	-0.91	129, 130, 138
	457	2.75	118	36.9	7.29	-1.21	126
	57.2	0.70	8.16	3.53	37.5	0.66	134
TC	4.97	3.04	4.01	4.01	10.8	0.43	121
	25538	8.07	2152		167	-1.11	122, 141
	9000	nd	278	3.30	151	-0.27	125
	<5				2.94		84
	137	nd	46.8	31.1	3.00	-1.19	127
	<5				3.82		84
	114	nd	28.0		6.21	-0.65	129, 130, 138
	49.6	3.28	13.9	10.5	5.38	-0.41	126
	13.1	4.20	7.15	5.83	19.3	0.43	135
CTC	4.38	2.87	3.63	3.63	5.74	0.20	121
	68870				60.5	-2.35	122
	122	0.30	27.2	11.7	1.66	-0.85	127, 128
	143	nd	28.1		1.05	-1.43	129, 130, 138
	767	2.81	97.5	9.98	1.62	-0.79	132
	7.46	0.04	1.99	1.71	4.19	0.32	134
DC	3.00	1.42	2.21	2.21	107	1.68	121
	66.5	2.80	11.4	4.80	28.8	0.40	127
	112	nd	12.5		20.6	0.22	129, 130
	3.71	0.62	1.75	2.22	125	1.75	134

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
NFX	617		132		1659	1.10	122, 123, 141
	156	nd	28.6		5913	2.32	124
	123	nd			2056		123
	327	5.00	98.0	90.0	649	0.82	142
	228	36.5	116	118	727	0.80	126
	<5				128		84
	134	5.10	39.2	22.7	339	0.94	127
	<5				114		84
	6.50	nd	2.25		291	2.11	129, 130, 138
	500	nd	31.0		389	1.10	109, 127
	6.70	<1.13	3.57	3.75	142	1.60	126
	290	0.20	21.3	4.49	360	1.23	134
	137	4.70	61.3	65.7	1631	1.43	135, 136, 139
CFX	551	nd	206		1120	0.74	122, 123
	2150	3.75	184	3.75	1099	0.78	124, 125
	6.00	nd			211		123
	234	45.0	107	91.9	45.3	-0.38	126
	<5				11.8		84
	<5				39.2		84
	43.6	nd	5.75		16.5	0.46	129, 138
	54.6	1.82	5.85	1.82	97.8	1.22	134
OFX	11735	2.02	793		602	-0.12	122, 123, 141
	860	1.75	88.3	1.75	480	0.74	124, 125
	6.00	nd			299		123
	10.0	nd			131		123
	264	5.00	81.0	80.5	9.72	-0.92	142
	45.4	1.20	14.8	12.0	33.8	0.36	126

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
OFX	74.0	< 5			7.21		84
	135	0.85	16.5	7.00	13.3	-0.09	127, 128
	7.00	6.00			10.2		84
	82.8	nd	19.4		21.6	0.05	129, 138
	85.0		48.7		51.9	0.03	109, 143
	46.2	6.50	27.7	30.5	21.8	-0.10	126, 131
	46.1	5.32	17.8	10.7	46.1	0.41	135, 136
LFX	<5				84.0		84
	13.1	2.60	5.00	3.65	250	1.70	127
	<5				75.8		84
EFX	979	nd	332		546	0.22	122
	4.42	nd	1.28		546	2.63	124
	22.5	2.50	11.8	12.4	23.7	0.30	126
	53.1	2.00	14.3	13.0	11.4	-0.10	127
	14.6	nd	2.80		7.65	0.44	129
			14.6		49.2	0.53	143
	60.8	15.1	29.6	20.4	13.5	-0.34	131
	6.70	2.70	4.70	4.35	21.2	0.65	136
FL	6.40	nd			439		124
CTM	13.4	0.75	5.36	2.70	140	1.42	126
	15.8	0.60	2.03	1.20	58.8	1.46	127
	17.8	0.16	2.51	0.79	10.6	0.63	133
	0.72	0.26			15.8		137
RTM	3.29	2.30	2.80	2.80	16.6	0.77	121
	2552	nd	622		86.6	-0.86	122, 123
	4500	2.25	735	130	180	-0.61	124, 125
	48.0	nd			378		123

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
RTM	92.0	4.00			31.0		123
	95.0	nd	28.2	17.0	4.87	-0.76	142
	159	0.48	49.7	42.5	20.6	-0.38	126
	29.0	<5			5.33		84
	9.80	0.43	3.35	2.90	11.0	0.52	127, 128
	39.0	<5			13.4		84
	50.7	0.76	11.6	1.90	15.2	0.12	129, 130, 138
	379	0.29	32.9	2.95	9.38	-0.54	133
	1952	0.12	75.9	3.97	39.2	-0.29	134
	1070	0.70	104	3.60	42.9	-0.38	136, 139
	0.53	nd			5.68		137
TYL	44.6		13.4		194	1.16	122
	1.88	nd	0.10		503	3.70	124
	75.0	nd			20.4		84
	187	9.00			24.2		84
	0.61	nd		0.17	31.1		130
	67.1	7.45	14.1	11.2	28.5	0.31	134
ERY-H_2O	1.51	1.05	1.28	1.28	799	2.80	121
	253		98.1		490	0.70	122
	4100	1.50	145	1.50	2397	1.22	125
	102	4.00	27.6	10.0	453	1.21	142
	182	0.72	50.0	15.7	599	1.08	126
	24.0	8.00			132		84
	382	0.20	47.1	3.90	375	0.90	127, 128
	85.0	19.0			125		84
	643	nd	56.5		298	0.72	129, 138
	174	2.60	23.5	8.50	81.1	0.54	133

Chemicals	MEC (ng/L)				PEC (ng/L)	Log-diff	References
	MAX	MIN	Mean	Median			
ERY-H_2O	1110	3.33	45.8	21.2	174	0.58	134
	826	6.00	63.8	21.7	990	1.19	135, 136, 139
	50.9	1.10			128		137
FF	2.20	0.24	1.22	1.22	2578	3.32	121
	46.7	10.5	22.4	16.3	667	1.47	128
	241	nd	45.6		446	0.99	129, 130
	26.4	0.32	9.88	9.19	295	1.47	131
CAP	1.30	0.90	1.10	1.10	355	2.51	121
	3.03	0.97	2.00	2.00	138	1.84	91
	3.90	nd	0.40		97.9	2.39	129
LCM	19.0	<5			75.1		84
	23.0	<5			75.8		84
CPX	10.0	nd			207		109
PEN	1.65	1.46	1.56	1.56	771	2.70	121
	2.16	0.50	0.84	0.50	220	2.42	140
	450	nd			448		109
KZ			10.0		0.49	-1.31	109

B. Sediment

Chemicals	MEC (ng/g)				PECs (ng/g)	Log-diff	Reference
	MAX	MIN	Mean	Median			
SDZ	11.0	0.00	0.78	0.00	0.02	-1.61	144
	5.60	0.30	0.40	0.39	0.07	-0.74	122, 144
	34.0	0.00	5.08	5.40	0.17	-1.49	144124, 125
	0.36	0.00	0.36	0.36	0.19	-0.28	144
	22.0	0.11	0.47	0.31	0.01	-1.63	144
	0.71	0.07	0.40		0.03	-1.09	129
	0.07	0.04	0.05	0.04	0.01	-0.60	133
	1.70	0.25	0.66	0.95	0.04	-1.18	134
	98.0	0.58	3.00	3.08	0.15	-1.30	139
SMZ	0.46	nd	0.06	nd	0.01	-0.93	144
	2.89	1.32	1.98	1.80	0.03	-1.87	144
	5.69	0.22	1.24	0.66	0.10	-1.08	144

Chemicals	MEC (ng/g)				PECs (ng/g)	Log-diff	Reference
	MAX	MIN	Mean	Median			
SMZ	0.42	nd	0.21	0.21	0.05	-0.65	144
	0.97	0.97	0.97	0.97	0.07	-1.15	144
	998	nd	39.8		0.01	-3.51	138
	3.35	0.08	0.55	0.70	0.02	-1.40	134
	248	0.26	6.65	7.38	0.07	-1.98	135, 145
SMX	1.08	nd	0.07	nd	0.04	-0.27	144
	59.0	0.28	2.78	0.90	0.23	-1.09	124, 125
	258	2.10	16.2	12.0	0.03	-2.67	129, 138, 140
	2.16	0.50	1.33	1.33	0.08	-1.23	134
	0.70	nd	0.38	0.29	0.18	-0.32	145
STZ	5.94	nd	0.64		0.07	-0.93	124
	51.7	nd	9.00		0.02	-2.67	129, 138
SCP	39.0	0.05	9.79	4.40	0.38	-1.41	125
	6310	126	2351	1933	0.55	-3.63	146
	15.8	nd	7.30		0.08	-1.95	138
SMM	0.50	nd	0.06		0.27	0.65	124
SQX	0.90	0.08			0.09		129
TMP	9.84	nd	2.10	0.78	0.34	-0.79	144
	5.63	nd	2.63	2.75	1.88	-0.15	122, 144
	28.0	0.50	6.51	4.40	3.69	-0.25	124, 125, 144
	3502	97.0	1547	1121	2.78	-2.75	146
	2.86	nd	0.23	0.10	0.07	-0.53	144
	130	9.30	60.5	42.0	0.97	-1.80	138, 140
	1.07	0.08	0.39	0.38	0.37	-0.02	133
	51.0	0.32	2.90	1.11	2.71	-0.03	134
	196	0.09	6.00	7.15	4.00	-0.18	145
OTC	653	nd	27.8	2.24	1.08	-1.41	144
	162673	2.03	187	3.46	9.46	-1.30	122, 141, 144
	57.0	nd	2.02	0.75	4.85	0.38	125, 144
	2.40	0.00	1.20	1.20	4.52	0.58	144
	48.5	nd	48.5	nd	3.06	-1.20	144
	184	nd	7.21	nd	0.12	-1.79	144
	197	nd	29.9		1.91	-1.19	129, 138
	1643	1.74	13.4	12.7	0.11	-2.07	134
	84.1	0.40	10.8	1.91	16.8	0.19	135, 145
TC	4.82	nd	0.88	0.26	1.43	0.21	144
	16799	1.79	1035	5.52	31.6	-1.51	122, 141, 144
	10.7	1.06	2.61	1.30	18.2	0.84	125, 144
	1.34	1.19	1.27	1.27	6.89	0.74	144
	5.27	nd	5.27	nd	15.4	0.46	144
	18.0	nd	1.50	nd	0.33	-0.65	144
	112	nd	25.7		7.34	-0.54	129, 138
	48.5	nd	10.7		1.01	-1.03	129, 138
	661	3.01	36.7	13.3	55.7	0.18	134
CTC	32.5	nd	2.93	nd	0.56	-0.72	144
	698	nd	49.5	3.26	5.24	-0.98	122, 144
	4.17	nd	0.82	nd	3.41	0.62	144

Chemicals	MEC (ng/g)				PECs (ng/g)	Log-diff	Reference
	MAX	MIN	Mean	Median			
CTC	3.99	nd	3.99	nd	1.60	-0.40	144
	21.3	nd	7.00		49.4	0.85	129
	60.2	3.00	10.0	6.20	8.74	-0.06	134
DC	2.80	nd	0.16	nd	29.5	2.28	144
	7.00	nd	1.75	nd	258	2.17	144
	16.4	3.50	5.14	4.29	295	1.76	134
	1120	2.10	75.8	7.17	5.42	-1.15	135, 145
NFX	177	nd	27.1	3.32	0.51	-1.72	144
	801	104	390		2.08	-2.27	122, 141, 144
	1140	nd	142	13.9	5.89	-1.38	124, 144
	20.3	5.95	11.0	13.1	7.66	-0.16	144
	225	nd	225	nd	7.60	-1.47	144
	142	nd	15.8	8.34	0.33	-1.68	144
	28.4	nd	9.90		0.99	-1.00	138
	4131	0.86	138	11.0	1.21	-2.06	134
	197	1.00	23.7	50.8	84.4	0.55	138, 145
CFX	28.7	nd	5.31	nd	30.3	0.76	144
	1287	30.1	265	306	334	0.10	122, 144
	55.0	nd	14.1	nd	199	1.15	124, 125, 144
	9.89	2.05	5.97	5.97	501	1.92	144
	7812	723	3286	2987	57.5	-1.76	146
	116	nd	116	nd	98.9	-0.07	144
	32.8	nd	2.40	nd	3.46	0.16	144
	25.3	nd	9.80		60.8	0.79	138
	151	2.02	27.1	8.52	363	1.13	134
	1560	0.74	214	5.59	77.4	-0.44	135, 145
OFL	50.5	nd	8.95	3.56	11.1	0.09	144
	653	nd	82.2	8.18	160	0.29	122, 141, 144
	69.0	nd	11.4	nd	78.8	0.84	124, 125, 144
	10.7	1.96	6.35	6.35	49.2	0.89	144
	59.5	nd	59.5	nd	57.5	-0.02	144
	124	0.14	12.2	3.07	1.74	-0.85	144
	52.8	nd	10.3		55.1	0.73	129, 138
LFX	5.82	nd	0.67	nd	1.32	0.29	144
	298	nd	68.2	0.72	2.77	-1.39	144
	46.2	nd	9.02	3.05	9.73	0.03	144
	1.67	nd	0.84	0.84	26.3	1.50	144
	26.2	nd	26.2	nd	14.2	-0.27	144
	44.3	44.3	44.3	44.3	2.44	-1.26	134
	1.43	1.03	1.17	1.05	142	2.08	135
ENR	82.1	nd	12.4		479	1.59	122, 144
	13.0	nd	0.33		291	2.95	124, 144
	7708	109	1627	721	140	-1.06	146
	14.6	nd	2.80		85.5	1.49	129
	0.89	0.09	0.40	0.40	0.10	-0.61	133
	39.8	0.35	6.73	3.46	529	1.90	134
CTM	0.89	0.09	0.33	0.40	0.07	-0.77	133

Chemicals	MEC (ng/g)				PECs (ng/g)	Log-diff	Reference
	MAX	MIN	Mean	Median			
ROX	29.6	nd	8.10	5.51	5.16	0.02	144
	2582		121		30.6	-0.45	122, 144
	64.9	0.75	4.26	0.75	42.2	1.12	124, 125
	1.67	nd	0.83	0.83	89.8	2.22	144
	5622	456	2134	751	23.2	1.51	144, 146
	6.80	nd	1.00	nd	0.78	0.10	144
	45.2	nd	8.90		25.8	0.55	129, 130, 138
	2.16	0.19	0.93	0.87	7.15	1.03	133
	133	0.09	34.1	18.0	57.1	0.33	135, 145
TYL	385	0.04	28.4	6.79	107	0.58	135, 145
ERY-H_2O	40.3	nd	6.73	3.61	6.52	0.28	144
	67.2	nd	20.4	nd	11.2	-0.01	122, 144
	22.2	0.50	2.17	0.50	65.6	1.48	125, 144
	1.41	nd	1.41	nd	77.1	1.74	144
	49.8	nd	5.82	1.28	4.52	-0.11	144
	120		18.7		32.8	0.24	129138
	2.58	0.30	1.36	1.14	4.57	0.53	133
	195	0.58	25.1	11.2	17.0	-0.17	134
	385	0.04	28.4	6.79	69.4	0.39	135, 145
FF	0.70	nd	0.30		0.00	-1.99	129
CAP			0.63		3.14	0.70	129

Remark: The PECs are compared preferably with the mean values, and then with available median values if the mean values are not available. No comparison is given when there are no reported mean and median values.

Table S9 Bacterial resistance of five bacterial species to ciprofloxacin (a), sulfamethoxazole/trimethoprim (b) and tetracycline (c) in hospitals in the seven regions of China (A), and bacterial resistance of *E. coli* to seven respective antibiotics in the hospitals and corresponding rivers (B).

A.

Species	Bacterial resistance (%)					
	East China	North China	Central-south China	Northeast China	Northwest China	Southwest China
E. col [a]	63.90	65.80	67.80	70.70	70.40	61.40
E. col [b]	67.20	68.10	74.90	76.60	77.50	73.70
E. col [c]	69.40	72.30	80.60	78.40	75.30	64.60
K. pneumoniae [a]	24.00	24.70	35.70	23.60	24.60	28.50
K. pneumoniae [b]	37.10	35.60	54.30	37.70	65.80	68.30
K. pneumoniae [c]	32.80	34.20	49.70	32.00	34.60	26.30
C. freundii [a]	31.30	28.60	42.30	52.10	34.50	55.20
C. freundii [b]	39.80	41.40	64.20	18.80	76.10	73.50
C. freundii [c]	48.80	30.20	64.00	49.50	61.30	50.00
A. Baumannii [a]	64.70	61.50	66.20	74.30	80.40	31.10
A. Baumannii [b]	67.00	64.40	67.80	82.10	80.40	89.40
A. Baumannii [c]	76.50	62.10	60.60	46.60	77.00	75.00
H. influenzae [a]	31.60	16.70	21.70	20.50	5.30	4.80
H. influenzae [b]	58.70	67.60	68.20	42.10	49.10	62.20
H. influenzae [c]	23.00	54.40	56.60	41.70	30.00	18.60

B.

Antibiotics		Bacterial resistance (%)				
		Pearl River Delta	Dongjiang River	Haihe River	Liaohe River	Yellow River
Ampicillin	Hospital	85.9	85.9	85	91.1	94.7
	River	43	43.3	48	57	52
Piperacillin	Hospital	75.1	75.1	74.2	83.4	89.5
	River	29	34.9	28	39	45
Ceftazidime	Hospital	28.1	28.1	52.5	58.5	21.4
	River	3	10.2	3	2	24
Cephazolin	Hospital	92	92	60.2	64.6	70.7
	River	20	2.71	26	24	46
Gentamicin	Hospital	45.3	45.3	56.1	65	80
	River	9	16.7	11	9	14
Ciprofloxacin	Hospital	60	60	69.2	59.1	85.7
	River	16	19	12	15	9
Sulfamethoxazole /Trimethoprim	Hospital	62.3	62.3	70.8	77.6	90.5
	River	31	40.6	29	42	39

Table S10 The standard deviation of the modelling parameters.

A. The standard deviations used for all the basins.

Parameters	Values	Parameters	Values	Parameters	Values	Parameters	Values	Parameters	Values
h_1	1.71	X_{2f}	2.30	T_{23h}	2.30	BCF_f	1.00	L_3	2.30
h_3	1.71	Y_f	2.30	T_{02p}	2.30	B_1	1.17	L_4	2.30
h_4	1.71	ρ_{23}	1.71	T_{03p}	2.30	B_2	1.17	K_p	1.15
X_{13}	1.30	ρ_{33}	1.56	T_{02c}	2.30	B_4	1.17	Sc	1.15
X_{31}	1.71	ρ_{43}	1.71	T_{03c}	2.30	K_{12}	1.17	K_s	2.08
X_{32}	1.71	ρ_f	1.22	T_{02o}	2.30	K_{13}	1.17	K_r	2.08
X_{33}	1.71	H	2.30	T_{03o}	2.30	K_{21}	1.17	K_l	2.30
X_{42}	1.71	Ps	2.30	t_1	2.30	K_{24}	1.17	K_e	2.30
X_{43}	1.71	T_{02h}	2.30						

B. The standard deviations used for all the basins relating to the chemicals.

Chemical/ Parameters	K_{OC}	t_2	t_3	t_4	f
	Values	Values	Values	Values	Values
SDZ	2.30	2.30	4.40	2.30	1.31
SMZ	1.68	1.07	2.30	2.30	2.09
SMX	2.30	2.41	2.30	2.54	1.53
STZ	2.30	2.30	2.30	2.30	1.17
SCP	2.30	2.30	1.37	2.30	1.18
SM	2.30	2.30	2.30	2.30	1.21
SMM	2.30	2.30	2.30	2.30	1.06
SQX	2.30	2.30	2.30	2.30	1.96
SG	2.30	2.30	2.30	2.30	2.30
TMP	2.30	2.30	2.30	1.23	1.78
OMP	2.30	2.30	2.30	2.30	2.30
OTC	2.30	2.30	1.56	2.14	1.40
TC	3.49	2.30	2.30	2.30	1.29
CTC	1.05	2.30	1.23	2.30	1.19
DC	2.30	2.30	2.30	2.30	1.23
MT	2.30	2.30	2.30	2.30	1.80
NFX	2.30	2.30	2.30	2.30	1.26
CFX	1.96	2.30	2.30	2.30	1.48
OFX	2.30	2.30	2.30	2.30	1.57
LFX	2.30	2.30	2.30	2.30	1.49
EFX	4.75	2.30	3.69	2.30	1.16
FL	2.30	2.30	2.30	2.30	2.47
PEF	2.30	2.30	2.30	2.30	1.26
DIF	2.30	2.30	2.30	2.30	1.05
LCM	2.30	2.30	2.30	2.30	2.30
CTM	2.30	2.30	2.30	2.30	1.37
RTM	2.30	2.30	2.30	2.30	1.53
TYL	2.90	2.30	3.65	5.14	1.73

Chemical/ Parameters	K_{OC}	t_2	t_3	t_4	f
	Values	Values	Values	Values	Values
ETM-H2O	2.30	2.30	2.30	2.30	1.66
FF	1.52	2.30	1.51	2.30	2.30
CAP	2.30	2.30	2.30	2.30	1.14
LIN	2.30	2.30	2.30	2.30	2.16
CPX	2.30	2.30	2.30	2.30	1.19
AMOX	2.30	2.30	2.30	2.30	1.16
PEN	2.30	2.30	2.30	2.30	1.91
CFZ	2.30	2.30	2.30	2.30	1.10

C. The standard deviation related to the environment.

Basin ID/Parameter	A_2	A_3	h_2	X_{23}	O_{23}	O_{33}	O_{43}	Q_{20t}	T	K_w
1	1.71	1.71	1.90	1.71	2.43	2.78	2.02	1.62	1.64	1.15
2	1.98	1.98	4.16	2.05	3.44	1.09	2.29	1.62	1.55	1.52
3	1.62	1.62	1.62	2.05	2.05	2.05	2.05	1.62	2.12	1.20
4	1.62	1.62	1.62	2.05	1.42	1.39	1.42	1.62	0.00	1.78
5	1.62	1.62	1.62	2.05	1.29	1.32	1.29	1.62	0.00	1.78
6	1.08	1.08	2.30	2.05	1.15	2.78	1.15	1.62	0.00	1.78
7	2.09	2.09	2.13	4.39	1.93	2.26	3.61	1.62	1.39	1.42
8	1.62	1.62	1.62	1.33	2.26	2.26	2.26	1.62	1.21	1.40
9	1.62	1.62	1.62	4.39	2.26	2.26	2.26	1.62	0.58	1.78
10	1.78	1.78	1.89	4.39	2.26	2.26	2.26	1.62	1.82	1.12
11	1.62	1.62	1.62	1.33	2.26	2.26	2.26	1.62	3.01	2.03
12	1.62	1.62	1.62	1.33	2.34	2.34	2.34	1.62	2.67	1.20
13	1.11	1.11	1.62	13.95	1.74	1.58	2.53	1.62	1.19	1.06
14	3.38	3.38	3.38	1.33	1.44	1.58	1.93	1.62	1.51	1.97
15	1.62	1.62	1.62	1.33	1.44	1.58	1.67	1.62	0.87	1.59
16	1.62	1.62	1.62	1.33	2.10	2.10	2.10	2.25	0.75	1.29
17	1.92	1.92	1.92	1.20	1.89	0.01	2.12	1.62	2.92	1.97
18	1.62	1.62	1.62	5.82	1.63	1.59	2.24	1.62	4.38	4.04
19	1.01	1.01	1.62	1.14	1.01	2.68	1.01	1.62	0.00	1.78
20	2.44	2.44	4.56	2.06	2.48	2.16	4.69	1.62	4.06	3.97
21	1.62	1.62	1.62	1.33	2.10	2.10	2.10	1.62	0.69	1.22
22	1.62	1.62	1.62	1.65	1.29	1.29	1.29	1.62	0.67	2.35
23	1.62	1.62	1.62	1.33	1.29	1.29	1.29	1.62	0.71	1.20
24	1.28	1.28	1.62	1.33	1.64	1.64	1.64	1.62	7.63	1.16
25	1.99	1.99	1.92	1.80	1.29	2.10	1.29	1.62	6.67	1.27
26	1.62	1.62	1.62	2.48	2.52	1.45	2.04	1.62	3.00	1.19
27	1.80	1.80	1.85	1.00	2.10	2.10	2.10	1.62	2.62	1.33
28	1.06	1.06	1.62	1.72	1.29	2.10	1.29	1.62	6.42	1.28
29	1.07	1.07	1.62	2.45	1.29	2.10	1.29	1.62	5.81	1.18
30	1.21	1.21	1.62	4.29	2.16	2.16	2.16	1.62	2.19	1.22
31	1.28	1.28	3.45	6.90	1.67	1.67	1.67	1.62	5.22	1.54
32	1.18	1.18	1.77	3.63	2.16	2.16	2.16	1.62	1.56	1.23

Basin ID/Parameter	A_2	A_3	h_2	X_{23}	O_{23}	O_{33}	O_{43}	Q_{20t}	T	K_w
33	1.53	1.53	1.68	1.62	2.01	2.01	2.01	1.62	4.95	1.22
34	1.13	1.13	1.20	2.22	1.64	1.64	1.64	1.62	7.30	1.17
35	2.21	2.21	1.37	1.33	2.01	2.01	2.01	1.62	0.32	1.22
36	1.66	1.66	1.53	1.22	2.01	2.01	2.01	1.62	0.67	1.18
37	1.78	1.78	1.96	1.33	1.74	1.74	1.74	1.62	0.00	1.78
38	3.45	3.45	3.16	1.33	1.74	1.74	1.74	1.62	0.00	1.78
39	1.62	1.62	1.17	1.33	1.92	1.92	1.92	1.62	8.94	1.00
40	1.62	1.62	1.19	1.33	1.38	1.38	1.38	1.62	5.10	2.99
41	1.62	1.62	1.18	1.33	1.38	1.38	1.38	1.62	2.06	1.45
42	1.07	1.07	2.43	2.81	2.23	1.38	2.64	3.31	1.23	1.31
43	2.66	2.66	1.07	1.33	1.80	1.38	2.58	7.79	0.30	1.07
44	1.29	1.29	1.26	1.33	1.38	1.38	1.38	1.31	0.00	1.78
45	1.09	1.09	2.50	1.94	1.94	1.94	1.94	1.15	0.25	4.55
46	1.22	1.22	2.27	1.33	2.38	2.42	2.38	3.32	1.27	1.36
47	1.16	1.16	3.28	1.33	2.38	2.42	2.38	1.62	7.79	1.94
48	1.18	1.18	3.34	1.33	2.38	2.42	2.38	1.62	7.96	2.05
49	1.07	1.07	2.20	1.33	2.42	2.42	2.42	1.62	4.24	1.64
50	1.32	1.32	2.67	1.33	2.42	2.42	2.42	1.62	0.00	1.78
51	1.28	1.28	1.28	1.33	2.61	2.61	2.61	1.02	0.00	1.78
52	1.62	1.62	1.62	1.33	2.05	2.05	2.05	3.06	0.00	1.59
53	1.62	1.62	1.62	1.62	2.24	2.24	2.24	1.62	3.40	3.25
54	1.08	1.08	1.62	1.93	2.92	2.92	2.92	1.62	4.51	2.86
55	1.62	1.62	1.62	1.54	2.61	2.61	2.61	1.62	4.01	2.00
56	1.62	1.62	1.62	1.33	2.61	2.61	2.61	1.62	0.00	1.78
57	1.62	1.62	1.62	1.06	2.61	2.61	2.61	1.62	1.67	3.30
58	1.62	1.62	1.62	1.06	2.42	2.42	2.42	1.62	6.07	3.29