Supplementary Data for

Occurrence, Distribution and Risks of Antibiotics in Urban Surface Water in Beijing, China

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Captions:

Table S1 Physicochemical characteristics of the target antibiotics

Table S2 Experimental conditions of electrospray tandem mass spectrometry

Table S3 Correlation coefficients (r^2), linear range, recoveries (%) and limits of detection (LODs, S/N=3) of 22 antibiotics

Table S4 Usage of some antibiotics in China in 2013.

Table S5 Acute toxicity data for selected antibiotics on aquatic organisms.

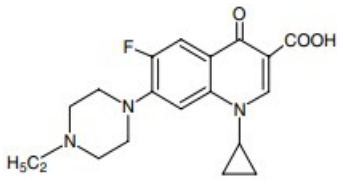
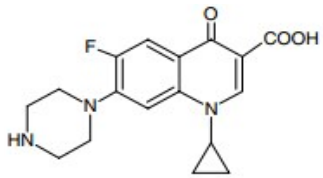
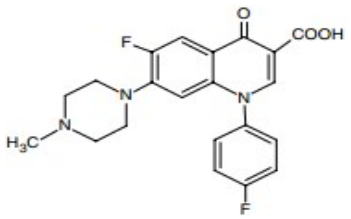
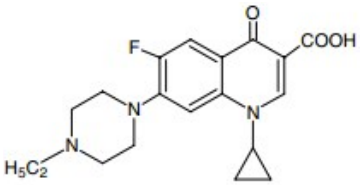
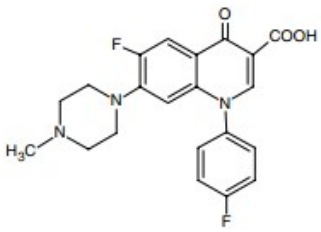
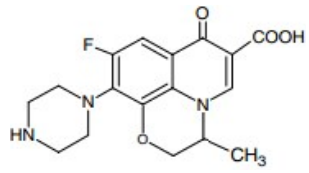
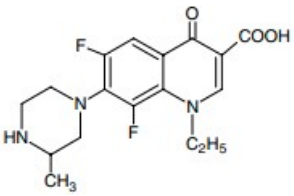
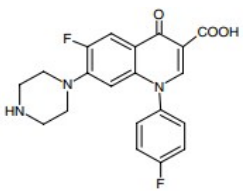
Table S6 Chronic toxicity data for selected antibiotics on aquatic organisms.

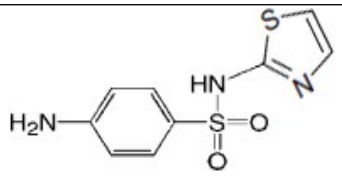
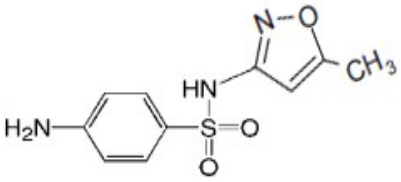
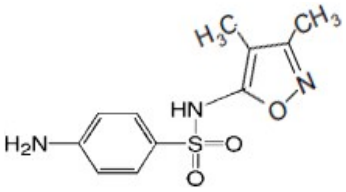
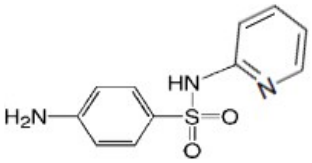
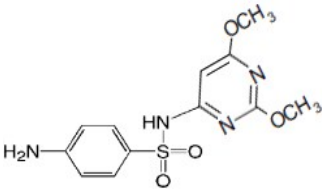
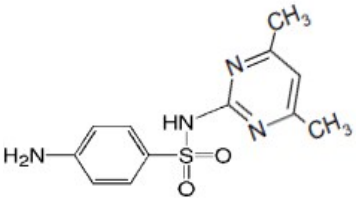
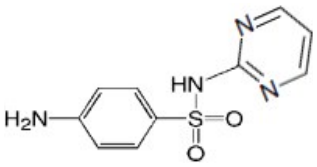
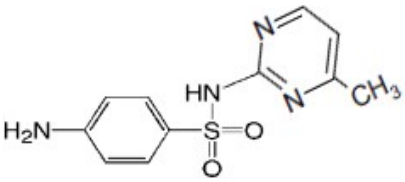
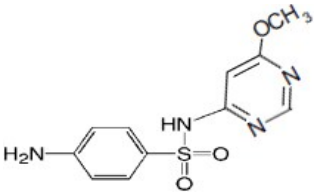
Fig. S1 Concentration-percent composition of antibiotics in 36 surface water samples

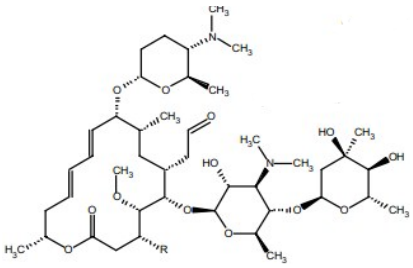
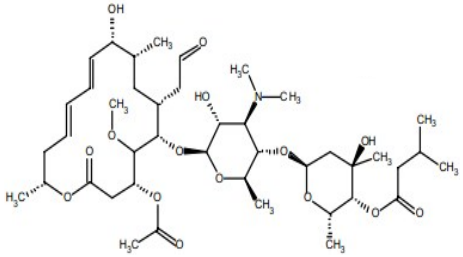
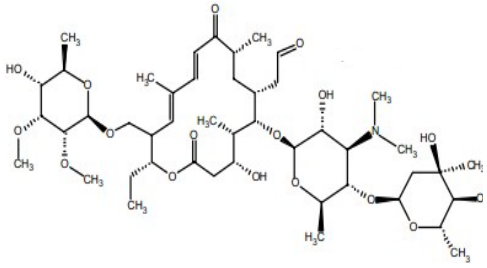
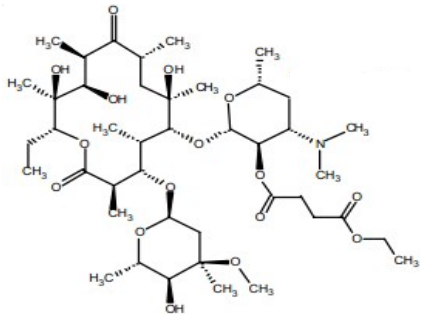
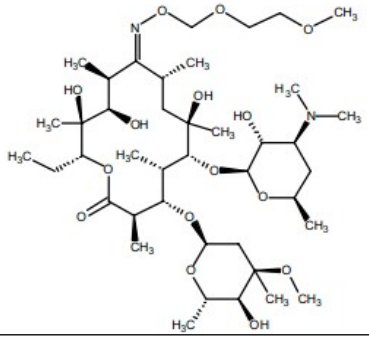
Fig. S2 Locations of animal farms in urban Beijing

Fig. S3 Distribution map of risk quotients (HQs) of OFL, SMX, ERY, and CIP in the surface water of Beijing.

Table S1 Physicochemical characteristics of the test antibiotics

Analytes	Structure	MW (g/mo1)	S_W(mg/L)	pKa	Log Kow
Norfloxacin (NOR)		319.3	540[1]	6.27; 8.3[2]	-1.03[3]
Ciprofloxacin (CIP)		331.3	700[1]	5.90; 8.89 [2]	-0.73[3]
Difloxacin (DIF)		399.4	n.a.	5.66; 7.24[2]	2.349
Enrofloxacin (ENR)		359.4	849.7[4]	5.86; 8.24[2]	1.1[4]
Fleroxacin (FLE)		369.4	na	5.46; 8.00[2]	1.08[5]
Ofloxacin (OFL)		361.3	230[1]	5.97; 8.28[6]	-0.70[3]
Lomefloxacin (LOM)		351.4	n.a.	6.56; 8.47[2]	-0.3[5]
Sarafloxacin (SAR)		385.4	100	6.0; 8.6[6]	0.84[7]

Sulfathiazole (STZ)		277.3	373[8]	2.08; 7.07[2]	0.72[8]
Sulfamethoxazole (SMX)		253.3	1382[4]	1.83; 5.57[2]	-0.43[3]
Sulfisoxazole (SIA)		267.3	300[8]	4.7[9]	1.01[8]
Sulfapyridine (SPD)		249.3	270	2.90; 8.54[2]	-1.18[3]
Sulfadimethoxine (SDM)		332.3	343[4]	2.4; 6.2[2]	1.63[4]
Sulfamethazine (SMZ)		278.3	1500[4]	2.28; 7.42 [2]	0.89[4]
Sulfadiazine (SDZ)		250.3	77	2.10; 6.28[2]	-0.092[10]
Sulfamerazine (SMR)		286.3	n.a.	2.17; 6.77[2]	0.21[5]
Sulfamonomethoxine (SMM)		280.0	4030[11]	2.0; 6.0[11]	0.7[12]

Spiramycin (SPI)		842.4	20[13]	8.0[9]	2.891
Josamycin (JOS)		827.3	n.a.	7.1[14]	4.169
Tylosin (TYL)		917.1	5000[15]	7.5[2]	3.074
Erythromycin (ERY)		733.9	1.4[16]	8.9[2]	2.362
Roxithromycin (ROX)		836.4	0.02[16]	9.2[2]	3.073

The table includes information on the hydrophobicity (log Kow); aqueous solubility (Sw) at neutral pH; acid-base reactivity (pKa); n.a.: not available.

Table S2 Experimental conditions of electrospray tandem mass spectrometry

Analytes	Parent ion (m/z)	Daughter ion (m/z)	Declustering Potential/ V	Entrance Potential/ V	Collision cellent potential/V	Collision Energy/ eV	Collision cell exit potential/ V
NOR	320.1	276.3	45	8.0	11	23	10
		302.2[a]	40	8.0	11	28	10
CIP	332.1	231.1	58	4.5	14	49	9.5
		314.3 [a]	55	5.0	11	28	6.0
DIF	400.0	299.1	60	4.0	13	41	12
		356.2 [a]	60	4.0	13	28	13
ENR	360.0	245.2	55	5.0	12	39	9.5
		316.2 [a]	58	5.0	11	28	11
FLE	370.0	269.2	45	4.5	20	34	10
		326.2 [a]	45	4.5	12	27	12
OFL	362.2	261.2	55	5.0	24	38	10
		318.2 [a]	55	5.0	12	27	11
LOM	352.0	265.2 [a]	53	5.0	12	34	10
		308.2	55	4.0	37	32	12
SAR	386.0	299.2	65	4.5	13	37	6.5
		368.2 [a]	60	4.5	14	31	7.0
NOR-d_5	325.3	281.4	50	8.5	11	23	6.0
		307.3 [a]	40	7.5	11	27	6.5
OFL-d_3	365.2	261.2	55	6	12	39	10
		321.2 [a]	55	6	12	28	11.5
SAR-d_8	394.2	350.3	60	6	13	28	12
		376.2 [a]	59	6	12	33	14
STZ	256.0	108.0	43	4.5	10	36	4.5
		156.0 [a]	42	4.2	10	21	4.5
SMX	254.0	156.0 [a]	45	4.0	9	23	5.2
		160.1	47	4.5	9	27	6.0
SIA	268.1	108.0	46	4.5	12	37	4.5
		156.0 [a]	46	4.5	9	21	5.0
SPD	250.1	108.0	38	7.0	11	36	4.5
		156.0 [a]	41	4.7	9	24	5.5
SDM	311.2	108.0	55	4.5	12	41	4.5
		156.1 [a]	57	4.0	12	30	6.0
SMZ	279.2	156.0	47	4.5	9	27	6.0
		186.1 [a]	49	4.0	10	25	6.5
SDZ	251.1	108.0	42	4.3	11	35	4.2
		156.0 [a]	43	3.5	9	23	5.0
SMR	265.2	107.9 [a]	47	4.5	11	37	4.5
		156.0	48	5.0	10	24	5.5

[a] quantitative ion

Table S2 Experimental conditions of electrospray tandem mass spectrometry (continued)

Analytes	Parent ion (m/z)	Daughter ion (m/z)	Declustering Potential/ V	Entrance Potential/ V	Collision cellent potential/V	Collision Energy/ eV	Collision cell exit potential/ V
SMM	281.2	156.0 [a]	50	5.0	10	26	5.5
		215.1	48	5.0	9	25	7.0
SMZ-d_4	283.1	160.0 [a]	48	4.5	10	28	6.0
		186.0	48	4.5	10	26	6.5
SMX-d_4	257.9	112.0	44	4.5	11	36	4.8
		160.0 [a]	44	4.5	9	25	5.5
SPI	843.4	174.1 [a]	87	10	30	50	8.0
		318.3	85	9.5	30	42	8.0
JOS	828.3	174.2 [a]	79	10	30	47	7.5
		229.1	77	10	28	43	8.5
TYL	916.3	174.0 [a]	83	10	33	55	8.0
		772.3	85	9.0	29	43	17
ERY	734.3	158.2 [a]	60	4.8	27	41	6.0
		576.3	58	4.8	23	28	12
ROX	837.4	158.1 [a]	62	7.0	30	48	7.0
		679.4	62	6.5	26	30	14
SPI I-d_3	846.4	174.1 [a]	85	10	30	52	8
		432.3	30	4.5	27	18	15
ERY-$^{13}C_3d_3$	738.0	162.1 [a]	55	5.0	25	45	7.0
		580.3	55	5.0	23	28	12

[a] quantitative ion

Table S3 Correlation coefficients (r), linear range, recoveries (%) and limits of detection (LODs，S/N=3) of 22 antibiotics

Groups	Analytes	Surrogates	r	Linear range (μg L^{-1})	Recovery (%)	LODs (μg L^{-1})
FQs	NOR	NOR-d_5	0.9974	0.1-500	87.5±7.4	0.1
	CIP	NOR-d_5	0.9987	0.05-500	82.7±11.4	0.1
	DIF	OFL-d_3	0.9985	0.05-500	74.3±10.3	0.1
	ENR	OFL-d_3	0.9990	0.05-500	97.4±8..9	0.1
	FLE	OFL-d_3	0.9984	0.1-500	97.6±6.8	0.15
	OFL	OFL-d_3	0.9988	0.1-500	104.0±8.5	0.2
	LOM	OFL-d_3	0.9967	0.05-500	72.4±3.3	0.1
	SAR	SAR-d_8	0.9992	0.05-200	95.9±4.6	0.1
SAs	STZ	SMX-d_4	0.9974	0.01-500	84.2±5.9	0.02
	SMX	SMX-d_4	0.9991	0.1-500	101.0±4.3	0.15
	SIA	SMX-d_4	0.9987	0.02-500	88.3±2.7	0.05
	SPD	SMZ-d_4	0.9985	0.02-500	98.0±5.3	0.04
	SDM	SMZ-d_4	0.9996	0.01-500	121.0±5.6	0.01
	SMZ	SMZ-d_4	0.9993	0.01-500	102.0±3.7	0.02
	SDZ	SMZ-d_4	0.9986	0.05-500	101.0±3.5	0.05
	SMR	SMZ-d_4	0.9977	0.02-500	107.0±7.1	0.05
	SMM	SMZ-d_4	0.9985	0.02-500	112.0±7.3	0.1
MCs	SPI	SPI I-d_3	0.9980	0.1-500	104.0±5.2	0.1
	JOS	SPI I-d_3	0.9934	0.05-200	84.4±5.6	0.05
	TYL	SPI I-d_3	0.9934	0.05-200	90.0±7.1	0.05
	ROX	SPI I-d_3	0.9905	0.05-500	101.0±6.1	0.1
	ERY	ERY-$^{13}C,d_3$	0.9992	0.1-500	109.0±5.3	0.15

Table S4 Usage of some antibiotics in China in 2013

Groups	Analytes	Primary usage	Usage (tons) [17]				
			Human	Pig	Chicken	Others	Total
FQs	NOR	Human, animal	1013	2820	961	644	5440
	CIP	Human, animal	455	3110	1060	712	5340
	DIF	Animal	0	378	172	117	667
	ENR	Animal	0	3090	1150	940	5180
	FLE	Human, animal	119	60.6	21.6	15.1	216
	OFL	Human, animal	1286	2440	832	557	5110
	LOM	Human, animal	228	650	222	149	1250
	SAR	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
	Total		**3101**	**12549**	**4419**	**3134**	**23203**
SAs	STZ	Animal	0.66	40.2	13.7	9.18	63.7
	SMX	Human, animal	2	198	67.6	45.3	313
	SIA	Human	n.a.	n.a.	n.a.	n.a.	n.a.
	SPD	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
	SDM	Animal [18]	n.a.	n.a.	n.a.	n.a.	n.a.
	SMZ	Human, animal	68.4	388	132	88.7	677
	SDZ	Human, animal (Animal forbidden)[19]	238	648	221	148	1260
	SMR	Human [18]	n.a.	n.a.	n.a.	n.a.	n.a.
	SMM	Animal	9.93	1400	477	320	2210
	Total		**319**	**2674**	**911**	**611**	**4524**
MCs	SPI	Human [19]	n.a.	n.a.	n.a.	n.a.	n.a.
	JOS	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
	TYL	Animal	0	3090	1050	706	4850
	ERY	Human, animal	1244	1580	565	377	3770
	ROX	Human, animal	184	112	67.3	22.5	386
	Total		**1428**	**4782**	**1682**	**1106**	**9006**

n.a.: not available

Table S5 Acute toxicity data for selected antibiotics on aquatic organisms.

Groups	Analytes	Taxonomic group	Species	L(E)C_{50}s (mg/L)	PNEC[a] (ng/L)	Reference
FQs	NOR	Algae	*S. obliquus*	50.18 (96 h)	50,180	[20]
		Invertebrate	*D. magna*	194.98 (48 h)	194,980	[20]
	CIP	Algae	*M. aeruginosa*	0.017 (24h)	17	[21]
		Algae	*P. subcapitata*	18.7 (24h)	18,700	[21]
		Plant	*L. minor*	0.203 (24h)	203	[21]
	ENR	Algae	*M. aeruginosa*	0.049 (24h)	49	[21]
		Algae	*P. subcapitata*	3.10 (24h)	3,100	[21]
		Plant	*L. minor*	0.114 (24h)	114	[21]
		Invertebrate	*D. magna*	56.7 (48h)	56,700	[4]
		Invertebrate	*M. macrocopa*	>200 (48h)	200,000	[4]
		Fish	*O. latipes*	>100 (48h)	100,000	[4]
	LOM	Algae	*M. aeruginosa*	0.186(24h)	186	[21]
		Algae	*P. subcapitata*	22.7 (24h)	22,700	[21]
	OFL	Algae	*M. aeruginosa*	0.021 (24h)	21	[21]
		Algae	*P. subcapitata*	1.44 (72 h)	1,440	[22]
		Plant	*L. minor*	0.126 (24h)	126	[21]
		Plant	*L. gibba*	0.121 (72 h)	121	[23]
		Invertebrate	*C. dubia*	17.41 (48 h)	17,410	[22]
		Invertebrate	*D. magna*	31.75 (72h)	31,750	[24]
		Invertebrate	*T. platyurus*	33.98 (72h)	33,980	[24]
		Fish	*B. rerio*	>1000 (72h)	1000,000	[24]
SAs	SMX	Algae	*S. leopolensis*	0.03 (96h)	30	[22]
		Invertebrate	*C. dubia*	15.51 (48 h)	15,510	[22]
		Invertebrate	*D. magna*	177.3 (96h)	177,300	[25]
		Invertebrate	*D. magna*	25.20 (72h)	25,200	[24]
		Invertebrate	*T. platyurus*	35.36(72h)	35,360	[24]
		Fish	*B. rerio*	>1000 (72h)	1000,000	[24]
		Fish	*O. latipes*	562.5 (96h)	562,500	[25]
	SDZ	Algae	*M. aeruginosa*	0.135 (72h)	135	[26]
		Algae	*S. capricornotum*	2.19 (72h)	2,190	[27]
		Algae	*S. vacuolatus*	2.22 (24h)	2,220	[28]
		Invertebrate	*D. magna*	221 (48h)	221,00	[29]
		Plant	*L. minor*	0.07(72h)	70	[28]
	SMZ	Algae	*P. subcapitata*	0.103 (72h)	103	[27]
		Invertebrate	*D. magna*	215.9 (48h)	215,900	[27]
		Invertebrate	*M. macrocopa*	110.7 (48h)	110,700	[27]
		Fish	*O. latipes*	>100 (48h)	100,000	[27]
	SDM	Algae	*S. vacuolatus*	9.85(24h)	9,850	[28]
		Plant	*L. minor*	0.02(72h)	20	[28]
	SPD	Algae	*S. vacuolatus*	5.28(24h)	5,280	[28]
		Plant	*L. minor*	0.46(72h)	460	[28]

Groups	Analytes	Taxonomic group	Species	L(E)C_{50}s (mg/L)	PNEC[a] (ng/L)	Reference
MCs	ROX	Invertebrate	*D. magna*	7.1 (96 h)	7,100	[30]
		Invertebrate	*M. macrocopa*	39.3 (96 h)	39,300	[30]
		Fish	*O. latipes*	288.3 (96 h)	288,300	[30]
	ERY	Algae	*P. subcapitata*	0.02 (72h)	20	[22]
		Invertebrate	*B. calyciflorus*	0.94 (48 h)	940	[22]
		Invertebrate	*C. dubia*	10.23(72h)	10,230	[24]
		Invertebrate	*D. magna*	22.45 (72h)	22,450	[24]
		Invertebrate	*T. platyurus*	17.68 (72h)	17,680	[24]
		Fish	*B. rerio*	>1000 (72h)	1000,000	[24]

PNEC[a] = Lowest EC_{50}/ 1000 for acute toxicity

Brachionus calyciflorus=B. calyciflorus; Brachydanio rerio=B. rerio; Ceriodaphnia dubia=C. dubia; Daphnia Magna=D. magna; Lemna gibba=L. gibba; Lemna minor=L. minor; Microcystis aeruginosa=M. aeruginosa; Moina macrocopa=M. macrocopa; Oryzias latipes=O. latipes; Oncorhynchus mykiss=O. mykiss; Pseudokirchneriella subcapitata=P. subcapitata; Selenastrum capricornotum= S. capricornotum; Synechoccus leopolensis=S. leopolensis; Scenedesmus obliquus=S. obliquus;Scenedesmus vacuolatus=S. vacuolatus; Thamnocephalus platyurus=T. platyurus

Table S6 Chronic toxicity data for selected antibiotics on aquatic organisms.

Groups	Analytes	Taxonomic group	Species	L(E)C_{50}s (mg/L)	PNEC [b] (ng/L)	Reference
FQs	NOR	Plant	*L. gibba*	0.913 (7 d)	9,130	[31]
	CIP	Plant	*L. gibba*	0.698 (7 d)	6,980	[31]
	LOM	Plant	*L. minor*	0.106(7d)	1,060	[21]
	OFL	Plant	*L. gibba*	0.532 (7 d)	5,320	[31]
SAs	SMX	Plant	*L. gibba*	0.081 (7 d)	810	[31]
		Plant	*L. gibba*	0.21 (7 d)	2,100	[24]
	SMZ	Plant	*L. gibba*	1.277 (7 d)	12,770	[27]
MCs	ROX	Plant	*L. gibba*	>1 (7 d)	10,000	[31]
	ERY	Plant	*L. gibba*	>1 (7 d)	10,000	[31]
		Plant	*L. minor*	5.62 (7 d)	56,200	[32]

PNEC[b]= Lowest EC_{50}/ 100 for chronic toxicity

Lemna gibba=L. gibba; Lemna minor=L. minor

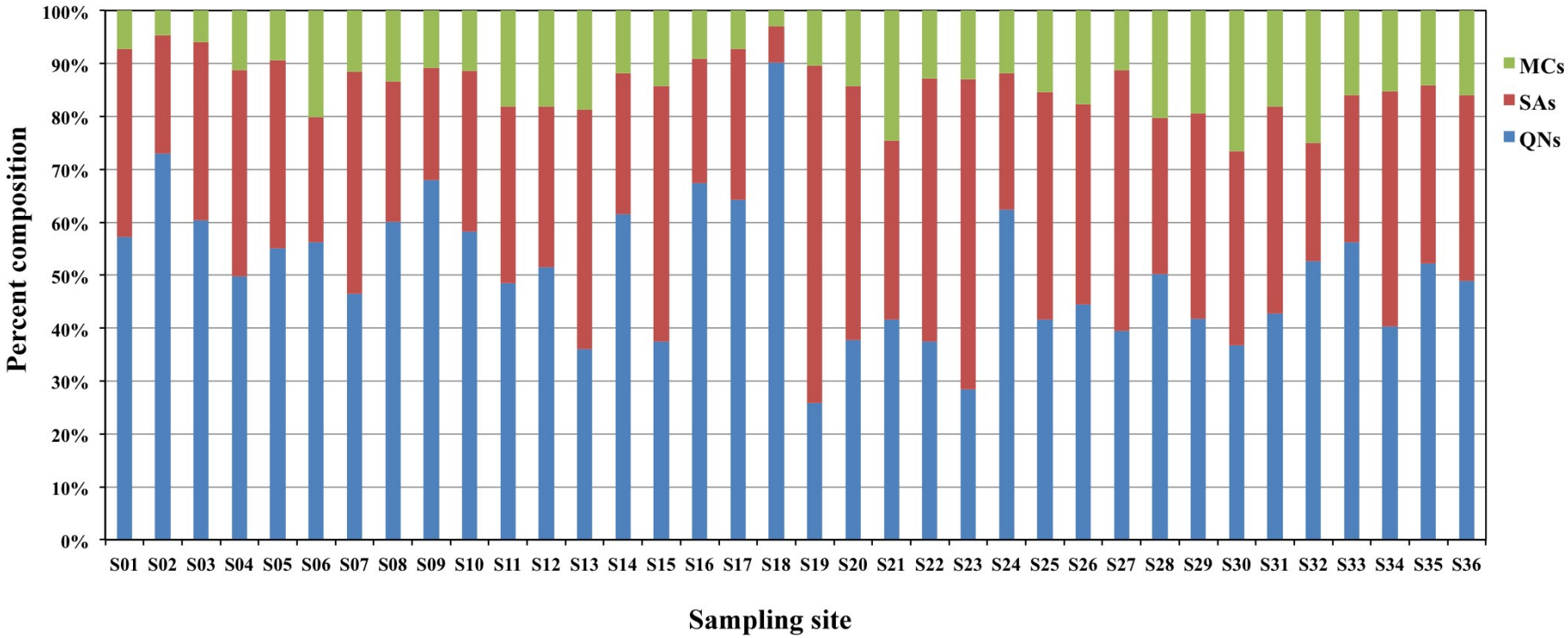


Fig.S1 Concentration-percent composition of antibiotics in 36 surface water samples

Fig. S2 Locations of animal farms in urban Beijing

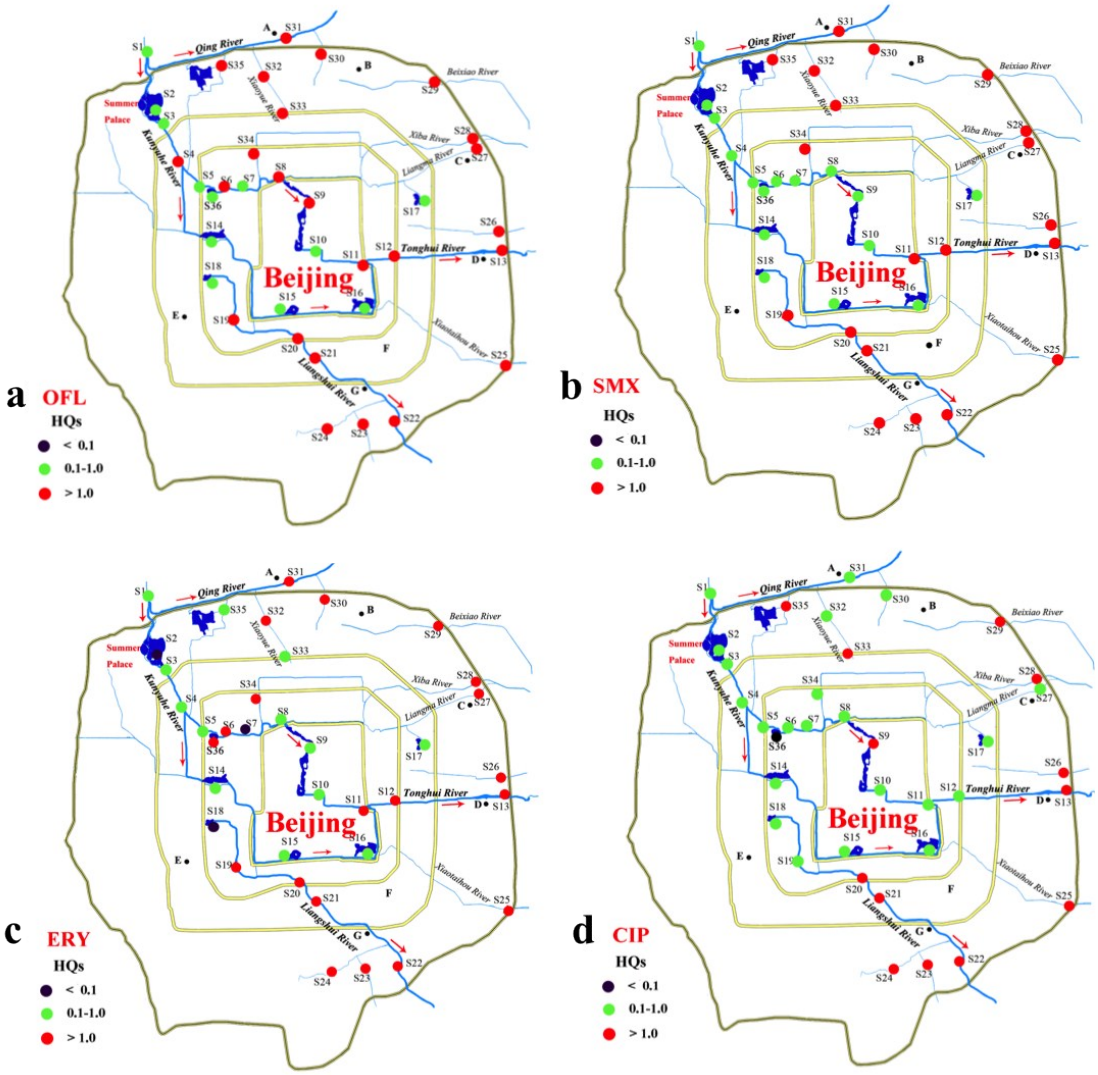


Fig. S3 Distribution map of risk quotients (HQs) of OFL (a), SMX (b), ERY (c), and CIP (d) in the surface water of Beijing.

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