Supporting information for

Environmental Science and Pollution Research

Identifying unknown persistent, bioaccumulative and risky antibiotics in river water in Beijing, China

Qingwei Bu[1,*], Hongmei Cao[1], Qingshan Li[1], Handan Zhang[1], Weiwei Jiang[2], Gang Yu[3]

[1] School of Chemical & Environmental Engineering, China University of Mining & Technology-Beijing, Beijing 100083, P.R. China

[2] Shanghai National Engineering Research Center of Urban Water Resources Co., Ltd, Shanghai 200082, P.R. China

[3] School of Environment, State Key Joint Laboratory of Environmental Simulation and Pollution Control, Beijing Key Laboratory for Emerging Organic Contaminants Control, Tsinghua University, Beijing 100084, P.R. China

***, Corresponding author**

[*]Address correspondence to Qingwei Bu, School of Chemical & Environmental Engineering, China University of Mining & Technology-Beijing, Beijing 100083, P.R. China. E-mail: qingwei.bu@cumtb.edu.cn

Number of pages: 10
Number of tables: 4
Number of figures: 3

Table S1. List of 95 human use antibiotics in China

CAS no.	Antibiotics	Therapeutic group	PV, kg	KOWWIN	BIOWIN1	HPV	P	B
085721-33-1	Ciprofloxacin	Fluoroquinolones	1745104	0	-0.3974	×	×	
000599-79-1	Sulfasalazine	Sulfonamides	49684	3.81	0.4541		×	×
005250-39-5	Flucloxacillin	β-Lactams	22453	3.42	-0.0972		×	×
062013-04-1	Dirithromycin	Macrolides	26384	3	-1.2900		×	×
081103-11-9	Clarithromycin	Macrolides	384338	3.18	-1.7926		×	×
083905-01-5	Azithromycin	Macrolides	772983	3.24	-1.6578		×	×
000057-62-5	Chlortetracycline	Sulfonamides	75257	-0.68	0.4211		×	
000057-68-1	Sulfadimidine	Sulfonamides	228266	0.76	0.4906		×	
000057-92-1	Streptomycin	Aminoglycosides	760611	-7.53	0.2881		×	
000068-35-9	Sulfadiazine	Sulfonamides	298158	-0.34	0.3946		×	
000114-07-8	Erythromycin	Macrolides	528338	2.48	-1.4385		×	
000723-46-6	Sulfamethoxazole	Sulfonamides	968684	0.48	0.4479		×	
001695-77-8	Spectinomycin	Aminoglycosides	71826	-0.82	-0.0047		×	
008025-81-8	Spiramycin	Macrolides	48902	1.87	-1.7448		×	
023155-02-4	Fosfomycin	others	557794	-1.53	0.3345		×	
024916-51-6	Acetylspiramycin	Macrolides	371356	2.03	-1.7494		×	
032385-11-8	Sisomicin	Aminoglycosides	663	-3.45	0.0477		×	
051940-44-4	Pipemidic acid	Fluoroquinolones	140188	-1.7	0.4260		×	
056391-56-1	Netilmicin	Aminoglycosides	127	-2.5	0.0344		×	
070458-96-7	Norfloxacin	Fluoroquinolones	537681	-0.31	-0.3916		×	
074011-58-8	Enoxacin	Fluoroquinolones	201098	-0.21	-0.5467		×	
078110-38-0	Aztreonam	others	172450	-3.36	0.4054		×	
080214-83-1	Roxithromycin	Macrolides	348732	2.75	-2.1892		×	
082419-36-1	Ofloxacin	Fluoroquinolones	174634	-0.2	-0.6388		×	
098079-51-7	Lomefloxacin	Fluoroquinolones	1238	0.31	-1.2169		×	
100986-85-4	Levofloxacin	Fluoroquinolones	519092	-0.2	-0.6388		×	
112811-59-3	Gatifloxacin	Fluoroquinolones	25922	0.5	-0.2864		×	
127045-41-4	Pazufloxacin	Fluoroquinolones	31016	-0.13	-0.2379		×	
127294-70-6	Balofloxacin	Fluoroquinolones	1972	0.99	-0.2931		×	
000061-72-3	Cloxacillin	β-Lactams	2777	3.22	0.7213			×
006990-06-3	Fusidic acid	others	1164	6.75	0.5141			×
000061-33-6	Benzylpenicillin	β-Lactams	2115750	1.85	1.0802	×		
000069-53-4	Ampicillin	β-Lactams	3268503	1.45	1.1722	×		
000079-57-2	Oxytetracycline	Sulfonamides	6831824	-2.87	0.7710	×		
000154-21-2	Lincomycin	Lincosamides	1350475	0.29	0.8465	×		
000738-70-5	Trimethoprim	Trimethoprims	1156363	0.73	0.5922	×		
026787-78-0	Amoxicillin	β-Lactams	15844961	0.97	1.1523	×		
038821-53-3	Cefradine	Cephalosporins	2266176	0.41	1.2280	×		
063527-52-6	Cefotaxime	Cephalosporins	1759217	0.64	0.9641	×		

CAS no.	Antibiotics	Therapeutic group	PV, kg	KOWWIN	BIOWIN1	HPV	P	B
069739-16-8	Cefodizime	Cephalosporins	1786466	0.71	0.9105	×		
073384-59-5	Ceftriaxone	Cephalosporins	1381391	-1.37	0.7428	×		
000056-75-7	Chloramphenicol	Amphenicols	474923	0.92	0.5935			
000059-01-8	Kanamycin	Aminoglycosides	158811	-6.70	0.8539			
000060-54-8	Tetracycline	Tetracyclines	880055	-1.33	0.6199			
000066-79-5	Oxacillin	β-Lactams	16818	2.57	1.0483			
000080-35-3	Sulfamethoxypyridazine	Sulfonamides	16051	0.20	0.5123			
000087-08-1	Phenoxymethylpenicillin	β-Lactams	679165	1.87	1.1498			
000519-02-8	Matrine	Others	6659	1.71	0.6342			
000564-25-0	Doxycycline	Tetracyclines	260877	-1.36	1.0172			
000914-00-1	Metacycline	Tetracyclines	6200	-1.37	0.9635			
001404-90-6	Vancomycin	Others	25749	-0.84	2.0137			
004697-36-3	Carbenicillin	β-Lactams	1641	1.19	1.1319			
005508-58-7	Andrographolide	Others	160320	1.90	0.8632			
015318-45-3	Thiamphenicol	Amphenicols	17990	-0.33	0.8828			
015686-71-2	Cefalexin	Cephalosporins	270693	0.40	1.3571			
016837-52-8	Ammothamnine	Others	142926	-1.35	0.8314			
018323-44-9	Clindamycin	Lincosamides	80050	2.01	0.5676			
021967-41-9	Baicalin	Others	187797	0.74	1.3669			
025953-19-9	Cefazolin	Cephalosporins	439144	-2.19	1.0788			
026973-24-0	Ceftezole	Cephalosporins	204913	-2.74	1.0308			
032986-56-4	Tobramycin	Aminoglycosides	6827	-5.76	0.6983			
033075-00-2	Cefathiamidine	Cephalosporins	185897	0.86	1.1897			
034444-01-4	Cefamandole	Cephalosporins	91647	-0.71	1.3072			
034787-01-4	Ticarcillin	β-Lactams	17668	1.01	1.0010			
035607-66-0	Cefoxitin	Cephalosporins	106774	0.22	0.6400			
037091-66-0	Azlocillin	β-Lactams	193733	1.71	0.8095			
037517-28-5	Amikacin	Aminoglycosides	351448	-8.78	1.1746			
050370-12-2	Cefadroxil	Cephalosporins	161670	-0.08	1.3372			
053994-73-3	Cefaclor	Cephalosporins	73302	0.35	1.2360			
055268-75-2	Cefuroxime	Cephalosporins	925752	0.29	1.1180			
056796-20-4	Cefmetazole	Cephalosporins	51606	-0.94	0.7918			
058152-03-7	Isepamicin	Aminoglycosides	354	-7.17	0.8396			
058569-36-1	Sulbenicillin	β-Lactams	18461	0.81	1.0958			
061270-58-4	Cefonicid	Cephalosporins	3695	-3.93	1.3774			
061477-96-1	Piperacillin	β-Lactams	417065	1.83	1.1484			
061622-34-2	Cefotiam	Cephalosporins	135673	-1.40	0.6060			
062893-19-0	Cefoperazone	Cephalosporins	688303	-0.42	1.2591			
064544-07-6	Cefuroxime axetil	Cephalosporins	303584	0.11	1.3527			
065243-33-6	Cefetamet pivoxil	Cephalosporins	24651	1.86	0.8550			

CAS no.	Antibiotics	Therapeutic group	PV, kg	KOWWIN	BIOWIN1	HPV	P	B
068373-14-8	Sulbactam	β-Lactams	370552	0.50	0.7354			
068401-81-0	Ceftizoxime	Cephalosporins	124882	0.55	0.8243			
070797-11-4	Cefpiramide	Cephalosporins	12497	0.30	1.2907			
072558-82-8	Ceftazidime	Cephalosporins	416731	-1.36	0.6344			
079350-37-1	Cefixime	Cephalosporins	245004	0.12	0.8636			
080370-57-6	Ceftiofur	Cephalosporins	669	1.57	0.7575			
084305-41-9	Cefminox	Cephalosporins	321919	-4.37	0.6884			
084957-29-9	Cefpirome	Cephalosporins	12714	2.67	0.8707			
088376-58-3	Cefepime	Cephalosporins	70257	0.20	0.7770			
089786-04-9	Tazobactam	β-Lactams	19369	-1.72	0.7035			
091700-98-0	Norvancomycin	Others	391	-1.31	2.0203			
091832-40-5	Cefdinir	Cephalosporins	20666	1.47	0.8185			
096036-03-2	Meropenem	β-Lactams	86658	-1.25	1.3705			
120410-24-4	Biapenem	β-Lactams	360	-2.97	1.0213			
756762-35-3	Mezlocillin	β-Lactams	484431	2.98	0.9073			
783258-71-9	Houttuyfonate	Others	39224	-0.57	0.9964			

Table S2. Number of antibiotics in each therapeutic group

Therapeutic group	Number of antibiotics		
	Total	P, B or P&B	not P and not B
Aminoglycosides	8	4	4
Amphenicols	2	0	2
Cephalosporins	28	0	28
Fluoroquinolones	10	10	0
Lincosamides	2	0	2
Macrolides	7	7	0
Others	10	3	7
Sulfonamides	7	5	2
Tetracyclines	3	0	3
Trimethoprims	1	0	1
β-Lactams	17	2	15
SUM	95	31	64

Table S3. Analytical conditions employed for targeted screening procedure

HPLC-MS/MS analytical conditions					
Instrument	Shimadzu high performance liquid chromatograph (LC-30A) coupled with a TSQ mass spectrometer (LCMS-8030)				
Column	Shim-pack XR-ODS C18, 2 mm × 75 mm, 2.2 μm				
Mobile phase	Formic acid:H_2O/Acetonitrile gradient elution				
Ionization mode	ESI negative/positive				
MS mode	Precursor/product ion spectra, multiple reaction monitoring (MRM)				
MS/MS parameters for target antibiotics					
Substances	Precursor ion (m/z)	Product ion (m/z)	Q1 Pre bias	CE (eV)	Q3 Pre Bias
Erythromycylamine	368.35	83.15 115.2	18	24	16
Ampicillin	350.2	106.2 192.2	17	19	19
Cefotaxime	456.15	395.95 323.9	22	11	28
Fusidic acid	539.3[a]	479.4	28	19	24

[a] It is the precursor ion of sodium fusidate as only this form is available for pharmaceutical use and analytical standards.

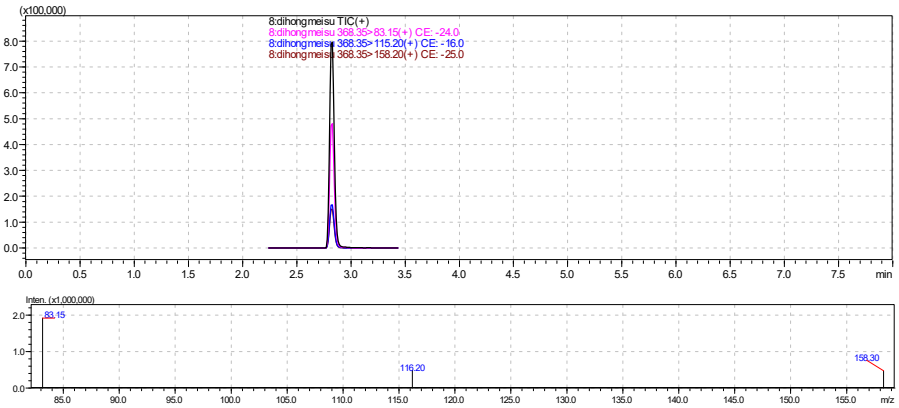
Table S4. Validation of method performance for determination of antibiotics in water samples with different spiked concentrations

Pharmaceutical	Recovery (Mean±SD, %) at varied spiked levels			LOD, ng/L	LOQ, ng/L	MDL, ng/L
	30 ng/L[a]	80 ng/L	150 ng/L			
Erythromycylamine	61.9±11.4	70.4±3.40	60.4±10.7	0.05	0.16	0.13
Ampicillin	54.4±7.50	53.2±9.10	54.1±4.50	0.08	0.26	0.43
Cefotaxime	119±5.40	104±8.00	104±10.5	0.20	0.60	0.66
Fusidic acid	92.3±6.10	91.3±10.8	90.9±5.80	0.86	2.60	3.97

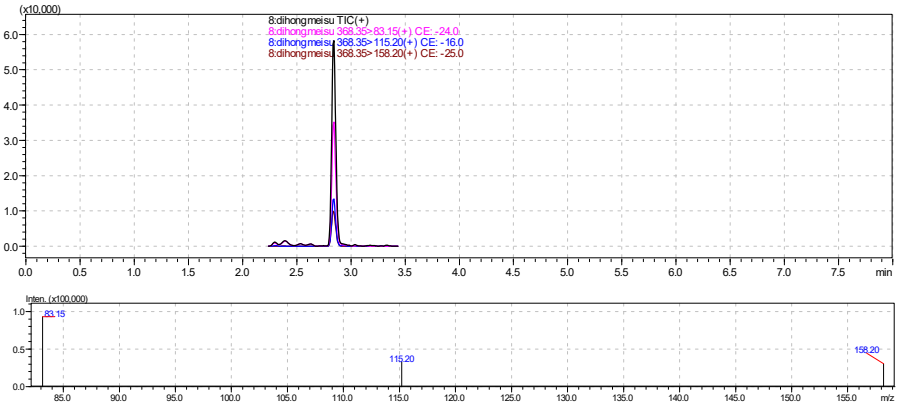
[a] Spiked concentration

LOD, limit of detection; LOQ, limit of quantification; MDL, method detection limit

A)



B)



C)

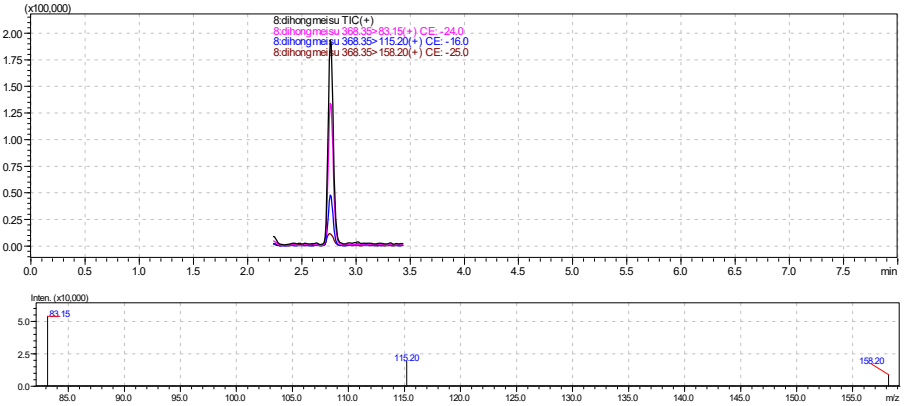
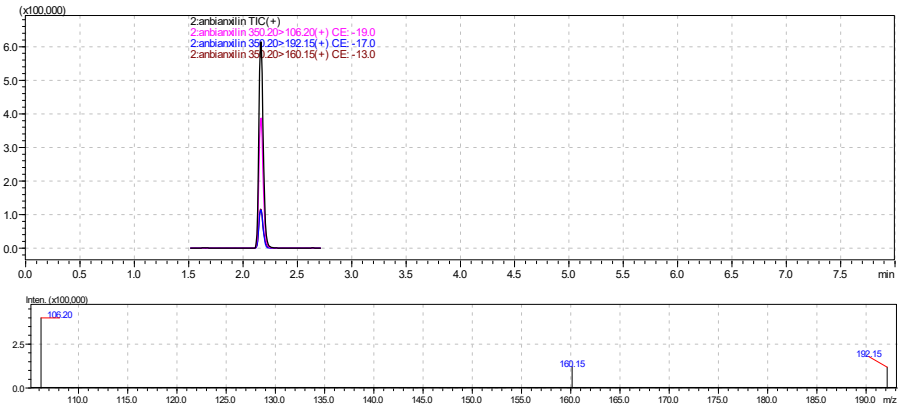


Figure S1. Chromatogram and mass spectra of erythromycylamine in: A) a standard solution; B) spikes samples; C) water from Qing River

A)



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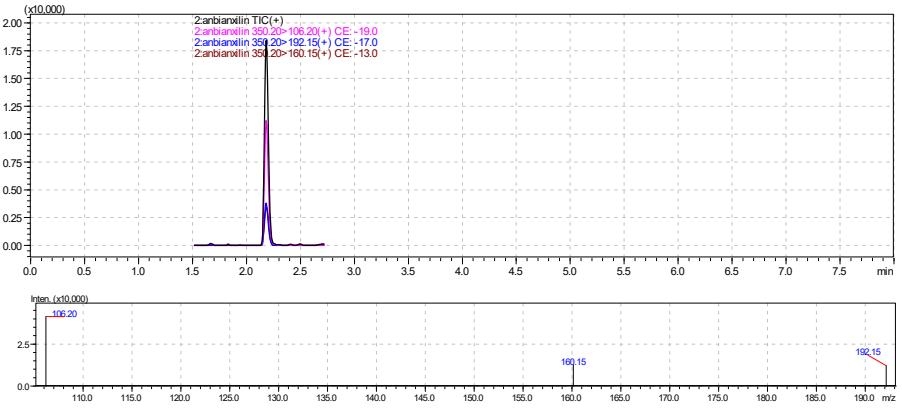


C)

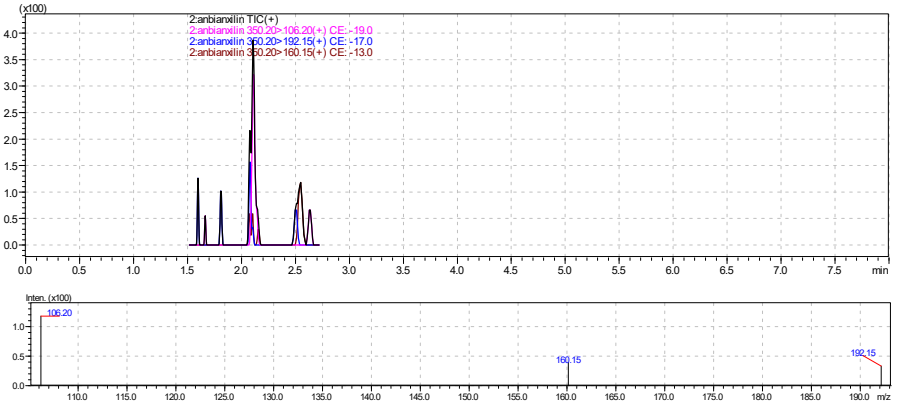
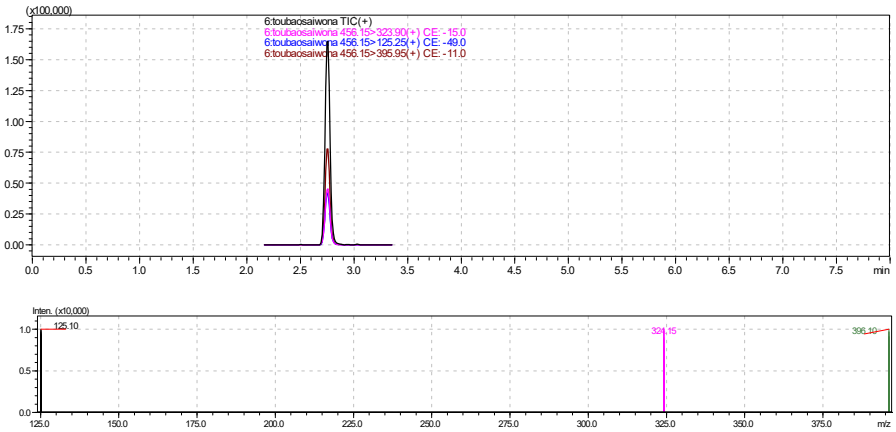
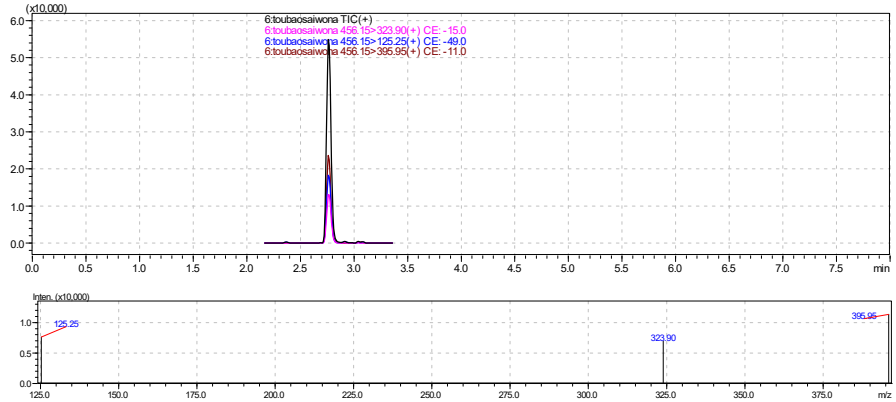


Figure S2. Chromatogram and mass spectra of ampicillin in: A) a standard solution; B) spikes samples; C) water from Qing River

A)



B)



C)

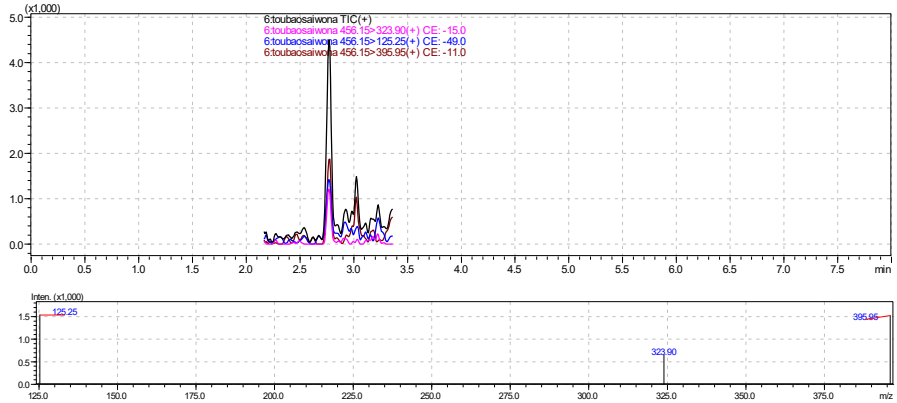


Figure S3. Chromatogram and mass spectra of cefotaxime in: A) a standard solution; B) spikes samples; C) water from Qing River