

Supporting Information

Spatio-temporal distribution and risk assessment of antibiotics in the aquatic environment in China nationwide

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Table S1 Physico-chemical properties of antibiotics investigated in this study

Class	Compound	Abbreviation	CAS NO.	Molecular formula	Molecular weight	logK _{ow}	pK _a
β-lactams	Penicillin V	PENV	87-08-1	C ₁₆ H ₁₈ N ₂ O ₅ S	350.389	1.88 ^a	2.73
	Penicillin G	PENG	61-33-6	C ₁₆ H ₁₈ N ₂ O ₄ S	334.390	1.83 ^b	2.74
	Cephalexin	CLX	15686-71-2	C ₁₆ H ₁₇ N ₃ O ₄ S	347.389	0.65	5.20
	Cefradine	CRD	38821-53-3	C ₁₆ H ₁₉ N ₃ O ₄ S	349.405	0.98	2.60
	Amoxicillin	AMOX	26787-78-0	C ₁₆ H ₁₉ N ₃ O ₅ S	365.404	0.87	3.20
	Mezlocillin	MEZ	51481-65-3	C ₂₁ H ₂₅ N ₅ O ₈ S ₂	539.582	1.18	- ^c
	Ampicillin	AMP	69-53-4	C ₁₆ H ₁₉ N ₃ O ₄ S	349.405	1.65	2.50
	Cefuroxime	CFO	55268-75-2	C ₁₆ H ₁₆ N ₄ O ₈ S	424.385	0.47	-
	Cefadroxil	CFD	50370-12-2	C ₁₆ H ₁₇ N ₃ O ₅ S	363.388	0.09	-
	Ceftriaxone	CER	73384-59-5	C ₁₈ H ₁₈ N ₈ O ₇ S ₃	554.580	0.77	-
	Cefotaxim	CTX	60846-21-1	C ₁₆ H ₁₇ N ₅ O ₇ S ₂	455.465	0.29	-
	Cefazolin	CFZ	25953-19-9	C ₁₄ H ₁₄ N ₈ O ₄ S ₃	454.507	1.13	-
	Cefmetazole	CFM	56796-20-4	C ₁₅ H ₁₇ N ₇ O ₅ S ₃	471.534	0.97	-
macrolides	Erythromycin	ERY	114-07-8	C ₃₇ H ₆₇ NO ₁₃	733.927	3.06	8.90
	Roxithromycin	ROX	80214-83-1	C ₄₁ H ₇₆ N ₂ O ₁₅	837.047	3.73	-
	Tylosin	TYL	1401-69-0	C ₄₆ H ₇₇ NO ₁₇	916.100	1.63	7.73
	Azithromycin	AZI	83905-01-5	C ₃₈ H ₇₂ N ₂ O ₁₂	748.984	4.02	8.74
	Spiramycin	SPI	8025-81-8	C ₄₃ H ₇₄ N ₂ O ₁₄	843.053	1.87	7.88
	Josamycin	JOS	16846-24-5	C ₄₂ H ₆₉ NO ₁₅	827.995	3.88	-
	Clarithromycin	CLR	81103-11-9	C ₃₈ H ₆₉ NO ₁₃	747.953	3.16	8.99
	Kitasamycin	KIT	1392-21-8	C ₄₀ H ₆₇ NO ₁₄	785.958	3.35	-
	Oleandomycin	ODM	3922-90-5	C ₃₅ H ₆₁ NO ₁₂	687.858	1.69	8.84
	Leucomycin	LCM	8025-81-8	C ₄₃ H ₇₄ N ₂ O ₁₄	843.053	1.87	7.88
sulfonamides	Sulfanilamide	SA	63-74-1	C ₆ H ₈ N ₂ O ₂ S	172.205	0.62	10.58
	Sulfapyridine	SP	144-83-2	C ₁₁ H ₁₁ N ₃ O ₂ S	249.289	0.35	8.43
sulfonamides	Sulfacetamide	SAAM	144-80-9	C ₈ H ₁₀ N ₂ O ₃ S	214.242	0.96	-
	Sulfadimethoxine	SDM	122-11-2	C ₁₂ H ₁₄ N ₄ O ₄ S	310.329	1.63	-
	Sulfameter	SM	651-06-9	C ₁₁ H ₁₂ N ₄ O ₃ S	280.303	0.41	-

Class	Compound	Abbreviation	CAS NO.	Molecular formula	Molecular weight	logK _{ow}	pK _a
fluoroquinolones	Sulfamethazine	SMZ	57-68-1	C ₁₂ H ₁₄ N ₄ O ₂ S	278.330	0.14	2.65
	Sulfaguanidine	SGD	57-67-0	C ₇ H ₁₀ N ₄ O ₂ S	214.245	1.22	11.25
	Sulfamethoxazole	SMX	723-46-6	C ₁₀ H ₁₁ N ₃ O ₃ S	253.278	0.89	1.60
	Sulfamerazin	SMR	127-79-7	C ₁₁ H ₁₂ N ₄ O ₂ S	264.304	0.14	-
	Sulfamonomethoxine	SMM	1220-83-3	C ₁₁ H ₁₂ N ₄ O ₃ S	280.303	0.70	-
	Sulfaquinoxaline	SQ	59-40-5	C ₁₄ H ₁₂ N ₄ O ₂ S	300.336	1.68	5.10
	Sulfachloropyridazine	SCP	80-32-0	C ₁₀ H ₉ ClN ₄ O ₂ S	284.722	3.25	-
	Sulfadiazine	SD	68-35-9	C ₁₀ H ₁₀ N ₄ O ₂ S	250.277	0.09	6.36
	Sulfathiazole	STZ	72-14-0	C ₉ H ₉ N ₃ O ₂ S ₂	255.317	0.05	2.20
	Sulfisoxazole	SIA	127-69-5	C ₁₁ H ₁₃ N ₃ O ₃ S	267.304	1.01	1.50
	Trimethoprim	TMP	738-70-5	C ₁₄ H ₁₈ N ₄ O ₃	290.318	0.91	7.12
	Sulfadoxine	SDX	2447-57-6	C ₁₂ H ₁₄ N ₄ O ₄ S	310.329	0.70	-
	Sulfamethoxypyridazine	SMP	80-35-3	C ₁₁ H ₁₂ N ₄ O ₃ S	280.303	0.32	6.70
	Sulfadimidine	SM2	57-68-1	C ₁₂ H ₁₄ N ₄ O ₂ S	278.330	0.89	7.59
	Sulfamethizole	SML	144-82-1	C ₉ H ₁₀ N ₄ O ₂ S ₂	270.331	0.54	-
	Sulfisomidine	SIM	515-64-0	C ₁₂ H ₁₄ N ₄ O ₂ S	278.330	0.33	-
	Sulfamethiazole	SMT	144-82-1	C ₉ H ₁₀ N ₄ O ₂ S ₂	270.331	0.54	-
	Pipemidicacid	PPA	51940-44-4	C ₁₄ H ₁₇ N ₅ O ₃	303.316	2.15	-
	Fleroxacin	FLE	79660-72-3	C ₁₇ H ₁₈ F ₃ N ₃ O ₃	369.338	0.24	-
	Ciprofloxacin	CIP	85721-33-1	C ₁₇ H ₁₈ FN ₃ O ₃	331.341	0.28	6.09
	Gatifloxacin	GAT	112811-59-3	C ₁₉ H ₂₂ FN ₃ O ₄	375.394	1.21	-
	Lomefloxacin	LOM	98079-51-7	C ₁₇ H ₁₉ F ₂ N ₃ O ₃	351.348	0.30	-
	Moxifloxacin	MXF	151096-09-2	C ₂₁ H ₂₄ FN ₃ O ₄	401.430	0.95	-
	Norfloxacin	NOR	70458-96-7	C ₁₆ H ₁₈ FN ₃ O ₃	319.331	0.46	6.34
	Ofloxacin	OFL	82419-36-1	C ₁₈ H ₂₀ FN ₃ O ₄	361.367	0.39	5.97
fluoroquinolones	Enrofloxacin	ENR	93106-60-6	C ₁₉ H ₂₂ FN ₃ O ₃	359.395	0.70	-
	Difloxacin	DIF	98106-17-3	C ₂₁ H ₁₉ F ₂ N ₃ O ₃	399.391	2.72	-
	Marbofloxacin	MAR	115550-35-1	C ₁₇ H ₁₉ FN ₄ O ₄	362.356	0.55	-
	Nalidixicacid	NDA	389-08-2	C ₁₂ H ₁₂ N ₂ O ₃	232.235	1.59	8.60

Class	Compound	Abbreviation	CAS NO.	Molecular formula	Molecular weight	logK _{ow}	pK _a
	Pefloxacin	PEF	70458-92-3	C ₁₇ H ₂₀ FN ₃ O ₃	333.357	0.27	-
	Sarafloxacin	SRA	98105-99-8	C ₂₀ H ₁₇ F ₂ N ₃ O ₃	385.364	1.07	5.60
	Danofloxacin	DAN	112398-08-0	C ₁₉ H ₂₀ FN ₃ O ₃	357.379	1.20	-
	Flumequine	FMQ	42835-25-6	C ₁₄ H ₁₂ FNO ₃	261.248	1.60	-
	Sparfloxacin	SPA	110871-86-8	C ₁₉ H ₂₂ F ₂ N ₄ O ₃	392.400	1.60	-
	Enoxacin	ENO	74011-58-8	C ₁₅ H ₁₇ FN ₄ O ₃	320.319	0.20	-
	Oxolinicacid	OLA	14698-29-4	C ₁₃ H ₁₁ NO ₅	261.230	0.94	6.87
	Orbifloxacin	ORB	113617-63-3	C ₁₉ H ₂₀ F ₃ N ₃ O ₃	395.380	2.37	-
	Pyrroleacid	PA	89059-06-3	C ₇ H ₉ NO ₂	139.152	0.96	-
	Flumequin	FLU	42835-25-6	C ₁₄ H ₁₂ FNO ₃	261.248	1.60	-
lincosamides	Lincomycin	LIN	154-21-2	C ₁₈ H ₃₅ ClN ₂ O ₆ S	442.998	0.20	7.60
chloramphenicols	Florfenicol	FF	73231-34-2	C ₁₂ H ₁₄ Cl ₂ FNO ₄ S	358.213	0.12	-
	Chloramphenicol	CAP	56-75-7	C ₁₁ H ₁₂ Cl ₂ N ₂ O ₅	323.129	1.14	-
	Thiamphenicol	TAP	15318-45-3	C ₁₂ H ₁₅ C ₁₂ NO ₅ S	356.222	0.33	-
imidazole	Metronidazole	MET	443-48-1	C ₆ H ₉ N ₃ O ₃	171.154	0.02	-
tetracyclines	Chlortetracycline	CTC	57-62-5	C ₂₂ H ₂₃ ClN ₂ O ₈	478.880	0.62	3.30
	Doxycycline	DOX	564-25-0	C ₂₂ H ₂₄ N ₂ O ₈	444.435	1.36	-
	Tetracycline	TET	60-54-8	C ₂₂ H ₂₄ N ₂ O ₈	444.435	1.37	3.30
	Oxytetracycline	OTC	79-57-2	C ₂₂ H ₂₄ N ₂ O ₉	460.434	0.90	9.50
glycopeptides	Vancomycin	VAN	1404-90-6	C ₆₆ H ₇₅ Cl ₂ N ₉ O ₂₄	1449.250	4.73	2.60

^a Values in black obtained from Chemical search engine in Chinese: <https://www.chemsrc.com/>.

^b Values in red obtained from U.S. National Library of Medicine: <http://toxnet.nlm.nih.gov/>.

^c Not available.

Table S2 abbreviation and full name index

Abbreviation	Full Name	Abbreviation	Full Name
AF	Appropriate Standard Assessment Factor of 1000	ENR	Enrofloxacin
AMOX	Amoxicillin	ERY	Erythromycin
AMP	Ampicillin	FF	Florfenicol
AZI	Azithromycin	FLE	Fleroxacin
BS	Bohai Sea	FLU	Flumequin
CAP	Chloramphenicol	FMQ	Flumequine
CC	Central China	GAT	Gatifloxacin
CER	Ceftriaxone	JOS	Josamycin
CFD	Cefadroxil	KIT	Kitasamycin
CFM	Cefmetazole	LC ₅₀	Lethal Concentration 50
CFO	Cefuroxime	LCM	Leucomycin
CFZ	Cefazolin	LIN	Lincomycin
CIP	Ciprofloxacin	LOM	Lomefloxacin
CLR	Clarithromycin	MAR	Marbofloxacin
CLX	Cephalexin	MCs	Macrolides
COVID-19	Corona Virus Disease 2019	MDL	Method Detection Level
CPs	Chloramphenicols	MEC	Measured Environmental Concentration
CRD	Cefradine	MET	Metronidazole
CTC	Chlortetracycline	MEZ	Mezlocillin
CTX	Cefotaxim	MXF	Moxifloxacin
DAN	Danofloxacin	NC	Northern China
DIF	Difloxacin	NDA	Nalidixicacid
DOX	Doxycycline	NEC	Northeastern China
EC	Eastern China	NOEC	No Observed Effect Concentration
EC ₅₀	Concentration for 50% of Maximal Effect	NOR	Norfloxacin
ENO	Enoxacin	NWC	Northwestern China

Abbreviation	Full Name	Abbreviation	Full Name
ODM	Oleandomycin	SIM	Sulfisomidine
OFL	Ofloxacin	SM	Sulfameter
OLA	Oxolinicacid	SM2	Sulfadimidine
ORB	Orbifloxacin	SML	Sulfamethizole
OTC	Oxytetracycline	SMM	Sulfamonomethoxine
PA	Pyrroleacid	SMP	Sulfamethoxypyridazine
PEF	Pefloxacin	SMR	Sulfamerazin
PENV	Penicillin V	SMT	Sulfamethiazole
PENG	Penicillin G	SMX	Sulfamethoxazole
PNEC	Predicted No Effect Concentration	SMZ	Sulfamethazine
PPA	Pipemidicacid	SP	Sulfapyridine
PPCPs	Pharmaceutical and Personal Care Products	SPA	Sparfloxacin
PRB	Pearl River Basin	SPI	Spiramycin
QNs	Fluoroquinolones	SQ	Sulfaquinoxaline
ROX	Roxithromycin	SRA	Sarafloxacin
RQs	Risk Quotients	STZ	Sulfathiazole
SA	Sulfanilamide	SWC	Southwestern China
SAAM	Sulfacetamide	TAP	Thiamphenicol
SAs	Sulfonamides	TCs	Tetracyclines
SC	Southern China	TET	Tetracycline
SCP	Sulfachloropyridazine	TMP	Trimethoprim
SD	Sulfadiazine	TYL	Tylosin
SDM	Sulfadimethoxine	VAN	Vancomycin
SDX	Sulfadoxine	WWTPs	Wastewater Treatment Plants
SGD	Sulfaguanidine	YS	Yellow Sea
SIA	Sulfisoxazole	YRB	Yangtze River Basin

Table S3 Risk quotients of antibiotics in seawater of China

year	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017
	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ
	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)
ROX PNEC=47 ng·L ⁻¹	0.640 ^a	0.424	0.001				0.053			3.841
	(30.07)	(19.95)	(0.06)				(2.50)			(180.53)
			0.029 ^b		1.495			0.191		
			(1.38)		(70.27)			(8.96)		
		0.056 ^c		0.018	0.020	0.258	0.007		0.209	
		(2.65)		(0.83)	(0.95)	(12.11)	(0.32)		(9.80)	
	0.119 ^d	0.060	0.191	0.046				0.018	0.199	
	(5.60)	(2.82)	(8.97)	(2.16)				(0.83)	(9.34)	
SMX PNEC=1540 ng·L ⁻¹	0.015	0.085	0.001						0.004	0.081
	(23.69)	(131.63)	(1.72)						(6.67)	(124.33)
			0.009	0.001		0.014		0.115		
			(14.490)	(1.28)		(22.00)		(177.52)		
		0.020	0.175	0.008	0.070	0.011	0.010	0.014	0.001	
		(30.22)	(270)	(12.18)	(108.47)	(17.16)	(15.08)	(20.91)	(1.45)	
	0.000	0.009	0.002	0.010				0.002	0.017	
	(0.51)	(14.06)	(3.55)	(15.89)				(3.50)	(26.30)	
SMZ PNEC=1740 ng·L ⁻¹	0.005	0.010							0.002	0.028
	(8.96)	(16.64)							(3.84)	(48.60)
				0.000		0.015		0.002		
				(0.34)		(25.50)		(3.97)		
		0.083		0.009		0.001	0.002	0.002	0.004	
		(144.13)		(15.3)		(1.52)	(3.55)	(4.22)	(6.95)	
	0.000	0.013		0.007				0.004	0.008	
	(0.04)	(23.3)		(12.86)				(6.15)	(14.5)	

year	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017
	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ
	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)
SD PNEC=2220 ng·L ⁻¹	0.005	0.012	0.000						0.002	0.023
	(10.19)	(25.95)	(0.05)						(4.39)	(51.00)
			0.000	0.000		0.037		0.032		
			(0.75)	(0.19)		(82.90)		(71.40)		
		0.006		0.005	0.016	0.002	0.006	0.001		
		(12.84)		(10.92)	(35.9)	(4.85)	(14.25)	(1.71)		
	0.000	0.001	0.004	0.001				0.001	0.000	
	(0.12)	(2.63)	(7.83)	(2.66)				(1.23)	(0.01)	
TMP PNEC=16400 ng·L ⁻¹	0.001	0.056	0.000							0.004
	(12.33)	(924.79)	(2.93)							(64.33)
			0.000					0.000		
			(2.97)					(7.20)		
		0.001		0.001		0.000	0.000	0.000	0.000	
		(10.9)		(10.24)		(3.83)	(0.37)	(6.85)	(0.15)	
	0.005	0.001	0.000	0.000				0.000	0.000	
	(76.6)	(13.13)	(1.08)	(5.96)				(3.68)	(6.52)	
NOR PNEC=108.3 ng·L ⁻¹	2.461	0.707					0.363			1.396
	(255.40)	(73.36)					(37.73)			(144.87)
			0.248		0.714			0.176		
			(25.72)		(74.15)			(18.25)		
		0.015	0.723	0.002	0.010	0.115	0.312			
		(1.54)	(75)	(0.23)	(1.02)	(11.95)	(32.39)			
	0.001	0.086	0.096	0.661				0.007	1.204	
	(0.06)	(8.94)	(10.01)	(68.61)				(0.69)	(125.00)	
	18.517	1.144					0.604		0.506	20.265

year	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017
	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ
	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)
DOX PNEC=316 ng·L ⁻¹			0.003 (1.00)	0.001 (0.26)		0.031 (9.70)				
		0.021 (6.64)		0.252 (79.75)	0.036 (11.30)					
TET PNEC=3310 ng·L ⁻¹	0.001 (3.80)	0.009 (30.89)					0.007 (23.55)		0.002 (6.22)	0.005 (16.53)
			0.000 (1.28)	0.000 (1.03)		0.003 (9.30)		0.001 (3.60)		
		0.005 (15.97)		0.006 (19.22)	0.001 (1.69)		0.004 (11.61)			
			0.001 (3.60)	0.001 (3.60)				0.001 (3.60)	0.001 (3.60)	
OTC PNEC=1040 ng·L ⁻¹	0.014 (14.11)	0.026 (27.09)				0.018 (18.53)			0.020 (20.93)	0.062 (64.23)
			0.003 (3.16)	0.002 (2.46)		0.022 (22.60)		0.023 (24.31)		
		0.016 (16.19)		0.037 (38.88)	0.027 (27.84)		0.018 (18.27)			
			0.006 (6.56)					0.001 (1.44)	0.034 (35.10)	

RQs and (MEC) in the seawater in ^a the Bohai Sea; ^b the Yellow Sea; ^c the Yangtze River Basin and ^d the Pearl River Basin.

Table S4 Risk quotients of antibiotics in surface water of China

year	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017
	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ
	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)
ROX PNEC=47 ng·L ⁻¹	0.247 ^a		0.313	0.060						
	(11.61)		(14.70)	(2.81)						
			0.001 ^b		0.101	0.102	0.728	0.127	0.045	0.014
			(0.05)		(4.74)	(4.83)	(3.71)	(5.96)	(2.10)	(0.67)
	0.597 ^c	8.387	0.065	0.058				0.029	0.035	
	(28.07)	(394.20)	(3.06)	(2.74)				(1.38)	(1.66)	
				0.102 ^d			0.728			
				(4.79)			(34.22)			
SMX PNEC=1540 ng·L ⁻¹	0.037		0.078	0.002		0.029				0.014
	(56.74)		(1200.77)	(3.68)		(45.00)				(21.59)
	0.039	0.021	0.002	0.001	0.006	0.010	0.002	0.015	0.002	0.004
	(60.00)	(31.7)	(3.67)	(1.15)	(9.02)	(16.11)	(2.85)	(22.69)	(3.68)	(5.96)
	0.015	0.033	0.013		0.006	0.012	0.001	0.001	0.007	
	(22.69)	(50.09)	(20.74)		(8.85)	(18.25)	(1.2)	(2.17)	(10.39)	
				0.001			0.010	0.036	0.066	
				(1.55)			(15.21)	(56.03)	(101.28)	
SMZ PNEC=1740 ng·L ⁻¹	0.003		0.002	0.001		0.146				0.015
	(5.70)		(3.33)	(1.61)		(253.84)				(26.44)
		0.015	0.098	0.003	1.191	0.001	0.000	0.001	0.001	0.001
		(25.64)	(170.86)	(5.53)	(2072.22)	(1.10)	(0.05)	(1.35)	(0.92)	(2.35)
	0.006	0.174	0.047		0.061	0.004	0.001		0.017	
	(11.15)	(301.93)	(82.40)		(105.30)	(6.30)	(2.03)		(29.56)	
				0.004		0.002	0.003	0.002	0.000	
				(7.68)		(4.15)	(5.49)	(3.63)	(0.67)	

year	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017
	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ	RQ
	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)	(MEC)
SD PNEC=2220 ng·L ⁻¹	0.008		0.027	0.002		0.044				0.004
	(18.55)		(60.79)	(4.04)		(97.31)				(8.79)
		0.006		0.001	0.041	0.000	0.001	0.003	0.006	0.000
		(13.34)		(2.34)	(90.31)	(1.10)	(2.28)	(5.55)	(14.26)	(0.08)
	0.002	0.089	0.024	0.012	0.002		0.001	0.049		
	(4.57)	(196.94)	(52.57)	(26.86)	(3.91)		(2.50)	(109.86)		
				0.002		0.001	0.007	0.068	0.048	
				(4.51)		(2.05)	(14.86)	(150.86)	(106.67)	
TMP PNEC=16400 ng·L ⁻¹	0.001					0.051				0.001
	(17.71)					(834.60)				(20.48)
			0.004		0.000	0.018		0.001	0.000	0.000
			(60.78)		(2.84)	(287.00)		(8.45)	(0.39)	(0.65)
	0.002		0.000	0.001				0.000		
	(32.79)		(4.74)	(8.35)				(6.53)		
				0.000			0.000	0.000	0.000	
				(3.99)			(4.73)	(0.76)	(0.39)	
NOR PNEC=108.3 ng·L ⁻¹	0.503	0.300	0.276	0.077		0.491				
	(52.25)	(31.17)	(28.60)	(8.00)		(51.43)				
		0.096	4.540	0.119	0.065	0.470	0.007	0.043		0.011
		(9.95)	(471.29)	(12.33)	(6.74)	(48.77)	(0.76)	(0.44)		(1.12)
	0.132	0.413	0.032		0.123	0.257		0.077		
	(13.66)	(42.82)	(3.35)		(12.80)	(26.68)		(8.02)		
				0.024			0.355	0.003	0.001	
				(2.54)			(36.88)	(0.36)	(0.15)	
	6.327	0.365	0.817	2.478		88.355				2.473

year	2008 RQ (MEC)	2009 RQ (MEC)	2010 RQ (MEC)	2011 RQ (MEC)	2012 RQ (MEC)	2013 RQ (MEC)	2014 RQ (MEC)	2015 RQ (MEC)	2016 RQ (MEC)	2017 RQ (MEC)
OFL PNEC=11.3 ng·L ⁻¹	(71.49)	(4.13)	(9.23)	(28.00)		(998.41)				(27.94)
		0.424 (4.79)	37.659 (425.55)	1.770 (20.00)	3.364 (38.01)	6.486 (73.29)	0.050 (0.57)	0.141 (1.59)	0.050 (0.56)	0.027 (0.31)
	8.489 (95.93)		5.167 (58.39)		0.996 (11.26)		0.101 (1.14)	0.276 (3.12)	0.727 (8.21)	
				0.440 (4.97)			0.756 (8.54)	3.256 (36.79)	3.415 (38.59)	
	0.161 (7.89)		0.026 (1.28)	0.122 (6.00)		1.140 (55.85)				
ENR PNEC=49 ng·L ⁻¹		0.101 (4.93)		2.218 (108.670)	0.578 (28.30)	2.380 (116.63)	0.065 (3.18)	0.118 (5.80)		
			0.027 (1.32)		0.204 (10.01)	0.371 (18.18)		0.037 (1.80)		
				0.330 (16.19)			0.260 (12.72)	0.009 (0.43)	0.018 (0.89)	
			0.001 (7.95)	0.000 (2.36)		0.004 (34.90)				0.001 (4.87)
CTC PNEC=9310 ng·L ⁻¹		0.019 (172.50)		0.010 (97.52)	0.043 (397.83)	0.036 (337.15)	0.000 (1.92)	0.003 (28.10)		0.000 (2.60)
			0.006 (56.49)		0.004 (39.02)	0.002 (22.85)		0.002 (16.16)		
				0.004 (33.90)			0.007 (66.63)	0.059 (553.18)	0.012 (114.44)	
			0.012 (3.82)	0.004 (1.41)						0.033 (10.43)

year	2008 RQ (MEC)	2009 RQ (MEC)	2010 RQ (MEC)	2011 RQ (MEC)	2012 RQ (MEC)	2013 RQ (MEC)	2014 RQ (MEC)	2015 RQ (MEC)	2016 RQ (MEC)	2017 RQ (MEC)
DOX PNEC=316 ng·L ⁻¹		0.079 (25.00)			0.378 (119.56)	0.004 (1.20)	0.010 (3.03)	0.027 (8.59)		0.001 (0.21)
			0.021 (6.63)			0.147 (46.35)	0.085 (27.00)		0.016 (5.11)	
				0.046 (14.57)			0.010 (3.16)	0.007 (2.20)		
		0.003 (10.02)	0.008 (26.52)	0.002 (4.97)	0.001 (2.99)	0.013 (43.17)				0.006 (20.84)
TET PNEC=3310 ng·L ⁻¹		0.002 (8.00)	0.154 (510.00)		0.004 (13.87)	0.080 (265.39)	0.072 (237.80)	0.000 (0.72)	0.005 (17.90)	0.000 (1.07)
		0.011 (37.18)		0.054 (177.94)		0.014 (47.09)		0.004 (13.71)	0.006 (18.47)	
				0.001 (4.89)			0.009 (29.56)	0.093 (308.07)	0.137 (453.58)	
		0.035 (36.30)	0.024 (25.23)	0.006 (6.16)	0.002 (1.63)	0.107 (111.49)				0.022 (22.55)
OTC PNEC=1040 ng·L ⁻¹			0.118 (122.50)		0.113 (117.97)	0.566 (588.70)	1.087 (1130.45)	0.003 (2.94)	0.011 (10.97)	0.004 (4.41)
		0.004 (4.34)		0.028 (29.36)		0.008 (8.69)	0.040 (41.48)	0.004 (4.42)		
				0.003 (3.06)			0.012 (12.14)	0.425 (442.10)	0.152 (158.00)	

RQs and (MEC) in the surface water in ^a Northern China; ^b Eastern China; ^c Southern China and ^d Central China