Supplementary information for

Development of a method for trace level determination of antibiotics in drinking water sources by high performance liquid chromatography-tandem mass spectrometry

Tables

Figures

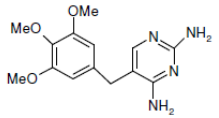
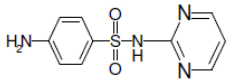
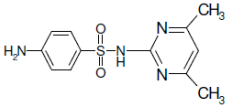
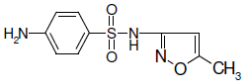
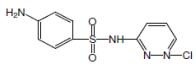
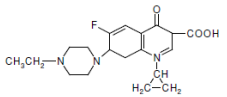
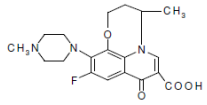
The signal suppression (or enhancement) for each antibiotic was calculated by the following equation:

$$\frac{A_{sp} - A_{non-sp}}{A_{sd}} - 1 \quad (1)$$

Where, A_{sp} is the peak area in drinking water sources extract spiked after extraction with 50 μg $L^{-1}$of each antibiotic; A_{non-sp} is the peak area in drinking water sources extract non-spiked after extraction; A_{sd} is the peak area of the antibiotic standard mixture of 50 μg L^{-1}.

A value of < 1 indicates signal suppression, and a value of > 1 indicates signal enhancement.

1 Table S1 Target antibiotics and their properties.

Group	Properties							
	Compounds	Log K_{ow}	pK_a	Molecular form	MW (g/mol)	CAS number	Structure	Excretion unchanged (%)
Sulfonamides	Trimethoprim (TMP)	0.91	7.1	$C_{14}H_{18}N_4O_3$	290.32	738-70-5		80-90
	Sulfadiazine (SD)	-0.09	6.4	$C_{10}H_{10}N_4O_2S$	250.28	68-35-9		30-40
	sulfamethazine (SMZ)	0.89	7.5	$C_{12}H_{14}N_4O_2S$	278.33	57-68-1		60-85
	Sulfamethoxazole (SMX)	0.89	5.7	$C_{10}H_{11}N_3O_3S$	253.30	723-46-6		20-40
	Sulfachloropyridazine (SCP)	0.28	5.1/7.4	$C_{10}H_9Cl\ N_4O_2S$	284.72	80-32-0		
Quinolones	Enrofloxacin (ENR)	1.10	6.3/8.3	$C_{19}H_{22}FN_3O_3$	359.39	93106-60-6		15-50
	Ofloxacin (OFL)	0.35	6.0/7.6	$C_{18}H_{20}FN_3O_4$	361.37	82419-36-1		30

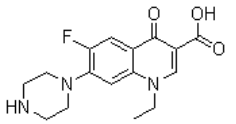
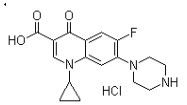
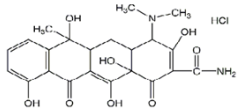
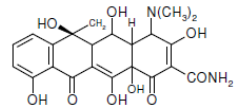
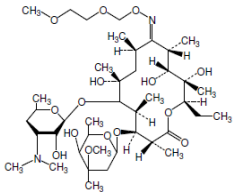
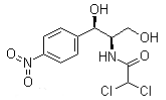
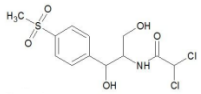
Tetracyclines	Norfloxacin (NOR)	0.28	6.3/8.7	$C_{16}H_{18}FN_3O_3$	319.24	70458-96-7		75-90
	Ciprofloxacin (CIP)	0.25	6.1/8.6	$C_{17}H_{18}FN_3O_3$	367.81	93107-08-5		29-44
	Tetracycline (TC)	0.09	3.7/7.8/9.6	$C_{22}H_{24}N_2O_8$	480.90	64-75-5		60-70
	Oxyetracycline (OTC)	0.08	3.2/7.8/9.6	$C_{22}H_{24}N_2O_9$	460.44	2058-46-0		70
Macrolides	Roxithromycin (ROX)	2.75	9.2	$C_{41}H_{76}N_2O_{15}$	837.05	80214-83-1		<10
Chloramphenicols	Chloramphenicol (CAP)	-	-	$C_{11}H_{12}Cl_2N_2O_5$	323.13	56-75-7		5-10
	Thiamphenicol (TAP)	-	-	$C_{12}H_{15}Cl_2NO_5S$	356.22	15318-45-3		70-90

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Table S2 Signal suppression of target antibiotics in the drinking water sources after extraction (antibiotics concentration, 50 μg L^{-1}).

antibiotics	Signal suppression (%)	RSD %
TMP	-6.7	0.9
SD	-7.0	1.8
SMZ	-4.8	1.2
SMX	-6.5	2.0
SCP	-9.1	4.0
ENR	-18.0	2.3
OFL	-15.3	1.7
NOR	-28.7	2.5
CIP	-27.4	1.3
TC	15.2	0.6
OTC	12.6	3.1
ROX	-1.2	2.4
CAP	-9.8	1.1
TAP	-5.2	0.7

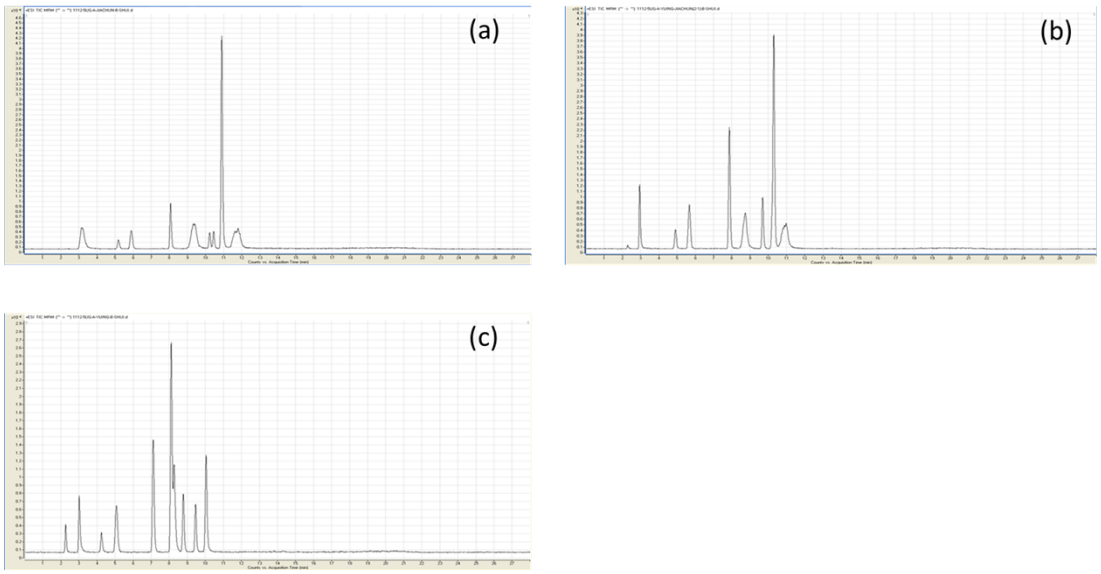

Figure S1 A total ion chromatogram reflecting the effect of organic mobile phase (mobile phase B) on chromatographic separation (a) methanol; (b) methanol-acetonitrile (2:1,v/v); (c) acetonitrile. Other parameters: mobile phase A: deionized water with 0.1% formic acid; flow rate: 0.2 mL min^{-1}; injection volume: 5 µL.

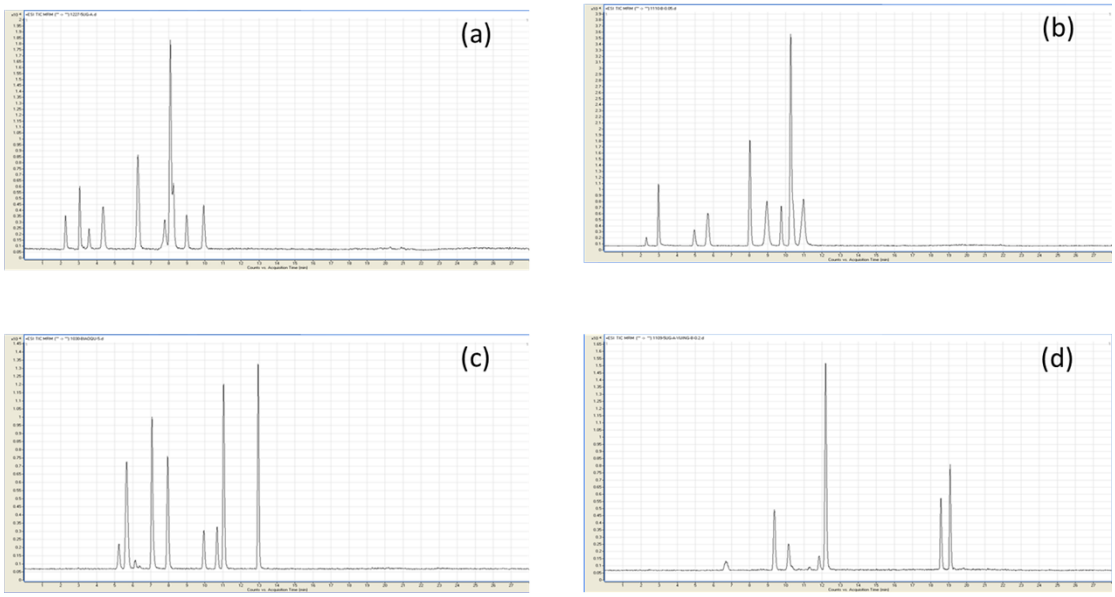

Figure S2 A total ion chromatogram reflecting the effect of formic acid concentration on chromatographic separation (a) 0%; (b) 0.05%; (c) 0.1%; (d) 0.2%. Other parameters: mobile phase B: acetonitrile; flow rate: 0.2 mL min^{-1}; injection volume: 5 µL.

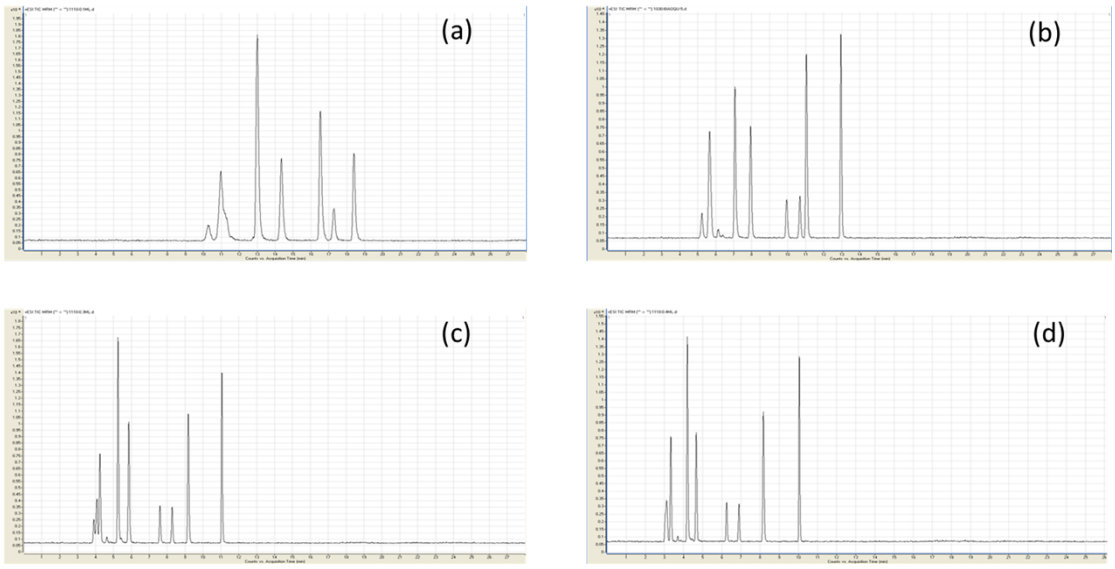

Figure S3 A total ion chromatogram reflecting the effect of flow rate on chromatographic separation (a) 0.1 mL min^{-1}; (b) 0.2 mL min^{-1}; (c) 0.3 mL min^{-1}; (d) 0.4 mL min^{-1}. Other parameters: mobile phase A: deionized water with 0.1% formic acid; mobile phase B: acetonitrile; injection volume: 5 µL.

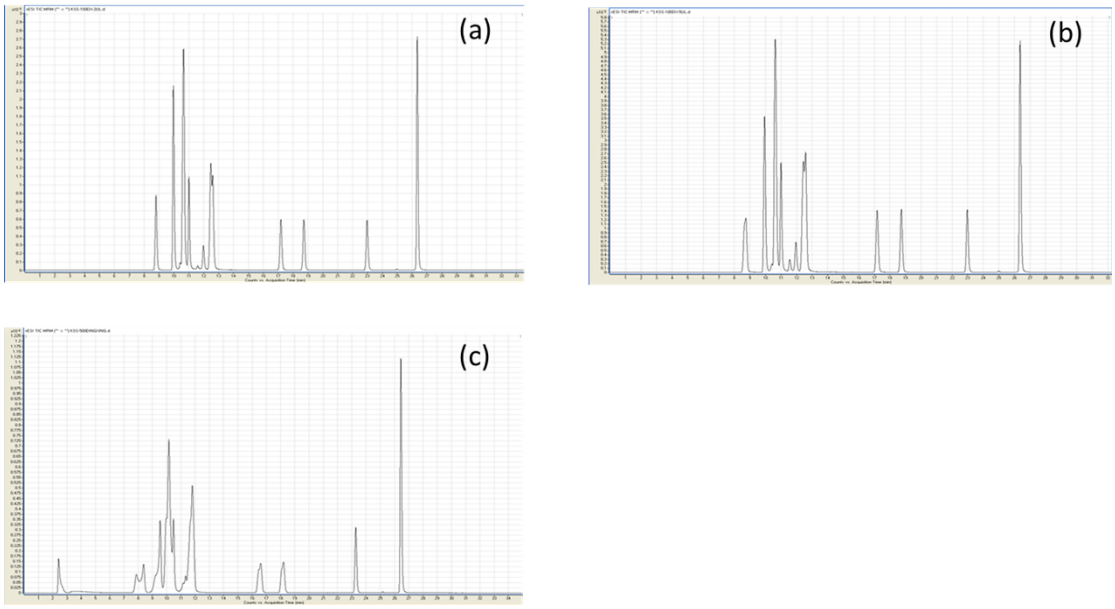

Figure S4 A total ion chromatogram reflecting the effect of injection volume chromatographic separation (a) 2 µL; (b) 5 µL; (c) 10 µL. Other parameters: mobile phase A: deionized water with 0.1% formic acid; mobile phase B: acetonitrile; flow rate: 0.2 mL min^{-1}.