Electronic Supplementary Material (ESI) for Analytical Methods.

Simultaneous Determination of 32 Antibiotics and 12 Pesticides in Sediment Using Ultrasonic-assisted Extraction and High Performance Liquid Chromatography-tandem Mass Spectrometry

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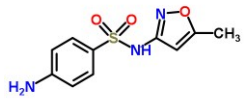
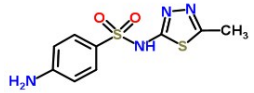
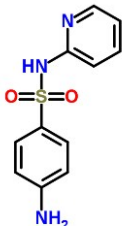
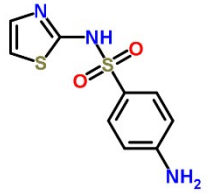
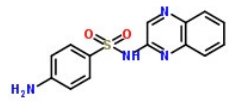
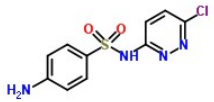
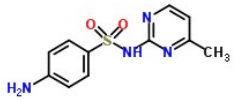
Supplementary data

Table S1 The physicochemical properties of the selected chemicals

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$[a]	pK_a[b]	Structure
Sulfonamides	Sulfamethoxazole (SMOZ)	723-46-6	253.28	$C_{10}H_{11}N_3O_3S$	610[c]	0.89[c]	1.85 5.6 5.9[e]	
	Sulfamethizole (SMTZ)	144-82-1	270.34	$C_9H_{10}N_4O_2S_2$	1,050[c]	0.54[c]	1.86 5.29[f]	
	Sulfapyridine (SPD)	144-83-2	249.29	$C_{11}H_{11}N_3O_2S$	268[c]	0.35[c]	2.58[e] 8.43[c]	
	Sulfathiazole (STZ)	72-14-0	255.32	$C_9H_9N_3O_2S_2$	373[c]	0.05[c]	2.0[e] 7.2 [c]	

22 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Sulfonamides	Sulfaquinoxaline (SQA)	59-40-5	300.34	$C_{14}H_{12}N_4O_2S$	120 [g]	1.68 [c]	2.3 6.0[g]	
	Sulfachlorpyridazine (SCPZ)	80-32-0	284.73	$C_{10}H_9ClN_4O_2S$	7,000 [c]	0.310 [c]	1.87 5.45[e]	
	Sulfamerazine (SMZ)	127-79-7	264.31	$C_{11}H_{12}N_4O_2S$	202 [c]	0.14 [c]	2.06 6.90[f]	
	Sulfadimethoxine (SDMX)	122-11-2	310.33	$C_{12}H_{14}N_4O_4S$	343 [c]	1.63 [c]	2.13 6.08[e]	

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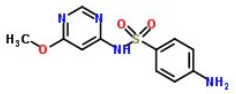
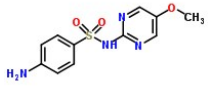
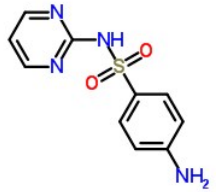
24 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Sulfonamides	Sulfamonomethoxine (SMMX)	1220-83-3	280.31	$C_{11}H_{12}N_4O_3S$	4,030 [c]	0.7 [c]	2.0 6.0[h]	
	Sulfameter (SMT)	651-06-9	280.31	$C_{11}H_{12}N_4O_3S$	730 [c]	0.41 [c]	1.84 6.69[i]	
	Sulfamethazine (SMA)	57-68-1	278.33	$C_{12}H_{14}N_4O_2S$	1,500 [c]	0.89 [c]	1.6 7.4[g]	
	Sulfadiazine (SDZ)	68-35-9	250.28	$C_{10}H_{10}N_4O_2S$	77 [c]	-0.09 [c]	1.6[e] 6.36 [c]	

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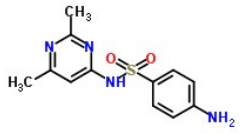
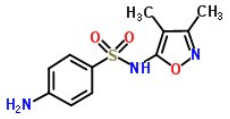
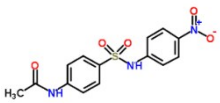
26 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Sulfonamides	Sulfisomidine (SMD)	515-64-0	278.33	$C_{12}H_{14}N_4O_2S$	1,620 [c]	-0.33 [c]	-[k]	
	Sulfisoxazole (SXZ)	127-69-5	267.31	$C_{11}H_{13}N_3O3S$	300 [c]	1.01 [c]	1.60 4.83[i]	
	Sulfanitran (SNT)	122-16-7	335.34	$C_{14}H_{13}N_3O5S$	36.6[d]	2.26 [c]	-	
	Sulfamethoxypyridazine (SMPZ)	80-35-3	280.31	$C_{11}H_{12}N_4O_3S$	147 [c]	0.32 [c]	2.08 7.19[i]	

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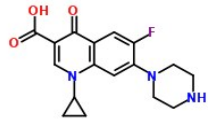
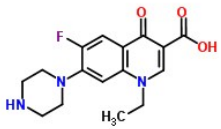
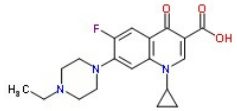
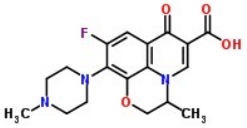
28 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Quinolones	Ciprofloxacin (CIP)	85721-33-1	331.35	$C_{17}H_{18}FN_3O_3$	30,000 [c]	0.28 [c]	3.01 6.14 8.70 10.58[e]	
	Norfloxacin (NOR)	70458-96-7	319.33	$C_{16}H_{18}FN_3O_3$	178,000 [c]	-1.03 [c]	3.11 6.10 8.6 10.56[e]	
	Enrofloxacin (ENR)	93106-60-6	359.40	$C_{19}H_{22}FN_3O_3$	3,400 [c]	0.70 [c]	3.85 6.19 7.59 9.86[e]	
	Ofloxacin (OFX)	82419-36-1	361.37	$C_{18}H_{20}FN_3O_4$	28,300 [c]	-0.39 [c]	5.97 8.28[e]	

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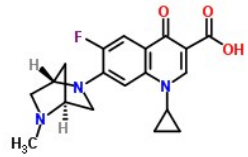
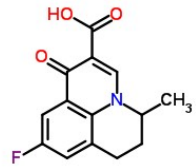
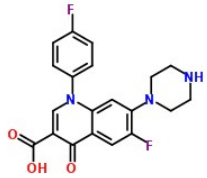
30 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Quinolones	Danofloxacin (DFX)	112398-08-0	357.38	$C_{19}H_{20}FN_3O_3$	5,818[d]	0.44[d]	2.73 9.13[e]	
	Flumequine (FLQ)	42835-25-6	261.25	$C_{14}H_{12}FNO_3$	2,190[c]	1.6[c]	6.29[j]	
	Marbofloxacin (MFX)	11550-35-1	362.36	$C_{17}H_{19}FN_4O_4$	1,000,000[c]	-2.92[d]	5.69 8.02[j]	
	Sarafloxacin (SFX)	98105-99-8	385.37	$C_{20}H_{17}F_2N_3O_3$	1,139[d]	1.07[c]	6.0 8.6[e]	

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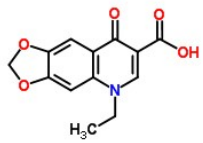
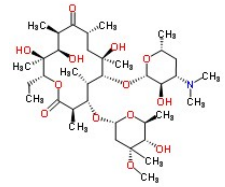
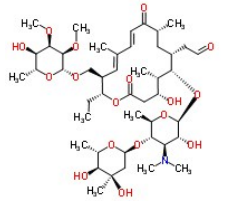
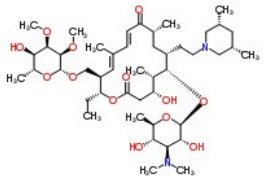
33 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Quinolones	Oxolinic Acid (OA)	14698-29-4	261.23	$C_{13}H_{11}NO_5$	3.2 [c]	0.94 [c]	6.87 [c]	
Macrolides	Erythromycin (ETM)	114-07-8	733.93	$C_{37}H_{67}NO_{13}$	1.44 [c]	3.06 [c]	8.88 [c]	
	Tylosin (TLS)	1401-69-0	916.10	$C_{46}H_{77}NO_{17}$	5 [c]	1.63 [c]	3.31 7.73 [f]	
	Tilmicosin (TMS)	108050-54-0	869.14	$C_{46}H_{80}N_2O_{13}$	0.015 [c]	3.8 [c]	8.18 [c]	

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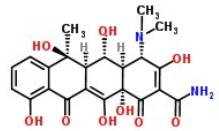
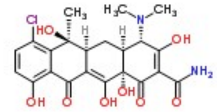
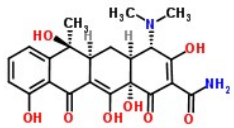
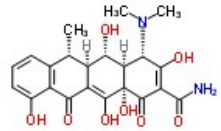
35 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Tetracyclines	Oxytetracycline (OTC)	79-57-2	460.44	$C_{22}H_{24}N_2O_9$	313 [c]	-0.9 [c]	3.22 7.46 8.94[e]	
	Chlortetracycline (CTC)	57-62-5	478.88	$C_{22}H_{23}ClN_2O_8$	630 [c]	-0.62 [c]	3.3 [c] 7.55 9.33[e]	
	Tetracycline (TCC)	60-54-8	444.44	$C_{22}H_{24}N_2O_8$	231 [c]	-1.30 [c]	3.3 [c] 7.78 9.58[e]	
	Doxycycline (DCC)	564-25-0	444.44	$C_{22}H_{24}N_2O_8$	630 [c]	-0.02 [c]	3.02 7.97 9.15[e]	

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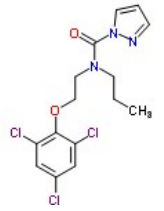
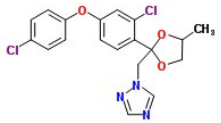
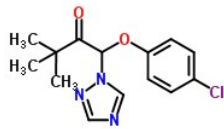
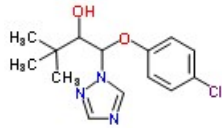
37 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Azoles	Prochloraz (PCA)	67747-09-5	376.67	$C_{15}H_{16}Cl_3N_3O_2$	34 [c]	4.1 [c]	3.8 [c]	
	Difenoconazole (DCZ)	119446-68-3	406.27	$C_{19}H_{17}Cl_2N_3O_3$	15 [c]	4.3 [c]	-	
	Triadimefon (TMF)	43121-43-3	293.75	$C_{14}H_{16}ClN_3O_2$	71.5 [c]	2.77 [c]	-	
	Triadimenol (TMN)	55219-65-3	295.77	$C_{14}H_{18}ClN_3O_2$	120 [c]	2.9 [c]	-	

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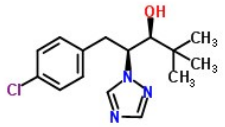
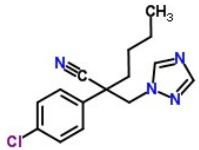
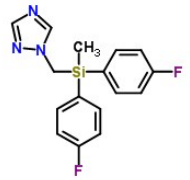
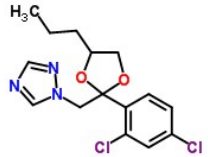
39 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Azoles	Paclobutrazol (PBZ)	76738-62-0	293.79	$C_{15}H_{20}ClN_3O$	26 [c]	3.2 [c]	-	
	Myclobutanil (MCB)	88671-89-0	288.78	$C_{15}H_{17}ClN_4$	142 [c]	2.94 [c]	-	
	Flusilazole (FSZ)	85509-19-9	315.40	$C_{16}H_{15}F_2N_3Si$	54 [c]	3.7 [c]	2.5 [c]	
	Propiconazole (PCZ)	60207-90-1	342.22	$C_{15}H_{17}Cl_2N_3O_2$	110 [c]	3.72 [c]	1.09 [c]	

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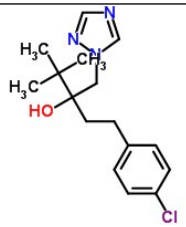
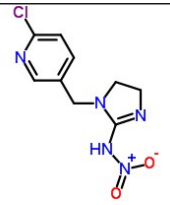
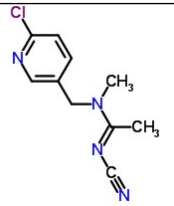
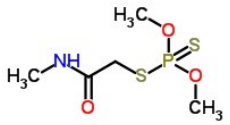
41 Table S1 (*Continued*)

Class	Compound	CAS	Molecular Weight	Formula	Solubility (in water, mg L^{-1})	$LogK_{ow}$	pK_a	Structure
Azoles	Tebuconazole (TCZ)	107534-96-3	307.82	$C_{16}H_{23}ClN_3O$	36 [c]	3.7 [c]	-	
Neonicotinoids	Imidacloprid (ICP)	138261-41-3	255.66	$C_9H_{10}ClN_5O_2$	610 [c]	0.57 [c]	-	
	Acetamiprid (AMP)	135410-20-7	222.68	$C_{10}H_{11}ClN_4$	4,200 [c]	2.55[d]	0.7 [c]	
Organophosphorus	Dimethoate (DMA)	60-51-5	229.26	$C_5H_{12}NO_3PS_2$	25,000 [c]	0.78 [c]	-	

42 [a] K_{ow}: the octanol-water partition coefficient, [b] pK_a: acidity constant, [c] U.S. National Medicine ChemIDPlus Advanced. http://chem.sis.nlm.nih.gov/chemidplus/ (November 10,
43 2014), [d] U.K. Royal Society of Chemistry-ChemSpider Search and Share Chemistry. http://www.chemspider.com/, [e] Reference [1], [f] Reference[2], [g] Reference[3], [g] Reference[4], [i] Reference[5],
44 [j] Reference[6], [k] Not available

Table S2 Optimization results of SPE clean-up (%)

Compound	Selection of SPE cartridge		Dilution volumes				Added of Na_2EDTA			
	GCB+HLB	SAX+HLB	200 mL	250 mL	300 mL	350 mL	0 g	0.2 g	0.4 g	0.6 g
SDZ-D4[a]	89.0	71.8	55.1	63.4	68.9	85.1	83.2	96.9	96.3	89.3
STZ-D4	83.5	111.6	71.3	72.0	73.1	85.9	74.6	95.8	86.4	86.8
NOR-D5	**0.0**[b]	42.4	78.3	114.0	94.6	104.3	89.5	81.4	90.9	92.4
SCZ	-[c]	-	92.8	94.9	85.4	101.0	91.7	96.5	98.0	94.0
SMOZ	106.6	87.7	87.7	88.4	79.9	94.4	78.3	96.0	93.5	92.7
SMTZ	82.2	99.4	84.8	81.6	77.3	90.6	71.5	94.5	80.9	87.6
SPD	95.8	105.5	66.4	77.4	71.8	92.7	74.7	92.7	99.7	91.1
STZ	90.7	92.3	70.2	83.2	71.8	90.3	74.2	94.6	87.7	86.5
SQA	60.5	80.7	89.2	84.5	77.1	90.7	61.4	109.7	72.6	90.0
SCPZ	-	-	89.6	88.1	79.9	92.6	75.5	98.0	93.6	92.7
SMZ	92.4	107.3	77.7	89.1	73.4	93.5	80.5	92.5	93.2	91.1
SDMX	92.3	97.7	89.5	84.3	78.6	94.9	71.7	98.9	83.7	90.1
SMMX	96.2	95.9	90.1	88.9	81.2	95.4	76.4	96.3	94.8	92.6
SMT	96.0	105.6	87.1	88.3	70.6	91.0	77.8	89.2	82.0	87.5
SMA	95.5	109.8	82.8	86.5	74.7	95.4	78.1	92.6	96.4	90.8
SDZ	95.0	73.5	58.2	67.9	69.5	83.6	83.3	95.7	92.4	87.0
SMD	98.1	40.4	**33.0**	**35.0**	41.8	60.4	69.8	75.1	80.1	72.8
SXZ	80.1	83.1	85.6	76.7	79.6	97.2	77.3	96.3	91.1	93.5
SNT	46.4	53.3	97.4	108.6	90.4	103.9	92.9	93.9	93.9	96.5
SMPZ	96.0	105.6	87.8	88.3	70.5	91.0	77.2	89.6	80.4	87.6
CIP	**0.0**	59.8	84.5	112.3	95.6	104.2	89.4	84.7	76.7	92.3
NOR	**0.0**	46.3	77.2	105.4	94.9	94.8	89.8	85.2	85.8	88.0
ENR	**0.0**	71.0	99.2	117.6	87.3	103.4	95.7	83.7	91.9	96.4
OFX	**0.0**	45.1	77.6	101.9	89.5	100.6	92.6	92.9	90.2	99.0
DFX	**0.0**	57.5	90.8	**135.1**	81.5	101.0	82.2	82.7	86.5	99.0
FLQ	**0.0**	113.1	105.2	117.6	99.5	105.8	86.9	89.9	104.9	97.4

Table S2 (*Continued*)

Compound	Selection of SPE cartridge		Dilution volumes				Added of Na_2EDTA			
	GCB+HLB	SAX+HLB	200 mL	250 mL	300 mL	350 mL	0 g	0.2 g	0.4 g	0.6 g
MFX	**0.0**	**23.3**	56.7	88.1	72.7	94.5	101.8	90.2	88.3	98.1
SFX	**0.0**	96.1	88.7	107.0	89.1	100.0	82.7	82.6	82.5	92.7
OA	**0.0**	115.7	104.1	133.7	99.7	110.7	83.3	85.3	94.2	100.2
ETM	-	-	74.0	84.7	77.0	84.8	94.1	99.0	103.9	103.8
TLS	-	-	*[d]	*	*	*	87.0	97.3	102.8	91.7
TMS	-	-	*	*	*	*	96.3	97.0	91.4	100.9
OTC	-	-	47.3	59.9	75.0	84.3	84.8	79.7	104.7	87.4
CTC	-	-	96.7	93.7	111.4	116.2	89.2	82.3	101.9	93.3
TCC	-	-	48.8	59.1	79.2	92.3	91.2	83.1	89.9	88.4
DCC	-	-	54.4	67.0	83.9	97.9	88.1	83.9	114.3	86.4
PCA	101.5	99.4	82.2	82.9	78.5	93.1	81.6	84.5	86.6	85.1
DCZ	71.1	80.7	49.8	51.5	**39.0**	59.4	60.7	70.7	45.6	54.0
TMF	-	-	93.4	88.6	87.0	103.5	96.2	90.5	93.7	98.5
TMN	-	-	99.4	102.8	93.4	103.8	99.9	87.3	104.3	99.4
PBZ	-	-	93.4	95.3	90.0	104.6	94.3	93.4	100.6	101.7
MCB	-	-	98.7	96.7	90.1	100.8	94.4	91.1	94.7	96.6
FSZ	-	-	77.4	76.7	76.9	96.1	75.1	83.2	83.1	82.7
PCZ	-	-	84.2	85.2	78.8	93.8	82.9	96.4	77.2	84.9
TCZ	-	-	88.1	90.9	85.9	103.6	83.7	87.5	86.0	92.4
ICP	100.7	112.0	94.3	98.5	93.8	102.8	96.4	96.2	112.0	103.1
AMP	127.9	101.6	92.4	96.8	88.7	102.4	96.4	96.8	107.3	99.0
DMA	113.0	106.6	85.9	87.0	87.6	101.2	96.0	99.1	104.6	101.0

[a] Italic letters in the table represent surrogate;

[b] Bold letters in the table represent those recoveries outside the range of 40%–130%;

[c] Not spiked;

[d] Not analysis

Table S3 Matrix effects and comparison of two quantification methods

Compound	ME (%)	Recovery (%)	
		Method of internal standard	Method of matrix-matched
SDZ-D4[a]	67.7	70.2	78.0
STZ-D4	61.7	61.3	79.2
NOR-D5	60.0	67.7	58.0
SCZ	84.6	**147.6**[b]	101.0
SMOZ	60.1	96.9	83.2
SMTZ	65.5	108.3	73.3
SPD	42.7	57.7	77.3
STZ	54.5	98.4	75.0
SQA	45.6	38.5	73.1
SCPZ	67.6	80.1	81.5
SMZ	37.3	64.5	80.7
SDMX	43.9	53.1	82.3
SMMX	74.6	81.7	81.4
SMT	48.2	67.5	71.5
SMA	45.4	79.6	81.4
SDZ	57.8	80.6	77.1
SMD	63.9	45.5	55.0
SXZ	64.6	69.9	81.4
SNT	47.5	**157.6**	102.6
SMPZ	48.1	77.8	71.7
CIP	53.0	92.7	52.9
NOR	62.2	95.9	55.8
ENR	66.4	82.9	47.8
OFX	51.8	72.8	55.0
DFX	62.0	87.6	53.8
FLQ	66.5	119.5	88.3
MFX	47.2	72.2	46.5
SFX	63.3	105.9	57.3
OA	48.8	89.1	77.8
ETM	45.5	73.3	89.0
TLS	98.5	**135.6**	82.5
TMS	89.3	**177.6**	73.0
OTC	294.4	**614.3**	72.4
CTC	257.5	**804.0**	85.9
TCC	156.7	**459.1**	73.4
DCC	275.0	**614.0**	82.2
PCA	61.4	52.6	86.5
DCZ	78.5	49.5	73.9
TMF	81.0	94.6	100.0
TMN	56.5	68.6	101.9
PBZ	75.0	96.5	100.2
MCB	75.6	99.5	99.2
FSZ	75.9	75.6	87.1
PCZ	82.9	100.9	91.6
TCZ	80.1	100.8	94.8
ICP	68.4	105.8	97.4
AMP	53.2	119.4	97.8
DMA	42.1	87.8	100.3

[a] Italic letters in the table represent surrogate;

[b] Bold letters in the table represent those recoveries outside the range of 40%–130%

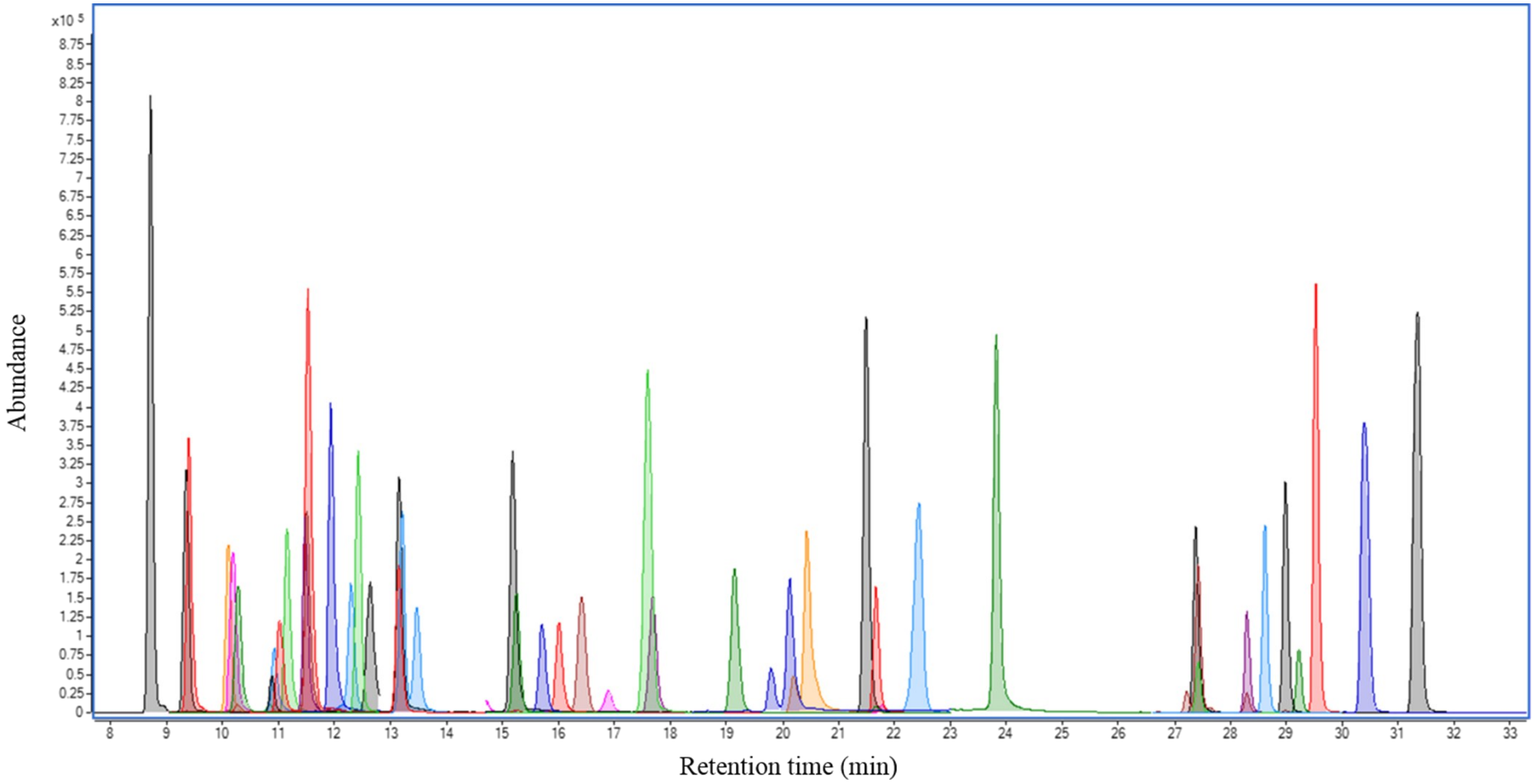


Figure S1 MRM chromatogram of target compounds and surrogates spiked in sediment extracts (50 ng·mL^{-1})

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