Electronic Supplementary Material 1

Targeted multi-analyte UHPLC-MS/MS methodology for emerging contaminants in septic tank wastewater and surface water

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Contents

S1 General and chemical information

Table S1: General and chemical information (Substance Class, Chemical, Cas Number, Molecular Formula, Molecular Weight, Water solubility, Log K_{OW}, pKa, Supplier) of target analytes, ordered by substance class, alphabetically.

Class	Chemical	Cas No.	Mol. Formular	Mol. Weight (g mol^{-1})	Solubility (mg L^{-1})	Log K_{OW}	pKa (most acidic)	pKa (most basic)	Supplier
Anaesthetics	Lidocaine	137-58-6	$C_{14}H_{22}N2O$	234.34	4100 [a]	2.44 [a]	13.78 [e]	7.75 [e]	Sigma Aldrich
Analgesics	3-Methoxy-Paracetamol	3251-55-6	$C_9H_{11}NO_3$	181.19	-	0.09 [c]	-	-	LGC standards
	Diclofenac	15307-79-6	$C_{14}H_{11}Cl_2NO_2$	296.15	2.37 [a]	4.51 [a]	4 [e]	-2.1 [e]	Sigma Aldrich
	Hydroxyibuprofen	51146-55-5	$C_{13}H_{18}O_3$	222.28	-	2.29 [c]	4.63 [d]	-	Sigma Aldrich
	Ibuprofen	15687-27-1	$C_{13}H_{18}O_2$	206.29	21 [a]	3.97 [a]	4.85 [e]	-	Sigma Aldrich
	Ketoprofen	22071-15-4	$C_{16}H_{14}O_3$	254.29	51 [a]	3.13 [a]	3.88 [e]	-7.5 [e]	Sigma Aldrich
	Naproxen	22204-53-1	$C_{14}H_{14}O_3$	230.27	15.9 [a]	3.18 [a]	4.19 [e]	-4.8 [e]	Sigma Aldrich
	Paracetamol	103-90-2	$C_8H_9NO_2$	151.17	30400 [b]	0.91 [a]	9.46 [e]	-4.4 [e]	Sigma Aldrich
Antibiotics	3-Desmethyltrimethoprim	27653-69-6	$C_{13}H_{16}N_4O_3$	276.29	-	-	-	-	LGC standards
	α-Hydroxytrimethoprim	29606-06-2	$C14_H_{18}N_4O_4$	306.32	-	-	-	-	LGC standards
	Amoxicillin	26787-78-0	$C_{16}H_{19}N_3O_5S$	365.4	3430 [b]	0.87 [a]	3.23 [e]	7.22 [e]	Sigma Aldrich
	Ciprofloxacin	85721-33-1	$C_{17}H_{18}FN_3O_3$	331.34	11500 [b]	0.28 [a]	5.56 [e]	8.77 [e]	Sigma Aldrich
	Clarithromycin	81103-11-9	$C_{38}H_{69}NO_{13}$	747.97	0.33 [a]	3.16 [a]	12.46 [e]	9 [e]	Sigma Aldrich
	Erythromycin	114-07-8	$C_{37}H_{67}NO_{13}$	733.93	0.52 [b]	2.6 [a]	12.45 [e]	9 [e]	Sigma Aldrich
	Ofloxacin	82419-36-1	$C_{18}H_{20}FN_3O_4$	361.37	28300 [a]	-0.39 [a]	5.35 [e]	6.72 [e]	Sigma Aldrich
	Sulfadiazine	68-35-9	$C_{10}H_{10}N_4O_2S$	250.28	77 [a]	-0.09 [a]	6.99 [e]	2.01 [e]	Sigma Aldrich
	Sulfamethoxazole	723-46-6	$C_{10}H_{11}N_3O_3S$	253.28	610 [a]	0.89 [a]	6.16 [e]	1.97 [e]	Sigma Aldrich
	Sulfanilamide	63-74-1	$C_6H_8N_2O_2S$	172.20	7500 [a]	-0.62 [a]	10.99 [e]	2.27 [e]	Sigma Aldrich
	Trimethoprim	738-70-5	$C_{14}H_{18}N_4O_3$	290.32	400 [a]	0.91 [a]	17.33 [e]	7.16 [e]	Sigma Aldrich
Anticoagulants	Warfarin	81-81-2	$C_{19}H_{16}O_4$	308.33	17 [a]	2.7 [a]	5.56 [e]	-6.9 [e]	Sigma Aldrich
Anticonvulsants	Carbamazepine	298-46-4	$C_{15}H_{12}N_2O$	236.28	17.7 [b]	2.77 [a]	15.96 [e]	-3.8 [e]	Sigma Aldrich

Class	Compound	CAS	Formula	MW	Solubility	logP	pKa1	pKa2	Source
	Carbamazepine-10,11-epoxide	36507-30-9	$C_{15}H_{12}N_2O_2$	252.27	-	0.95 [c]	13.91 [b]	-0.50 [b]	LGC standards
	Gabapentin	60142-96-3	$C_9H_{17}NO_2$	171.24	34000 [c]	1.25 [a]	4.63 [e]	9.91 [e]	Sigma Aldrich
	Lamotrigine	84057-84-1	$C_9H_7Cl_2N_5$	256.09	170 [a]	1.93 [a]	14.98 [e]	5.58 [e]	Sigma Aldrich
	Primidone	125-33-7	$C_{12}H_{14}N_2O_2$	218.25	500 [a]	0.91 [a]	11.5 [e]	-6.2 [e]	Sigma Aldrich
Antidepressants	Citalopram	59729-32-7	$C_{20}H_{21}FN_2O$	324.40	31.1 [b]	3.76 [a]	-	9.78 [a]	Sigma Aldrich
	Desmethylcitalopram	144025-14-9	$C_{19}H_{19}FN_2O$	310.37	-	3.53 [c]	-	10.54 [d]	LGC standards
	Desmethylvenlafaxine	93413-62-8	$C_{16}H_{25}NO_2$	263.38	-	2.69 [d]	10.04 [b]	9.33 [b]	Sigma Aldrich
	Fluoxetine	56296-78-7	$C_{17}H_{18}F_3NO$	309.33	60.3 [b]	4.05 [a]	-	9.8 [e]	LGC standards
	Venlafaxine	99300-78-4	$C_{17}H_{27}N_1O_2$	277.41	267 [b]	3.28 [b]	14.42 [e]	8.91 [e]	Sigma Aldrich
Anti-diabetics	Guanylurea	207300-86-5	$C_2H_6N_4O$	102.10	-	-3.57 [c]	-	-	Sigma Aldrich
	Metformin	1115-70-4	$C_4H_{11}N5$	129.17	1000000 [b]	-2.6 [a]	-	12.4 [a]	Sigma Aldrich
Anti-fungals	Climbazole	38083-17-9	$C_{15}H_{17}ClN_2O_2$	292.76	-	3.76 [c]	18.87 [e]	6.49 [e]	TCI
	Clotrimazole	23593-75-1	$C_{22}H_{17}ClN_2$	344.84	0.49 [a]	6.1 [a]	-	6.26 [e]	Sigma Aldrich
	Fluconazole	86386-73-4	$C_{13}H_{12}F_2N_6O$	306.27	-	0.5 [a]	12.68 [e]	2.3 [e]	TCI
	Miconazole	22916-47-8	$C_{18}H_{14}Cl_4N_2O$	416.13	-	6.25 [c]	-	6.48 [e]	Sigma Aldrich
Anti-helmintics	Mebendazole	31431-39-7	$C_{16}H_{13}N_3O_3$	295.29	71.3 [a]	2.83 [a]	8.44 [e]	3.93 [e]	TCI
Antihistamines	Cetirizine	83881-52-1	$C_{21}H_{25}ClN_2O_3$	388.9	101 [a]	2.8 [a]	3.59 [e]	7.42 [b]	Sigma Aldrich
	Chlorpheniramine	113-92-8	$C_{16}H_{19}ClN_2$	274.79	5500 [a]	3.38 [a]	-	9.13 [a]	Sigma Aldrich
	Fexofenadine	153439-40-8	$C_{32}H_{39}NO_4$	501.67	0.02 [b]	2.94 [e]	4.04 [e]	9.01 [e]	Sigma Aldrich
Anti-pruritic	Crotamiton	483-63-6	$C_{13}H_{17}NO$	203.28	-	2.9 [d]	-	-0.6 [e]	Sigma Aldrich
Antiulcer	4-Hydroxyomeprazole	301669-82-9	$C_{16}H_{17}N_3O_3S$	331.40	-	1.93 [c]	9.68 [d]	3.93 [d]	LGC standards
	Lansoprazole	103577-45-3	$C_{16}H_{14}F3N_3O_2S$	369.36	0.97 [a]	3.68 [c]	9.35 [e]	4.16 [e]	TCI
	Omeprazole	73590-58-6	$C_{17}H_{19}N_3O_3S$	345.52	359 [a]	2.23 [a]	9.29 [e]	4.77 [e]	Sigma Aldrich
	Ranitidine	66357-59-3	$C_{13}H_{22}N_4O_3S$	314.41	24700 [b]	0.2 [a]	-	8.2 [a]	Sigma Aldrich
Benzodiazepines	Lorazepam	846-49-1	$C_{15}H_{10}Cl_2N_2O_2$	321.16	80 [a]	2.39 [a]	10.61 [e]	-2.2 [e]	Sigma Aldrich
	Oxazepam	604-75-1	$C_{15}H_{11}ClN_2O_2$	286.71	179 [b]	2.24 [a]	10.61 [e]	-1.5 [e]	Sigma Aldrich

		CAS	Formula	MW					Supplier
	Temazepam	846-50-4	$C_{16}H_{13}ClN_2O_2$	300.75	164 [a]	2.19 [a]	10.68 [e]	-1.4 [e]	Sigma Aldrich
Betablockers	Acebutolol	34381-68-5	$C_{18}H_{28}N_2O_4$	336.43	259 [a]	1.71 [a]	13.91 [e]	9.65 [e]	Sigma Aldrich
	Atenolol	29122-68-7	$C_{14}H_{22}N_2O_3$	266.34	13300 [a]	0.16 [a]	14.08 [e]	9.67 [e]	Sigma Aldrich
	Bisoprolol	104344-23-2	$C_{18}H_{31}NO_4$	325.44	2240 [b]	2.2 [a]	14.09 [e]	9.67 [e]	Sigma Aldrich
	Metoprolol	56392-17-7	$C_{15}H_{25}NO_3$	267.37	4770 [b]	2.15 [a]	14.09 [e]	9.67 [e]	Sigma Aldrich
	Propranolol	318-98-9	$C_{16}H_{21}NO_2$	259.35	228 [e]	3.48 [a]	14.09 [e]	9.67 [e]	Sigma Aldrich
	Salbutamol	18559-94-9	$C_{13}H_{21}NO_3$	239.31	14100 [a]	1.4 [a]	10.12 [e]	9.4 [e]	Sigma Aldrich
	Sotalol	959-24-0	$C_{12}H_{20}N_2O_3S$	272.36	-	0.24 [c]	10.07 [e]	9.43 [e]	Sigma Aldrich
Chemotherapeutic	Ifosfamide	3778-73-2	$C_7H_{15}Cl_2N_2O_2P$	261.09	3780 [a]	0.86 [a]	14.64 [e]	-	Sigma Aldrich
Coccidiostat	Clopidol	2971-90-6	$C_7H_7Cl_2NO$	192.04	-	2.1 [c]	10.77 [d]	-	Sigma Aldrich
Hormones	17ß-Estradiol (E2)	50-28-2	$C_{18}H24O_2$	272.39	3.6 [a]	4.01 [a]	10.33 [e]	-0.88 [e]	Sigma Aldrich
	17α-Ethinylestradiol (EE2)	57-63-6	$C_{20}H24O_2$	296.41	11.3 [a]	3.67 [a]	10.33 [e]	-1.7 [e]	Sigma Aldrich
	Estriol (E3)	50-27-1	$C_{18}H_{24}O_3$	288.38	-	2.45 [a]	10.33 [e]	-3.2 [e]	Sigma Aldrich
	Estrone (E1)	53-16-7	$C_{18}H_{22}O_2$	270.37	0.76 [a]	2.6 [a]	10.33 [e]	-5.4 [e]	Sigma Aldrich
	Norethisterone	68-22-4	$C_{20}H_{26}O_2$	298.42	7.04 [c]	2.97 [c]	17.59 [e]	-1.7 [e]	Sigma Aldrich
Lipid regulators	Atorvastatin	344423-98-9	$C_{33}H_{35}FN_2O_5$	558.65	0.00112 [b]	6.36 [a]	4.31 [e]	-2.7 [e]	Sigma Aldrich
	Bezafibrate	41859-67-0	$C_{19}H_{20}ClNO_4$	361.83	1.2 [b]	4.25 [b]	3.83 [e]	-0.84 [e]	Sigma Aldrich
	Gemfibrozil	25812-30-0	$C_{15}H_{22}O_3$	250.33	4.96 [b]	4.39 [a]	4.42 [e]	-4.8 [e]	Sigma Aldrich
Wastewater	Caffeine	58-05-02	$C_8H_{10}N_4O_2$	194.19	21700 [a]	0.16 [b]	-	0.52 [b]	Sigma Aldrich
discharge marker	Cotinine	486-56-6	$C_{10}H_{12}N_2O$	176.22	999000 [b]	1.37 [d]	-	4.79 [d]	Sigma Aldrich
X-ray contrast	Amidotrizoic acid	117-96-4	$C_{11}H_9I_3N_2O_4$	613.91	-	3.3 [a]	2.17 [e]	-4.2 [ei]	Sigma Aldrich

[a] Drugbank [1], [b] Proctor et al., 2019 [2], [c] ChemSpider [3], [d] ChEMBL [4], [e] Drugbank using ChemAxon [1]

Table S2: CAS Number and supplier for deuterated pharmaceutical standards.

Compound	CAS	supplier
(±)-Acebutolol-d_5 hydrochloride	1189500-68-2	TRC
(±)-Atenolol-d_7	1202864-50-3	Analab
(±)-Bisoprolol-d_5	1189881-87-5	TRC
(±)-Chlorpheniramine-d_6 solution	129806-45-7	Sigma Aldrich
(±)-Citalopram-d_6 solution	1190003-26-9	Sigma Aldrich
(±)-Cotinine-d_3 solution	110952-70-0	Sigma Aldrich
(±)-Fluoxetine-d_6 solution	1173020-43-3	Sigma Aldrich
(±)-Ibuprofen-d_3	121662-14-4	Sigma Aldrich
(±)-Metoprolol-d_7 (+)-tartrate	2378803-75-7	Sigma Aldrich
(±)-Naproxen-d_3	958293-79-3	Sigma Aldrich
(±)-Propranolol-d_7 solution	1613439-56-7	Sigma Aldrich
(±)-Salbutamol-d_3	1219798-60-3	LGC standards
(±)-Sotalol-d_6 hydrochloride	1246820-85-8	LGC standards
(±)-Temazepan-d_5 solution	136765-51-0	Sigma Aldrich
(±)-Venlafaxine-D_6 solution	1062606-12-5	Sigma Aldrich
17β-Estradiol-d_4	66789-03-5	LGC standards
Acetaminophen-d_4	64315-36-2	Sigma Aldrich
Caffeine-^{13}C	202282-98-2	Sigma Aldrich
Carbamazepine-10,11-epoxide-d_{10}	1219804-16-6	LGC standards
Carbamazepine-d_{10} solution	132183-78-9	Sigma Aldrich
Clarithromycin-N-methyl-$^{13}C,d_3$	78088-19-4	LGC standards
Ciprofloxacin-d_8 Oxalate	1246819-94-2	TRC
Estrone-d_4	53866-34-5	Sigma Aldrich
Metformin-d_6 HCl	1185166-01-1	LGC standards
Ofloxacin-d_3	1173147-91-5	Sigma Aldrich
(±)-Oxazepam-d_5 solution	65854-78-6	Sigma Aldrich
Primidone-d_5	73738-06-4	Supelco

S2   Risk calculations

Risk calculations were performed for pharmaceuticals with annual prescription rates over 1,000,000 per item in Scotland in 2019 [5]. The risk quotient (RQ) is calculated by dividing the predicted and measured environmental concentrations in the UK by the predicted no effect concentration (PNEC). The PNEC was obtained from the lowest found value in the literature. A substance was included as a target analyte, if RQ > 1 [6,7].

S3   Sludge Sampler

Figure S1: Costume-made polyvinylchloride sludge sampler in its broken down form (a) and in use (b). For sampling, the sludge sampler was inserted into the septic tank until it reached the bottom, pulled up a few centimetres, and closed by pulling the cord up. It was then lifted up and the sludge was collected into a polypropylene bottle.

a)   b)
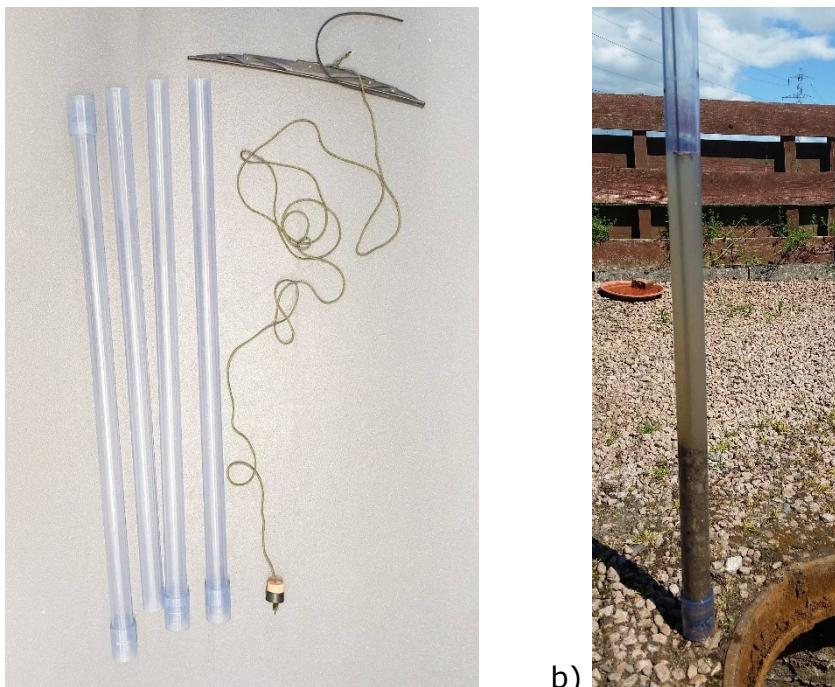
S4   LC Solvent gradient program

Table S3: LC solvent gradient program, mobile phase A: Water with additives, mobile phase B: methanol with additives. Additives were 5mM ammonium formate and 0.1% formic acid in the positive method, and 0.1mM ammonium fluoride in the negative method. The total run time was 14min for the positive, and 12min for the negative method.

Time /min	% A	
	positive	negative
0	95	95
0.5	95	95
8		20
9	20	20
9.1		95
11	20	95
11.1	95	95
12	95	95
14	95	

S5   Standard preparation

The standards were mainly purchased in solid form. Stock solutions were prepared by

dissolving 10 mg of the accurately weighted standard in HPLC grade methanol (MeOH, Fisher

Scientific) at a concentration of 1 mg mL^{-1}. The amoxicillin solution was prepared in water,

due to their limited solubility, sulfadiazine was dissolved in acetonitrile (ACN, Fisher

scientific), guanylurea sulphate was dissolved in MeOH/water (1/1, v/v), and mebendazole in

ACN/formic acid (9/1, v/v) [1]. The deuterated standards were mainly purchased as solutions. Otherwise, stock solutions were prepared as described for the standards. From the stock solutions, three separate mixtures of deuterated ECs (2 µg mL^{-1}), ECs except antibiotics (2 µg mL^{-1}), and antibiotics only (2 µg mL^{-1}) were prepared in MeOH. These were then further diluted to working solutions. Working solutions and antibiotic mixtures were prepared every 3 months. All solutions were stored in the dark at -20°C.

Table S4: Relevant concentrations in the method validation. 50 µL internal standard mixture (100 µg L^{-1}) and 50 µL standard working solutions of different concentrations were added to 0.4 mL direct injection sample, 50 mL influent and effluent, 100 mL river water, and 0.1 g sludge.

c (µg L^{-1}) standard working solution	c (µg L^{-1}) in water for direct injection	c (µg L^{-1}) before SPE (effluent, influent)	c (µg L^{-1}) before SPE (river water)	c (ng g^{-1}) in sludge	c (µg L^{-1}) in vial after extraction and in direct injection
0	0	0	0	0	0
10	1.25	0.01	0.005		1
100	12.5	0.1	0.05	50	10
500	62.5	0.5	0.25	250	50
1000				500	100

S6 Calculation of nominal dilution

The nominal dilution of the septic tank discharge into the river was calculated from the flow of the receiving river per day (f_{river}) and the calculated flow of the septic tank effluent per day (f_{ST}) following equation S1.

$$dilution = \frac{(f_{river} - f_{ST})}{f_{ST}}$$

(S1)

The flow of the septic tank effluent per day was calculated by multiplying the population equivalents (PE) by the average daily discharge per person per day (0.7252 m^3/day) (equation S2).[8]

$$f_{ST} = PE \cdot 0.7252 \, m^3 day^{-1}$$

(S2)

S7 MS/MS detection parameters

Table S5: MS/MS detection parameters for studied compounds (precursor ion, cone voltage (CV), quantifier and qualifier ions with collision energies (CE)), sorted according to retention times (RT).

RT /min	Analyte	Precursor Ion /m/z	CV /V	Quantifier Ion	CE /eV	Qualifier Ion	CE /eV
Positive Ionisation							
0.7	Guanylurea	103.1	16	60.1	10	86.1	8
0.8	Metformin	130.2	27	60.1	12	71.2	17
0.8	Metformin-d$_6$	136.3	28	60.1	13	-	-
1.2	Sulfanilamide	173.1	27	92.1	16	108.1	14
1.7	Cotinine-d$_3$	180.2	13	80.1	22	-	-
1.7	Cotinine	177.1	34	80.1	19	98.1	21
2.0	Amidotrizoic acid	631.9	29	361.2	26	233.2	46
2.2	Amoxicillin	366.1	29	114.1	19	208.2	12
2.2	Sotalol-d$_6$	279.2	24	214.1	17	-	-
2.3	Sotalol	273.2	25	133.2	28	213.2	17
2.3	Paracetamol-d$_4$	156.1	23	114.1	16	-	-
2.4	Paracetamol	151.9	26	110.0	16	92.9	24
2.5	Salbutamol-d$_3$	243.0	21	151.2	21	-	-
2.5	Salbutamol	240.2	27	148.1	20	166.1	12
2.5	Ranitidine	315.1	31	176.1	16	130.1	25
2.5	Atenolol-d$_7$	274.2	23	145.1	24	-	-
2.5	Atenolol	267.3	38	145.1	30	190.1	16
2.6	Sulfadiazine	251.1	18	156.1	15	92.1	26
2.9	3-Methoxy Paracetamol	182.2	22	108.1	16	80.1	29
3.0	3-Desmethyl Trimethoprim	277.2	30	261.2	25	123.2	35
3.1	alpha-Hydroxy Trimethoprim	307.2	22	289.2	14	274.2	20
3.3	Clopidol	192.1	27	101.1	24	87.1	28
3.3	Gabapentin	172.2	23	154.2	12	137.2	15
3.6	Trimethoprim	291.2	23	230.1	15	261.2	23
3.6	Caffeine	195.1	16	138.1	17	110.1	23
3.6	Caffeine-^{13}C	198.1	31	140.1	19	-	-
3.7	Ofloxacin-d$_8$	365.1	30	261.2	27	-	-
3.7	Ofloxacin	362.2	30	318.2	18	261.2	25
3.9	Ciprofloxacin	332.1	17	314.2	21	288.2	17
4.0	Lidocaine	235.2	29	86.1	17	-	-
4.1	Sulfamethoxazole	254.1	32	156.1	16	92.2	28
4.2	Ciprofloxacin-d$_8$	340.1	24	322.2	21	-	-
4.5	Desmethylvenlafaxine	264.3	29	246.3	12	107.1	30
4.7	Acebutolol	337.3	20	116.2	18	319.3	16
4.7	Acebutolol-d$_5$	342.3	19	121.2	23	-	-
4.7	Lamotrigine	256.1	24	211.1	25	187.1	27
4.8	Primidone-d$_5$	227.1	14	164.2	12	-	-
4.8	Metoprolol	268.2	30	159.1	22	191.2	17
4.8	Metoprolol-d$_7$	275.3	29	123.2	18	-	-
4.8	Primidone	219.1	28	162.1	12	91.1	25
4.8	Fluconazole	307.1	29	238.2	15	220.1	18
5.4	Ifosfamide	261.1	15	92.1	23	154.0	18
5.5	4-Hydroxy Omeprazole	316.2	22	168.1	24	149.2	24
5.8	Carbamazepine-10,11-epoxide-d$_{10}$	263.1	26	190.2	22	-	-

5.8	Chlorpheniramine	275.2	30	230.1	18	167.1	43
5.8	Chlorpheniramine-d$_6$	281.1	26	230.1	16	-	-
5.8	Venlaflaxine-d$_6$	284.3	34	266.3	12	-	-
5.9	Bisoprolol-d$_5$	331.2	23	121.2	17	-	-
5.9	Carbamazepine-10,11-epoxide	253.1	20	180.1	20	210.2	14
5.9	Venlafaxine	278.3	36	260.3	10	215.2	16
5.9	Bisoprolol	326.3	20	116.2	16	222.2	10
6.0	Propranolol-d$_7$	267.1	22	189.2	18	-	-
6.1	Propranolol	260.2	50	116.1	16	183.1	18
6.2	Citalopram	325.2	24	262.2	20	116.1	25
6.2	Citalopram-d$_6$	331.2	24	109.1	31	-	-
6.2	Desmethylcitalopram	311.2	22	109.1	20	262.2	17
6.4	Omeprazole	346.2	21	198.1	11	180.1	23
6.8	Hydroxyibuprofen	240.2	25	205.2	12	163.2	16
6.9	Carbamazepine-d$_{10}$	247.1	33	204.2	20	-	-
6.9	Carbamazepine	237.2	33	194.2	18	179.2	32
7.1	Mebendazole	296.1	19	264.2	23	105.1	33
7.3	Fexofenadine	502.4	37	466.5	25	171.2	35
7.3	Lansoprazole	370.1	29	252.1	11	119.2	20
7.4	Erythromycin	734.5	37	158.2	30	576.4	19
7.5	Oxazepam-d$_5$	292.1	26	246.2	25	-	-
7.5	Oxazepam	287.1	26	241.1	25	269.1	17
7.6	Lorazepam	321.1	25	275.1	22	303.1	16
7.7	Fluoxetine-d$_6$	316.1	19	154.2	9	-	-
7.7	Climbazole	293.1	23	69.2	21	41.2	26
7.7	Fluoxetine	310.2	34	44.1	10	148.1	10
7.8	Temazepam-d$_5$	306.1	24	260.2	21	-	-
7.8	Temazepam	301.1	24	255.2	21	283.2	14
7.8	Ketoprofen	255.2	50	209.2	15	105.1	22
7.8	Cetirizine	389.2	30	201.2	22	166.1	40
8.1	Clarithromycin	748.5	29	158.2	32	558.4	24
8.1	Clarithromycin-^{13}C-d$_3$	752.6	25	162.2	29	-	-
8.1	N-Desmethylclarithromycin	734.6	28	144.2	30	576.5	18
8.1	Norethisterone	299.2	16	231.2	18	109.2	26
8.1	Bezafibrate	362.1	25	139.1	25	316.2	14
8.1	Clotrimazole	277.1	27	165.2	20	242.2	20
8.2	Crotamiton	204.2	27	69.1	22	136.2	17
8.2	Warfarin	309.1	32	163.1	14	251.2	19
9.0	Atorvastin-d$_5$	564.4	27	445.4	22	-	-
9.0	Atorvastatin	559.2	28	440.3	23	250.2	43
9.3	Miconazole	417.0	18	159.1	30	161.1	28

Negative ionisation

5.7	Estriol	287.1	36	171.1	37	145.1	39
6.0	Naproxen	229.0	9	170.1	14	185.1	5
7.0	Diclofenac	294.1	21	250	10	178.1	29
7.4	E2-d$_4$	275.2	35	147.3	37	160.2	30
7.4	E2	271.2	25	145.1	40	183.2	40
7.5	Estrone	269.1	35	145.1	38	159.2	34
7.5	Estrone-d$_4$	273.2	39	147.1	36	160.1	36
7.5	EE2	295.1	20	159.1	36	145.1	38

7.6	Ibuprofen	205.1	12	161.3	12	-	-
7.6	Ibuprofen-d$_3$	208.1	13	164.2	8	-	-
8.7	Gemfibrozil	249.0	13	121.1	20	-	-

S8 Instrument performance

For each analyte, the ratios of the peak area against the peak area of the internal standard (area ratio, ar), were plotted against the standard concentrations (c) above the IQL. A linear regression model (equation S3) was fitted, where m was the slope of the calibration line and b was the intercept with the y-axis.

$$ar = m \cdot c + b$$

(S3)

The coefficient of determination (R^2) was calculated.

Table S6: Instrument performance information for analytes with the selected internal standard (IS), correlation coefficient (R2), linear concentration range, and instrument detection (IDL) and quantification limits (IQL), ordered by method and retention time.

RT	compound	IS	R^2	cali range (μg L^{-1})	IDL (μg L^{-1})	IQL (μg L^{-1})
0.7	Guanylurea	Salbutamol-d$_3$	0.997	0.5 – 100	0.25	0.5
0.8	Metformin	Metformin-d$_6$	0.997	0.1 – 500	0.05	0.1
1.2	Sulfanilamide	Primidone-d$_5$	0.999	1 – 100	0.5	1
1.7	Cotinine	Cotinine-d$_3$	0.992	0.05 – 100	0.005	0.02
2.0	Amidotrizoic acid	Salbutamol-d$_3$	1.000	0.5 – 100	0.1	0.3
2.2	Amoxicillin	Paracetamol-d$_4$	0.998	1 – 100	0.8	1
2.3	Sotalol	Sotalol-d$_6$	1.000	0.05 – 100	0.005	0.04
2.4	Paracetamol	Paracetamol-d$_4$	0.998	1 – 500	0.1	0.2
2.5	Salbutamol	Salbutamol-d$_3$	1.000	0.05 – 100	0.005	0.04
2.5	Ranitidine	Paracetamol-d$_4$	0.998	0.1 – 100	0.05	0.1
2.5	Atenolol	Atenolol-d$_7$	1.000	0.1 – 100	0.03	0.1
2.6	Sulfadiazine	Caffeine-^{13}C	0.997	0.5 – 100	0.02	0.07
2.9	3-Methoxy Paracetamol	Cotinine-d$_3$	1.000	0.1 – 100	0.03	0.1
3.0	3-Desmethyl Trimethoprim	Cotinine-d^3	0.999	0.05 – 100	0.01	0.02
3.1	α-Hydroxy Trimethoprim	Caffeine-^{13}C	0.994	0.1 – 100	0.05	0.1
3.3	Clopidol	Caffeine-^{13}C	0.999	5 – 100	0.3	1.1
3.3	Gabapentin	Caffeine-^{13}C	0.997	1 – 100	0.5	1
3.6	Trimethoprim	Paracetamol-d$_4$	0.999	0.05 – 100	0.01	0.05
3.6	Caffeine	Caffeine-^{13}C	0.995	1 – 100	0.08	0.3

3.7	Ofloxacin	Ofloxacin-d$_8$	0.991	0.1 – 100	0.05	0.1
3.9	Ciprofloxacin	Ofloxacin-d$_8$	0.991	0.05 – 100	0.02	0.05
4.0	Lidocaine	Carbamazepine-d$_{10}$	0.999	0.05 – 100	0.002	0.005
4.1	Sulfamethoxazole	Caffeine-^{13}C	0.997	0.1 – 100	0.05	0.1
4.5	Desmethylvenlafaxine	Venlafaxine-d$_6$	1.000	0.05 – 100	0.005	0.01
4.7	Acebutolol	Acebutolol-d$_5$	1.000	0.05 – 100	0.005	0.01
4.7	Lamotrigine	Carbamazepine-d$_{10}$	1.000	0.05 – 100	0.002	0.005
4.8	Metoprolol	Metoprolol-d$_7$	0.998	0.5 – 100	0.1	0.5
4.8	Primidone	Primidone-d$_5$	0.999	0.5 – 100	0.1	0.2
4.9	Fluconazole	Caffeine-^{13}C	0.997	0.1 – 100	0.03	0.1
5.4	Ifosfamide	Venlafaxine-d$_6$	0.999	0.5 – 100	0.05	0.25
5.5	4-Hydroxy Omeprazole	Carbamazepine-d$_{10}$	1.000	0.1 – 100	0.01	0.1
5.9	Chlorpheniramine	Chlorpheniramine-d$_6$	0.999	0.1 – 100	0.05	0.1
5.9	Carbamazepine-10,11-epoxide	Carbamazepine-10,11-epoxide-d$_{10}$	0.998	0.5 – 100	0.03	0.1
5.9	Venlafaxine	Venlafaxine-d$_6$	1.000	0.5 – 100	0.1	0.25
5.9	Bisoprolol	Bisoprolol-d$_5$	1.000	0.05 – 100	0.01	0.03
6.1	Propranolol	Propranolol-d$_7$	1.000	0.5 – 100	blank	0.1
6.2	Citalopram	Citalopram-d$_6$	0.999	0.1 – 100	0.02	0.1
6.2	Desmethylcitalopram	Citalopram-d$_6$	0.998	0.1 – 100	0.03	0.1
6.5	Omeprazole	Caffeine-^{13}C	0.995	1 – 100	0.7	1
6.8	Hydroxyibuprofen	Paracetamol-d$_4$	0.999	1 – 100	0.5	1
6.9	Carbamazepine	Carbamazepine-d$_{10}$	0.999	0.05 – 100	0.005	0.02
7.1	Mebendazole	Carbamazepine-d$_{10}$	0.999	5 – 100	blank	5
7.3	Fexofenadine	Venlafaxine-d$_6$	1.000	0.5 – 100	0.03	0.11
7.4	Erythromycin	Clarithromycin-^{13}C-d$_3$	1.000	0.05 – 50	0.01	0.05
7.5	Lansoprazole	Citalopram-d$_6$	0.998	1 – 100	0.05	1
7.6	Oxazepam	Oxazepam-d$_5$	0.998	0.5 – 100	0.2	0.5
7.6	Lorazepam	Temazepam-d$_5$	0.999	0.5 – 100	0.1	0.5
7.7	Climbazole	Clarithromycin-^{13}C-d$_3$	0.942	0.5 – 100	0.1	0.25
7.7	Fluoxetine	Fluoxetine-d$_6$	0.999	0.1 – 100	0.03	0.1
7.8	Temazepam	Temazepam-d$_5$	1.000	0.1 – 100	0.04	0.1
7.8	Ketoprofen	Temazepam-d$_5$	0.999	0.5 – 100	0.15	0.5
7.9	Cetirizine	Metoprolol-d$_7$	0.998	0.5 – 100	0.06	0.2
8.1	Clarithromycin	Clarithromycin-^{13}C-d$_3$	0.999	0.05 – 100	0.005	0.01
8.1	Norethisterone	Carbamazepine-d$_{10}$	1.000	0.5 – 100	0.15	0.5
8.1	Bezafibrate	Carbamazepine-d$_{10}$	1.000	0.5 – 100	0.15	0.5
8.2	Crotamiton	Carbamazepine-d$_{10}$	0.999	0.05 – 100	0.002	0.005
8.2	Clotrimazole	Clarithromycin-^{13}C-d$_3$	0.978	0.5 – 100	0.05	0.1
8.2	Warfarin	Carbamazepine-d$_{10}$	1.000	0.1 – 100	0.05	0.1

9.0	Atorvastatin	peak area	1.000	0.05 – 100	0.002	0.005
9.4	Miconazole	peak area	0.938	0.5 – 100	blank	0.5
5.6	Estriol	Estrone-d_4	1.000	0.5 – 100	0.1	0.5
6.0	Naproxen	Ibuprofen-d_3	0.996	1 – 100	0.05	1
7.1	Diclofenac	Ibuprofen-d_3	0.994	0.5 – 100	blank	0.5
7.4	17β-Estradiol	17β-Estradiol-d_4	1.000	0.5 – 100	0.1	0.3
7.5	Estrone	Estrone-d_4	1.000	0.5 – 100	0.1	0.3
7.5	17α-Ethinylestradiol	17β-Estradiol-d_4	0.999	1 – 100	0.5	1
7.5	Ibuprofen	Ibuprofen-d_3	0.994	0.5 - 500	0.1	0.5
8.7	Gemfibrozil	Ibuprofen-d_3	0.995	0.1 – 100	0.05	0.1

For precision, the relative standard deviation of the replicates was calculated. Accuracies were determined from the percentage deviation of the standards from the calibration curve. Therefore, concentrations (c_{calc}) of the 1, 10, and 50 µg L^{-1} standards were calculated from the area ratios (ar) following subtraction of the calculated concentration (c_0) of the blank using equation S4.

$$c_{calc} = \frac{(ar - b)}{m} - c_0$$

(S4)

Accuracy was then calculated from the ratio of the calculated and standard concentration (c_{std}) according to equation S5.

$$accuracy = \frac{c_{calc}}{c_{std}} \cdot 100\,\%$$

(S5)

Table S7: Intra- and Inter-day accuracy and precision (both in %) with p-values (two sample t-test with rstatix in R) for the repeated injection of 1, 10, and 50 µg L^{-1} standards.

RT	Analyte	Accuracy (/%)							Precision (/%)						
		Intra day			Inter day				Intra day			Inter day			
		1 µg L^{-1}	10 µg L^{-1}	50 µg L^{-1}	1 µg L^{-1}	10 µg L^{-}	50 µg L^{-1}	p-value	1 µg L^{-1}	10 µg L^{-1}	50 µg L^{-1}	1 µg L^{-1}	10 µg L^{-}	50 µg L^{-1}	p-value
0.7	Guanylurea	105	101	89	120	104	106	0.173	7	2	3	8	1	5	0.752
0.8	Metformin	90	98	106	90	100	108	0.891	9	1	4	3	1	5	0.532
1.2	Sulfanilamide	76	91	104	98	99	97	0.428	10	8	4	4	6	9	0.734
1.7	Cotinine	102	100	106	98	99	97	0.100	3	4	7	7	6	4	0.513
2.0	Amidotrizoic acid	100	102	99	94	100	105	0.794	13	7	6	5	11	11	0.858
2.2	Amoxicillin	99	110	100	118	100	113	0.336	9	10	4	20	15	10	0.117
2.3	Sotalol	100	100	98	108	90	99	0.961	7	2	2	2	8	3	0.843
2.4	Paracetamol	84	112	107	101	110	111	0.559	5	6	2	5	8	4	0.334
2.5	Salbutamol	100	101	96	97	96	91	0.160	9	1	4	9	5	7	0.461
2.5	Ranitidine	95	110	102	74	89	90	0.054	15	10	14	9	9	14	0.395
2.5	Atenolol	100	101	100	107	96	98	0.932	8	7	6	12	2	2	0.730
2.6	Sulfadiazine	106	101	90	93	92	84	0.199	7	4	3	7	4	6	0.491
2.9	3-Methoxy Paracetamol	122	98	100	124	97	110	0.722	6	6	2	4	8	5	0.755
3.0	3-Desmethyl Trimethoprim	101	96	94	116	101	109	0.098	7	4	5	4	11	5	0.602
3.1	α-Hydroxy Trimethoprim	107	101	92	111	108	97	0.441	3	8	5	16	7	1	0.609
3.3	Clopidol	a	104	94	a	108	96	0.711	a	6	8	a	6	7	0.674
3.3	Gabapentin	119	95	92	98	99	97	0.694	5	8	5	11	7	1	0.868
3.6	Trimethoprim	102	106	95	126	112	112	0.053	6	6	5	3	5	6	0.240
3.6	Caffeine	79	93	93	94	116	97	0.186	15	6	5	15	5	5	0.921
3.7	Ofloxacin	80	98	100	94	93	96	0.825	9	8	5	6	4	29	0.536
3.9	Ciprofloxacin	97	97	99	104	109	132	0.185	6	7	10	19	5	21	0.280

13

4.0	Lidocaine	100	100	101	95	93	93	0.004	6	1	4	16	10	4	0.206
4.1	Sulfamethoxazole	101	106	100	95	102	100	0.273	12	8	5	4	11	6	0.719
4.5	Desmethylvenlafaxine	85	99	100	97	100	94	0.650	6	3	5	10	6	2	0.632
4.7	Acebutolol	99	100	94	99	96	97	0.750	8	5	4	4	4	1	0.205
4.7	Lamotrigine	112	103	97	113	102	98	0.906	7	5	7	9	8	5	0.458
4.8	Primidone	102	99	104	104	108	106	0.100	6	4	8	3	5	3	0.225
4.8	Metoprolol	111	100	104	99	95	100	0.136	7	3	3	3	3	7	0.936
4.9	Fluconazole	102	100	94	98	94	94	0.367	6	7	2	7	5	2	0.954
5.4	Ifosfamide	90	99	93	95	93	88	0.615	9	1	6	2	8	7	0.843
5.5	4-Hydroxy Omeprazole	112	101	98	108	96	95	0.521	6	6	6	1	1	4	0.062
5.9	Chlorpheniramine	72	108	102	68	112	97	0.939	1	5	5	6	1	2	0.830
5.9	Carbamazepine-10,11-epoxide	106	101	95	96	101	96	0.513	12	6	7	10	1	6	0.488
5.9	Venlafaxine	97	102	101	94	103	98	0.590	7	6	4	5	5	5	0.625
5.9	Bisoprolol	100	101	100	100	100	103	0.426	2	4	6	6	5	4	0.423
6.1	Propranolol	100	100	98	101	111	94	0.626	7	10	5	4	7	3	0.185
6.2	Citalopram	98	98	96	94	101	101	0.634	5	4	5	7	3	3	0.907
6.2	Desmethylcitalopram	99	97	95	107	107	103	0.007	6	4	9	6	10	7	0.615
6.5	Omeprazole	[a]	99	103	[a]	106	98	0.773	18	21	16	[a]	13	21	0.752
6.8	Hydroxyibuprofen	98	99	94	97	105	108	0.178	23	5	7	18	5	4	0.722
6.9	Carbamazepine	102	100	99	100	96	99	0.288	4	6	5	4	3	5	0.132
7.1	Mebendazole	[a]	100	96	86	85	90	0.046	2	4	5	10	5	6	0.189
7.3	Fexofenadine	91	106	102	93	115	108	0.503	6	3	5	10	3	6	0.410
7.4	Erythromycin	110	99	[b]	105	87	[b]	0.523	8	9	2	2	2	9	0.498
7.5	Lansoprazole	125	100	101	136	121	84	0.794	28	11	7	36	14	30	0.287
7.6	Oxazepam	120	99	100	102	98	95	0.376	6	7	9	7	13	2	1.000

7.6	Lorazepam	108	104	112	103	108	101	0.233	9	10	13	5	1	8	0.085
7.7	Climbazole	a	82	110	a	116	106	0.451	10	1	7	4	1	5	0.479
7.7	Fluoxetine	96	107	93	80	105	92	0.514	5	5	4	2	4	5	0.520
7.8	Temazepam	107	103	102	104	106	103	0.639	6	4	8	9	5	6	0.717
7.8	Ketoprofen	93	102	104	84	97	91	0.169	5	5	10	12	11	1	0.786
7.9	Cetirizine	82	100	107	126	219	235	0.098	7	4	6	3	3	7	0.405
8.1	Clarithromycin	94	98	87	97	98	89	0.748	5	2	6	2	4	2	0.282
8.1	Norethisterone	116	101	99	105	105	106	0.967	15	4	3	16	9	12	0.299
8.1	Bezafibrate	115	100	98	97	94	92	0.194	7	3	6	2	7	3	0.541
8.2	Crotamiton	99	100	97	82	92	91	0.062	9	2	4	9	7	4	0.573
8.2	Clotrimazole	a	75	103	a	111	83	0.728	7	8	8	3	2	5	0.036
8.2	Warfarin	108	101	99	97	101	95	0.220	6	7	4	7	2	6	0.697
9.0	Atorvastatin	101	103	81	117	112	94	0.255	11	7	5	15	1	9	0.881
9.4	Miconazole	112	102	88	87	91	92	0.265	7	8	13	5	12	2	0.535
5.6	Estriol	101	102	98	76	83	85	0.012	14	3	4	12	6	3	0.947
6.0	Naproxen	115	96	104	106	106	111	0.703	4	8	6	5	2	15	0.798
7.1	Diclofenac	110	110	106	104	100	100	0.018	4	10	9	4	13	12	0.571
7.4	17β-Estradiol	101	105	102	105	101	102	0.846	15	6	6	17	13	12	0.222
7.5	Estrone	109	98	101	103	105	106	0.662	8	6	4	3	2	6	0.313
7.5	17α-Ethinylestradiol	112	109	99	115	101	108	0.834	4	3	5	2	13	5	0.570
7.5	Ibuprofen	a	106	98	a	112	92	0.981	9	2	11	10	11	10	0.829
8.7	Gemfibrozil	86	102	98	89	91	91	0.389	6	5	6	10	15	13	0.034

a) c ≤ IQL, b) c ≥ calibration range

S9   Method performance

Table S8: Absolute recoveries (REC) and relative standard deviation (sd) (both in %) from spiked wastewater (c = 10ng/mL) using polytetrafluoroethylene (PTFE), cellulose acetate (CA), polyvinylidene fluoride hydrophilic (PVDF-HL), and polyvinylidene fluoride hydrophobic (PVDF) syringe filters (n = 3). Sorted according to method and retention times.

RT /min	Analyte	PTFE		CA		PVDF		PVDF-HL	
		REC	sd	REC	sd	REC	sd	REC	sd
positive									
0.7	Guanylurea	99	3	101	3	95	3	91	2
0.8	Metformin	97	4	97	4	88	4	88	2
1.2	Sulfanilamide	91	7	93	6	87	5	82	9
1.7	Cotinine	102	4	100	3	94	4	93	5
2.2	Amoxicillin	120	7	42	19	82	9	83	6
2.3	Sotalol	103	4	96	4	86	6	86	3
2.4	Paracetamol	100	3	98	2	104	2	101	3
2.5	Salbutamol	102	5	98	5	86	2	86	2
2.5	Ranitidine	99	4	99	7	85	4	83	4
2.5	Atenolol	96	5	95	7	85	6	83	3
2.6	Sulfadiazine	99	2	95	6	84	4	79	3
3.3	Gabapentin	103	5	100	6	88	2	88	5
3.6	Trimethoprim	102	3	97	3	88	3	87	4
3.6	Caffeine	95	9	91	8	88	10	89	11
3.7	Ofloxacin	100	4	97	7	79	3	83	1
3.9	Ciprofloxacin	99	2	93	7	84	3	79	3
4.0	Lidocaine	94	5	94	6	83	3	85	3
4.1	Sulfamethoxazole	98	4	97	7	88	3	87	3
4.5	Desmethylvenlafaxine	96	5	93	7	84	2	84	3
4.7	Acebutolol	92	5	91	6	73	3	84	4
4.7	Lamotrigine	100	6	94	5	87	4	85	4
4.8	Metoprolol	97	3	95	4	81	6	86	4
4.8	Primidone	106	4	100	4	91	4	87	6
4.8	Fluconazole	97	5	98	6	86	5	85	3
5.4	Ifosfamide	99	5	93	8	89	5	86	5
5.8	Chlorpheniramine	59	3	73	4	12	2	72	7
5.9	Carbamazepine-10,11-epoxide	101	4	96	6	88	3	88	4
5.9	Venlafaxine	76	10	87	11	59	3	79	3
5.9	Bisoprolol	88	7	90	6	67	4	83	3
6.1	Propranolol	55	3	52	5	42	4	57	7
6.2	Citalopram	27	47	39	3	6	15	49	6
6.2	Desmethylcitalopram	24	48	35	61	16	13	38	7
6.4	Omeprazole	98	3	91	6	87	2	87	4
6.8	Hydroxyibuprofen	100	3	95	6	91	2	90	3
6.9	Carbamazepine	100	3	94	6	87	2	87	3
7.1	Mebendazole	104	4	67	13	89	2	89	3

7.3	Fexofenadine	88	7	93	7	59	4	85	5
7.4	Erythromycin	56	34	82	16	18	12	79	5
7.5	Oxazepam	94	4	85	6	82	6	83	5
7.6	Lorazepam	96	3	79	6	81	5	82	3
7.7	Climbazole	81	6	58	15	69	4	68	5
7.7	Fluoxetine	5	13	26	13	7	22	11	12
7.8	Temazepam	96	3	88	4	80	2	84	4
7.8	Ketoprofen	106	4	103	4	95	2	91	4
7.8	Cetirizine	50	15	52	4	31	3	56	8
8.1	Clarithromycin	27	54	61	26	6	12	65	6
8.1	Norethisterone	102	3	76	5	85	4	84	3
8.1	Bezafibrate	101	9	98	4	89	15	89	22
8.1	Clotrimazole	28	39	13	59	9	14	10	31
8.2	Warfarin	100	7	96	4	93	11	90	12
9.0	Atorvastatin	88	4	65	6	71	3	75	2
9.3	Miconazole	8	28	11	22	4	7	11	28
negative									
5.7	Estriol	119	14	112	4	107	19	110	25
6.0	Naproxen	101	13	103	7	91	9	91	23
7.0	Diclofenac	96	9	98	5	91	15	101	16
7.4	E2	101	12	63	7	97	22	80	14
7.5	Estrone	95	12	37	6	84	17	71	9
7.6	Ibuprofen	98	11	99	5	91	12	92	19
8.7	Gemfibrozil	97	9	96	3	94	13	90	12

Table S9: Absolute recoveries (Rec) and relative standard deviation (sd) (both in %) for each analyte in influent, effluent, river water, and sludge (n = 3). If not otherwise stated all spiked samples were used in the calculation.

RT /min	Analyte	Direct inject.						SPE						Sludge	
		Influent		Effluent		River		Influent		Effluent		River			
		Rec	sd	Rec	sd	Rec	sd	Rec	sd	Rec	sd	Rec	sd	Rec	sd
0.7	Guanylurea	52	7	55	6	184	13	4	2	3[a]	4	2	1	[d]	-
0.8	Metformin	161	74[b]	192[a]	60[b]	186	86[b]	16	2	[b]	-	4[c]	3	[d]	-
0.8	Metformin-d$_6$	209	7	164	8	241	11	9	5	7	4	3	2	[d]	-
1.2	Sulfanilamide	84[a]	9	77	6	98	7	11[a]	2	15[a]	7	16	14	5[d]	5
1.7	Cotinine-d$_3$	96	8	100	6	98	8	89	11	82	4	91	12	108	30
1.7	Cotinine	94	3	103	9	95	5	80	6	[b]	-	90	10	100	14

2.0	Amidotrizoic acid	95	8	98	11	92	7	0	0	1	0	0	0	0[d]	-
2.2	Amoxicillin	87	7	96	9	98	11	11[a]	9	31[a]	6	1	1	0[d]	-
2.2	Sotalol-d_6	98	4	106	6	98	4	87	5	89	4	90	9	23	5
2.3	Sotalol	101	6	99	3	99	7	79	10	78	3	87	13	28	3
2.3	Paracetamol-d_4	84	5	96	3	87	7	58	2	40	2	51	12	33	2
2.4	Paracetamol	86[a]	5	b	-	90[a]	9	b	-	b	-	33[a]	11	b	-
2.5	Salbutamol-d_3	96	6	104	5	92	3	92	7	95	6	79	7	17	8
2.5	Salbutamol	101	4	107	6	101	6	112	18	88	4	79	7	13	3
2.5	Ranitidine	121	35	142	18	118	37	59	11	98	19	85	21	2[d]	1
2.5	Atenolol-d_7	97	5	103	6	98	7	100	4	93	6	91	7	31	9
2.5	Atenolol	107	7	103	6	107	12	88	11	84[a]	8	92	12	37	9
2.6	Sulfadiazine	94	3	105	14	97	9	70	4	55	11	75	4	20	9
2.9	3-Methoxy Paracetamol	98[a]	8	105[a]	12	99	11	81[c]	3	b	-	87	10	79	18
3.0	3-Desmethyl Trimethoprim	102	6	104	5	105	9	85	7	63	16	79	11	63	9
3.1	α-Hydroxy Trimethoprim	104	5	105	4	107	5	91	11	81	4	86	11	44	10
3.3	Clopidol	86[a]	6	99[a]	8	94[a]	13	78[a]	10	74[a]	5	70[a]	5	77	9
3.3	Gabapentin	89	8	112	18	92	12	7	5	b	-	2	2	7[d]	2
3.6	Trimethoprim	103	10	109	4	105	9	69	6	50[a]	7	75	10	53	19
3.6	Caffeine	59	29	99[c]	23	73	27	b	-	b	-	64[a]	20	101[e]	1
3.6	Caffeine-[13]C	90	7	105	5	93	6	86	8	82	5	92	8	97	4
3.7	Ofloxacin	47	6	116	5	41	4	17	2	34	13	4	2	15	2
3.7	Ofloxacin-d_8	95	1	128	8	91	15	37	5	71	7	10	2	12	3
3.9	Ciprofloxacin	59	28	106	34	50	20	194	36	43	8	87	4	18	6
4.0	Lidocaine	96	3	99	5	101	6	57	2	43	5	75	10	50	16
4.1	Sulfamethoxazole	94	4	103	4	100	7	81	4	75	9	88	11	47	19
4.5	Desmethylvenlafaxine	93	3	98	6	98	6	49	3	64[a]	13	76	11	54	13

4.7	Acebutolol-d$_5$	102	8	106	7	105	11	80	8	76	3	79	7	22	5
4.7	Acebutolol	104	6	112	10	107	10	83	2	83	7	78	8	22	4
4.7	Lamotrigine	93	7	100	5	98	6	46	5	61	11	71	11	29[c]	10
4.8	Metoprolol-d$_7$	96	4	98	4	99	5	62	4	66	4	75	9	24	4
4.8	Metoprolol	97	10	102	8	106	8	55	8	71	13	77	8	22	4
4.8	Primidone-d$_5$	92	13	99	4	93	10	74	11	85	6	90	12	75	9
4.8	Primidone	96	8	95	3	98	8	72	8	78	5	92	10	84	9
4.9	Fluconazole	89	6	97	4	96	7	67	7	75	5	84	4	91	9
5.4	Ifosfamide	88	3	102	9	94	7	57	5	71	8	85	8	77	6
5.5	4-Hydroxy Omeprazole	89	6	102	2	97	9	57[a]	13	55[a]	2	69	9	86	26
5.8	Chlorpheniramine-d$_6$	175	12	164	25	209	16	111	10	96	7	44	13	72	12
5.9	Chlorpheniramine	82	23	162	9	97	25	189	11	[b]	-	20	11	67	38
5.8	Carbamazepine-10,11-epoxide-d$_{10}$	89	10	108	16	87	8	77	10	92	18	89	15	73	9
5.9	Carbamazepine-10,11-epoxide	87	5	100	4	91	7	79	8	84	9	84	7	93	9
5.8	Venlafaxine-d$_6$	95	6	99	7	99	7	58	4	60	4	70	5	55	8
5.9	Venlafaxine	91	5	108	11	101	8	53	7	[b]	-	55	12	49[e]	20
5.9	Bisoprolol-d$_5$	107	4	103	11	103	4	101	4	93	7	88	13	24	4
5.9	Bisoprolol	109	4	111	10	108	6	105	5	84[a]	15	85	12	24	7
6.0	Propranolol-d$_7$	94	9	102	12	106	11	80	6	71	8	33	10	[d]	-
6.1	Propranolol	90	6	95	12	101	9	65	5	54[a]	6	25	6	32	12
6.2	Citalopram-d$_6$	84	7	96	18	113	8	117	5	108	16	13	5	65	10
6.2	Citalopram	85	12	103	6	118	13	69	14	[b]	-	12	4	73[c]	10
6.2	Desmethylcitalopram	88	12	99	9	118	12	62	9	54[a]	7	7	6	8	3
6.5	Omeprazole	26[a]	6	21[a]	13	23[a]	3	37[a]	19	30[a]	6	54[a]	19	[d]	-
6.8	Hydroxyibuprofen	90[a]	9	116[c]	20	95[a]	5	[b]	-	[b]	-	50[a]	13	34	1
6.9	Carbamazepine-d$_{10}$	91	8	103	6	93	10	52	6	51	5	79	10	72	14

RT	Compound														
6.9	Carbamazepine	89	5	101	5	91	5	53	5	45	7	72	10	64	5
7.1	Mebendazole	63[a]	2	41[a]	26	67[a]	2	52[a]	1	23[a]	5	33[a]	1	25	9
7.3	Fexofenadine	97	3	103	11	100	6	65[a]	2	[b]	-	71	4	112	31
7.4	Erythromycin	75	59	140	19	63	45	3	1	2	1	21	18	33[e]	22
7.5	Lansoprazole	23[a]	5	19[a]	8	19[a]	4	35	20	29[a]	20	19[a]	11	[d]	-
7.5	Oxazepam-d_5	90	8	102	17	83	16	143	32	60	22	68	11	107	16
7.6	Oxazepam	91	5	93	8	90	4	111	26	[b]	-	68	12	80	17
7.6	Lorazepam	93	15	94	11	101	22	88[a]	7	25[a]	8	75	14	84	21
7.7	Climbazole	88	5	100	4	89	6	60	14	9	7	18	7	36	16
7.7	Fluoxetine-d_6	26	7	35	10	73	13	34	6	13	5	1[a]	0	10	29
7.7	Fluoxetine	32	11	34	4	101	23	43	13	8	3	1[a]	3	5	2
7.8	Temazepam-d_5	94	6	105	5	92	9	102	5	32	13	72	7	108	13
7.8	Temazepam	95	7	100	5	99	6	99	14	19	7	72	7	79	13
7.8	Ketoprofen	94	5	100	9	96	7	101	8	27	11	92	13	112	13
7.9	Cetirizine	68	19	95	17	68	16	38	14	[b]	-	46	19	46	17
8.1	Clarithromycin	166	30	137	26	154	38	67	10	16	4	27	9	23[e]	7
8.1	Clarithromycin-^{13}C-d_3	144	25	104	34	140	42	68	16	17	5	21	7	39	9
8.1	Norethisterone	87	10	95	7	95	10	42	6	30	12	55	10	48	10
8.1	Bezafibrate	97	6	102	6	99	6	85	12	36	13	88	12	118	10
8.2	Clotrimazole	81	15	58	11	47	16	24	4	19	3	1	0	25[e]	11
8.2	Crotamiton	93	4	97	4	98	7	46	6	16[c]	4	63	6	42	12
8.2	Warfarin	95	4	98	4	97	8	63	5	33	9	83	7	86	15
9.0	Atorvastatin	84	7	105	5	79	5	27	9	[b]	-	31	7	40	5
9.4	Miconazole	85	30	43	8	27	17	8	2	11	6	1[a]	6	30[e]	11
5.6	Estriol	104	23	96[a]	4	95	18	64	5	132[c]	7	85	11	73	15
6.0	Naproxen	92[a]	8	102[a]	11	84	6	81[a]	7	[b]	-	104[a]	7	108[c]	17

RT	Analyte														
7.1	Diclofenac	96[a]	5	99[a]	4	96[a]	3	69[a]	4	92[a]	18	85[a]	5	49[e]	9
7.4	17β-Estradiol-d$_4$	98	7	96	6	95	3	73	5	81	3	46	5	39	11
7.4	17β-Estradiol	98	9	99	9	98	10	70	10	77	9	43	5	35	12
7.5	Estrone-d$_4$	99	4	102	7	99	6	72	3	79	4	43	5	33	7
7.5	Estrone	106	15	102	3	97	6	62	12	86[c]	5	41	6	36	11
7.5	17α-Ethinylestradiol	103	17	103[a]	7	107	18	71[a]	11	71[a]	11	19[a]	3	35	12
7.5	Ibuprofen	101[a]	5	89[a]	6	89[a]	5	b	-	b	-	77[a]	11	b	-
7.6	Ibuprofen-d$_3$	99	15	109	14	93	8	172	14	115	7	100	10	95	15
8.7	Gemfibrozil	91	10	102[a]	4	91	10	17	4	67[a]	4	75	9	36	7

a) calculated from c ≥ 10 µgL^{-1}, b) c too high in sample, c) calculated from c ≥ 50 µgL^{-1}, d) method not suitable, e) calculated from c ≥ 100 µgL^{-1}

If an EC concentration in the SPE sample was too high for the calculation of the absolute recovery ($REC_{SPE,matrix\ 1}$) to be practical (Table S9), a theoretical absolute recovery was calculated from the average ratios of the absolute recoveries in direct injection ($REC_{di,matrix}$) and SPE ($REC_{SPE,matrix}$) (equation S6) and used to determine MDL and MQL as described in equations S4 and S5, respectively. For ECs withisotopically labelled EC, the absolute recovery of the isotopically labelled EC was used.

$$REC_{SPE,\ matrix\ 1} = REC_{di,\ matrix\ 1} \cdot 0.5 \cdot \left(\frac{REC_{SPE,\ matrix\ 2}}{REC_{di,\ matrix\ 2}} + \frac{REC_{SPE,\ matrix\ 3}}{REC_{di,\ matrix\ 3}} \right)$$

(S6)

Relative recoveries (Figure 4) were calculated accordingly.

Table S10: Method detection (MDL) and quantitation limits (MQL) in influent, effluent, river water and sludge analysed by direct injection and SPE

RT	Analyte	Direct injection in µg L^{-1}						SPE in µg L^{-1}						Sludge in µg kg^{-1}	
/min		Influent		Effluent		River		Influent		Effluent		River			
		MDL	MQL	MDL	MQL	MDL	MQL	MDL	MQL	MDL	MQL	MDL	MQL	MDL	MQL

0.7	Guanylurea	0.53	1.1	0.51	1.0	0.15	0.30	a	a	a	a	a	a	a	a
0.8	Metformin	0.035	0.069	0.029	0.058	0.030	0.060	a	a	a	a	a	a	a	a
1.2	Sulfanilamide	0.66	1.3	0.72	1.4	0.57	1.1	0.045	0.091	0.033	0.067	0.016	0.031	a	a
1.7	Cotinine	$5.9 \cdot 10^{-3}$	0.019	$5.4 \cdot 10^{-3}$	0.017	$5.9 \cdot 10^{-3}$	0.019	$6.3 \cdot 10^{-5}$	$2.0 \cdot 10^{-4}$	$6.1 \cdot 10^{-5}$	$2.0 \cdot 10^{-4}$	$2.9 \cdot 10^{-5}$	$8.9 \cdot 10^{-5}$	0.025	0.080
2.0	Amidotrizoic acid	0.12	0.35	0.11	0.34	0.10	0.36	a	a	a	a	a	a	a	a
2.2	Amoxicillin	1.0	1.3	0.93	1.2	0.91	1.1	0.073	0.091	0.026	0.032	0.40	0.50	a	a
2.3	Sotalol	$5.5 \cdot 10^{-3}$	0.044	$5.6 \cdot 10^{-3}$	0.045	$5.6 \cdot 10^{-3}$	0.045	$5.8 \cdot 10^{-5}$	$4.6 \cdot 10^{-4}$	$5.6 \cdot 10^{-5}$	$4.5 \cdot 10^{-4}$	$2.9 \cdot 10^{-5}$	$2.3 \cdot 10^{-4}$	0.090	0.72
2.4	Paracetamol	0.086	0.29	0.077	0.26	0.082	0.27	$1.1 \cdot 10^{-3}$	$3.8 \cdot 10^{-3}$	$1.7 \cdot 10^{-3}$	$5.6 \cdot 10^{-3}$	$6.5 \cdot 10^{-4}$	$2.2 \cdot 10^{-3}$	1.0	3.1
2.5	Salbutamol	$5.5 \cdot 10^{-3}$	0.044	$5.2 \cdot 10^{-3}$	0.042	$5.5 \cdot 10^{-3}$	0.044	$5.4 \cdot 10^{-5}$	$4.3 \cdot 10^{-4}$	$5.3 \cdot 10^{-5}$	$4.2 \cdot 10^{-4}$	$3.2 \cdot 10^{-5}$	$2.5 \cdot 10^{-4}$	0.19	1.6
2.5	Ranitidine	0.046	0.092	0.039	0.078	0.047	0.094	$8.5 \cdot 10^{-4}$	$1.7 \cdot 10^{-3}$	$5.1 \cdot 10^{-4}$	$1.0 \cdot 10^{-3}$	$2.9 \cdot 10^{-4}$	$5.9 \cdot 10^{-4}$	a	a
2.5	Atenolol	0.026	0.10	0.027	0.11	0.026	0.10	$2.8 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$3.0 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$1.4 \cdot 10^{-4}$	$5.4 \cdot 10^{-4}$	0.33	1.3
2.6	Sulfadiazine	0.024	0.079	0.021	0.071	0.023	0.076	$2.9 \cdot 10^{-4}$	$9.5 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$1.3 \cdot 10^{-4}$	$4.4 \cdot 10^{-4}$	0.49	1.6
2.9	3-Methoxy Paracetamol	0.034	0.11	0.032	0.11	0.034	0.11	$3.7 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$3.4 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$1.7 \cdot 10^{-4}$	$5.7 \cdot 10^{-4}$	0.19	0.63
3.0	3-Desmethyl Trimethoprim	$5.6 \cdot 10^{-3}$	0.019	0.055	0.018	0.055	0.018	$6.1 \cdot 10^{-5}$	$2.0 \cdot 10^{-4}$	$8.2 \cdot 10^{-5}$	$2.7 \cdot 10^{-4}$	$3.3 \cdot 10^{-5}$	$1.1 \cdot 10^{-4}$	0.041	0.14
3.1	α-Hydroxy Trimethoprim	0.053	0.11	0.053	0.11	0.052	0.10	$5.5 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$6.2 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$2.9 \cdot 10^{-4}$	$5.8 \cdot 10^{-4}$	0.57	1.1
3.3	Clopidol	0.41	1.4	0.35	1.2	0.37	1.2	$4.0 \cdot 10^{-3}$	0.013	$4.3 \cdot 10^{-3}$	0.014	$2.3 \cdot 10^{-3}$	$7.5 \cdot 10^{-3}$	2.1	6.9
3.3	Gabapentin	0.62	1.2	0.50	0.99	0.60	1.2	a	a	a	a	a	a	a	a
3.6	Trimethoprim	0.013	0.045	0.013	0.042	0.013	0.044	$1.8 \cdot 10^{-4}$	$6.0 \cdot 10^{-4}$	$2.5 \cdot 10^{-4}$	$8.3 \cdot 10^{-4}$	$8.3 \cdot 10^{-5}$	$2.8 \cdot 10^{-4}$	0.12	0.39
3.6	Caffeine	0.099	0.35	0.090	0.31	0.096	0.33	$9.3 \cdot 10^{-4}$	$3.3 \cdot 10^{-3}$	$9.8 \cdot 10^{-3}$	$3.4 \cdot 10^{-3}$	$4.3 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$	0.40	1.4

3.7	Ofloxacin	0.058	0.12	0.043	0.087	0.14	0.27	$2.9 \cdot 10^{-3}$	$5.9 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$2.9 \cdot 10^{-3}$	$6.3 \cdot 10^{-3}$	0.013	1.6	3.2
3.9	Ciprofloxacin	0.038	0.094	0.021	0.052	0.044	0.11	$1.0 \cdot 10^{-4}$	$2.6 \cdot 10^{-4}$	$4.7 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$1.1 \cdot 10^{-4}$	$2.9 \cdot 10^{-4}$	0.56	1.4
4.0	Lidocaine	$6.3 \cdot 10^{-3}$	0.021	$6.1 \cdot 10^{-3}$	0.020	$6.0 \cdot 10^{-3}$	0.020	$9.6 \cdot 10^{-5}$	$3.2 \cdot 10^{-4}$	$1.3 \cdot 10^{-4}$	$4.2 \cdot 10^{-4}$	$3.6 \cdot 10^{-5}$	$1.2 \cdot 10^{-4}$	0.054	0.18
4.1	Sulfamethoxazole	0.059	0.12	0.054	0.11	0.056	0.11	$6.2 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$6.7 \cdot 10^{-4}$	$1.3 \cdot 10^{-3}$	$2.8 \cdot 10^{-4}$	$5.7 \cdot 10^{-4}$	0.54	1.1
4.5	Desmethylvenlafaxine	$6.0 \cdot 10^{-3}$	0.012	$5.7 \cdot 10^{-3}$	0.011	$5.7 \cdot 10^{-3}$	0.011	$1.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-4}$	$7.8 \cdot 10^{-5}$	$1.6 \cdot 10^{-4}$	$3.3 \cdot 10^{-5}$	$6.6 \cdot 10^{-5}$	0.046	0.093
4.7	Acebutolol	0.053	0.18	0.050	0.17	0.052	0.17	$6.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$6.0 \cdot 10^{-4}$	$2.0 \cdot 10^{-3}$	$3.2 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	1.1	3.7
4.7	Lamotrigine	0.21	0.70	0.20	0.65	0.20	0.67	$3.8 \cdot 10^{-3}$	0.013	$2.9 \cdot 10^{-3}$	$9.6 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$4.1 \cdot 10^{-3}$	3.1	10
4.8	Primidone	0.071	0.24	0.072	0.24	0.069	0.24	$8.5 \cdot 10^{-4}$	$2.8 \cdot 10^{-3}$	$7.8 \cdot 10^{-4}$	$2.6 \cdot 10^{-3}$	$3.3 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	0.36	1.2
4.8	Metoprolol	0.11	0.57	0.11	0.54	0.10	0.52	$1.8 \cdot 10^{-3}$	$9.1 \cdot 10^{-3}$	$1.4 \cdot 10^{-3}$	$7.0 \cdot 10^{-3}$	$6.5 \cdot 10^{-4}$	$3.2 \cdot 10^{-3}$	2.3	12
4.9	Fluconazole	0.037	0.12	0.034	0.11	0.035	0.12	$4.5 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$	$4.0 \cdot 10^{-4}$	$1.3 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$	$6.0 \cdot 10^{-4}$	0.17	0.55
5.4	Ifosfamide	0.063	0.32	0.054	0.27	0.059	0.30	$8.8 \cdot 10^{-4}$	$4.4 \cdot 10^{-3}$	$7.0 \cdot 10^{-4}$	$3.5 \cdot 10^{-3}$	$2.9 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$	0.32	1.6
5.5	4-Hydroxy Omeprazole	0.012	0.12	0.011	0.11	0.011	0.11	$1.8 \cdot 10^{-4}$	$1.8 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$	$1.8 \cdot 10^{-3}$	$7.2 \cdot 10^{-5}$	$7.2 \cdot 10^{-4}$	0.058	0.58
5.9	Chlorpheniramine	0.15	0.48	0.073	0.24	0.12	0.41	$5.7 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$	$1.1 \cdot 10^{-3}$	$3.7 \cdot 10^{-3}$	$2.7 \cdot 10^{-3}$	$8.9 \cdot 10^{-3}$	0.79	2.6
5.9	Carbamazepine-10,11-epoxide	0.038	0.13	0.033	0.11	0.037	0.12	$3.8 \cdot 10^{-4}$	$1.3 \cdot 10^{-3}$	$3.6 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	$1.8 \cdot 10^{-4}$	$6.0 \cdot 10^{-4}$	0.16	0.54
5.9	Venlafaxine	0.12	0.31	0.10	0.26	0.11	0.28	$1.9 \cdot 10^{-3}$	$4.7 \cdot 10^{-3}$	$1.6 \cdot 10^{-3}$	$4.1 \cdot 10^{-3}$	$9.1 \cdot 10^{-4}$	$2.3 \cdot 10^{-3}$	1.0	2.5
5.9	Bisoprolol	0.010	0.031	0.010	0.030	0.010	0.031	$9.5 \cdot 10^{-5}$	$2.9 \cdot 10^{-4}$	$1.2 \cdot 10^{-4}$	$3.6 \cdot 10^{-4}$	$5.9 \cdot 10^{-5}$	$1.8 \cdot 10^{-4}$	0.21	0.62
6.1	Propranolol	[b]	0.12	[b]	0.12	[b]	0.11	[b]	$1.3 \cdot$	[b]	$1.4 \cdot$	[b]	$2.0 \cdot$	[b]	1.6

pKa	Compound														
								10^{-3}		10^{-3}		10^{-3}		
6.2	Citalopram	0.026	0.13	0.022	0.11	0.019	0.094	$1.7 \cdot 10^{-4}$	$8.5 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	$9.3 \cdot 10^{-4}$	$8.3 \cdot 10^{-4}$	$4.2 \cdot 10^{-3}$	0.14	0.68
6.2	Desmethylcitalopram	0.032	0.13	0.028	0.11	0.024	0.094	$4.0 \cdot 10^{-4}$	$1.6 \cdot 10^{-3}$	$4.6 \cdot 10^{-4}$	$1.9 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$	$7.1 \cdot 10^{-3}$	1.7	6.6
6.5	Omeprazole	3.0	4.3	3.7	5.3	3.4	4.8	0.019	0.027	0.023	0.033	$6.5 \cdot 10^{-3}$	$9.3 \cdot 10^{-3}$	[a]	[a]
6.8	Hydroxyibuprofen	0.62	1.2	0.48	0.96	0.58	1.2	0.011	0.021	$8.2 \cdot 10^{-3}$	0.016	$5.0 \cdot 10^{-3}$	0.010	7.4	15
6.9	Carbamazepine	[b]	0.62	[b]	0.55	[b]	0.61	[b]	$9.4 \cdot 10^{-3}$	[b]	0.011	[b]	$3.5 \cdot 10^{-3}$	[b]	3.9
7.1	Mebendazole	[b]	8.8	[b]	14	[b]	8.3	[b]	0.096	[b]	0.22	[b]	0.076	[b]	49
7.3	Fexofenadine	0.038	0.13	0.036	0.12	0.037	0.12	$5.1 \cdot 10^{-4}$	$1.7 \cdot 10^{-3}$	$4.7 \cdot 10^{-4}$	$1.6 \cdot 10^{-3}$	$2.3 \cdot 10^{-4}$	$7.8 \cdot 10^{-4}$	0.15	0.49
7.4	Erythromycin	0.015	0.074	$7.9 \cdot 10^{-3}$	0.040	0.018	0.088	$3.3 \cdot 10^{-3}$	0.017	$5.0 \cdot 10^{-3}$	0.025	$2.4 \cdot 10^{-4}$	$1.2 \cdot 10^{-3}$	0.15	0.76
7.5	Lansoprazole	0.24	4.8	0.29	5.8	0.29	5.8	$1.4 \cdot 10^{-3}$	0.028	$1.7 \cdot 10^{-3}$	0.034	$1.3 \cdot 10^{-3}$	0.026	[a]	[a]
7.6	Oxazepam	0.24	0.61	0.24	0.60	0.25	0.62	$1.8 \cdot 10^{-3}$	$4.5 \cdot 10^{-3}$	$3.3 \cdot 10^{-3}$	$8.3 \cdot 10^{-3}$	$1.5 \cdot 10^{-3}$	$3.7 \cdot 10^{-3}$	1.3	3.1
7.6	Lorazepam	0.12	0.60	0.12	0.59	0.11	0.55	$1.1 \cdot 10^{-3}$	$5.7 \cdot 10^{-3}$	$4.0 \cdot 10^{-3}$	0.020	$6.7 \cdot 10^{-4}$	$3.3 \cdot 10^{-3}$	0.60	3.0
7.7	Climbazole	0.13	0.32	0.11	0.28	0.12	0.31	$1.7 \cdot 10^{-3}$	$4.2 \cdot 10^{-3}$	0.011	0.028	$2.8 \cdot 10^{-3}$	$6.9 \cdot 10^{-3}$	1.4	3.5
7.7	Fluoxetine	0.087	0.35	0.082	0.33	0.028	0.11	$5.8 \cdot 10^{-4}$	$2.3 \cdot 10^{-3}$	$3.1 \cdot 10^{-3}$	0.013	0.013	0.050	2.5	10
7.8	Temazepam	0.018	0.058	0.017	0.056	0.017	0.056	$1.5 \cdot 10^{-4}$	$5.1 \cdot 10^{-4}$	$7.9 \cdot 10^{-4}$	$2.6 \cdot 10^{-3}$	$1.0 \cdot 10^{-4}$	$3.5 \cdot 10^{-4}$	0.095	0.32
7.8	Ketoprofen	0.18	0.59	0.17	0.56	0.17	0.58	$1.6 \cdot 10^{-3}$	$5.3 \cdot 10^{-3}$	$1.0 \cdot 10^{-3}$	$3.4 \cdot 10^{-3}$	$6.5 \cdot 10^{-4}$	$2.2 \cdot 10^{-3}$	0.67	2.2
7.9	Cetirizine	0.098	0.33	0.070	0.23	0.098	0.33	$1.5 \cdot 10^{-3}$	$5.0 \cdot 10^{-3}$	$5.6 \cdot 10^{-3}$	0.019	$8.2 \cdot 10^{-4}$	$2.7 \cdot 10^{-3}$	0.65	2.2
8.1	Clarithromycin	3.3 ·	6.7 ·	4.1 ·	8.1 ·	3.6 ·	7.2 ·	7.5 ·	1.5 ·	3.1 ·	6.3 ·	9.3 ·	1.9 ·	0.11	0.22

		10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-3}	10^{-5}	10^{-4}	10^{-4}	10^{-4}	10^{-5}	10^{-4}		
8.1	Norethisterone	0.19	0.64	0.18	0.58	0.18	0.58	$3.6 \cdot 10^{-3}$	0.012	$5.0 \cdot 10^{-3}$	0.017	$1.4 \cdot 10^{-3}$	$4.5 \cdot 10^{-3}$	1.6	5.2
8.1	Bezafibrate	0.64	2.1	0.61	2.0	0.62	2.1	$6.5 \cdot 10^{-3}$	0.022	0.015	0.051	$3.2 \cdot 10^{-3}$	0.011	2.4	7.9
8.2	Crotamiton	0.038	0.13	0.036	0.12	0.036	0.12	$6.9 \cdot 10^{-4}$	$2.3 \cdot 10^{-3}$	$2.0 \cdot 10^{-3}$	$6.6 \cdot 10^{-3}$	$2.5 \cdot 10^{-4}$	$8.4 \cdot 10^{-4}$	0.38	1.3
8.2	Clotrimazole	0.069	0.14	0.096	0.19	0.12	0.24	$2.1 \cdot 10^{-3}$	$4.2 \cdot 10^{-3}$	$2.6 \cdot 10^{-3}$	$5.3 \cdot 10^{-3}$	0.025	0.050	0.98	2.0
8.2	Warfarin	0.44	1.2	0.43	1.1	0.43	1.1	$6.0 \cdot 10^{-3}$	0.016	0.011	0.030	$2.3 \cdot 10^{-3}$	$6.0 \cdot 10^{-3}$	2.3	5.8
9.0	Atorvastatin	0.070	0.23	0.056	0.19	0.074	0.25	$1.9 \cdot 10^{-3}$	$6.5 \cdot 10^{-3}$	$1.4 \cdot 10^{-3}$	$4.7 \cdot 10^{-3}$	$8.5 \cdot 10^{-4}$	$2.8 \cdot 10^{-3}$	0.66	2.2
9.4	Miconazole	b	0.65	b	1.3	b	2.1	b	0.063	b	0.045	b	0.25	b	8.3
5.6	Estriol	0.11	0.53	0.12	0.58	0.12	0.59	$1.6 \cdot 10^{-3}$	$7.8 \cdot 10^{-3}$	$7.6 \cdot 10^{-4}$	$3.8 \cdot 10^{-3}$	$5.9 \cdot 10^{-4}$	$2.9 \cdot 10^{-3}$	0.68	3.4
6.0	Naproxen	0.060	1.2	0.054	1.1	0.066	1.3	$6.2 \cdot 10^{-4}$	0.012	$4.6 \cdot 10^{-4}$	$9.2 \cdot 10^{-3}$	$2.4 \cdot 10^{-4}$	$4.8 \cdot 10^{-3}$	0.25	4.9
7.1	Diclofenac	b	0.58	b	0.56	b	0.58	b	$7.2 \cdot 10^{-3}$	b	$5.4 \cdot 10^{-3}$	b	$2.9 \cdot 10^{-3}$	b	5.1
7.4	17β-Estradiol	0.11	1.1	0.11	1.1	0.11	1.1	$1.4 \cdot 10^{-3}$	0.014	$1.3 \cdot 10^{-3}$	0.013	$1.2 \cdot 10^{-3}$	0.012	1.4	14
7.5	Estrone	0.11	0.31	0.11	0.33	0.12	0.34	$1.6 \cdot 10^{-3}$	$4.8 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$3.5 \cdot 10^{-3}$	$1.2 \cdot 10^{-3}$	$3.7 \cdot 10^{-3}$	1.4	4.2
7.5	17α-Ethinylestradiol	0.54	1.1	0.54	1.1	0.52	1.0	$7.0 \cdot 10^{-3}$	0.014	$7.0 \cdot 10^{-3}$	0.014	0.013	0.026	7.2	14
7.5	Ibuprofen	0.10	0.34	0.087	0.29	0.11	0.36	$5.2 \cdot 10^{-4}$	$1.7 \cdot 10^{-3}$	$6.8 \cdot 10^{-4}$	$2.3 \cdot 10^{-3}$	$4.3 \cdot 10^{-4}$	$1.4 \cdot 10^{-3}$	0.47	1.6
8.7	Gemfibrozil	0.061	0.12	0.054	0.11	0.061	0.12	$2.9 \cdot 10^{-3}$	$5.9 \cdot 10^{-3}$	$7.5 \cdot 10^{-4}$	$1.5 \cdot 10^{-3}$	$3.3 \cdot 10^{-4}$	$6.7 \cdot 10^{-4}$	0.70	1.4

a) method not suitable, b) blank that could be corrected for

Table S11: Method accuracy and precision for direct injection (both in %), samples spiked with 1, 10, and 50 µg L^{-1} (n = 3).

RT	Analyte	Influent						Effluent						River					
		accuracy			precision			accuracy			precision			accuracy			precision		
		1	10	50	1	10	50	1	10	50	1	10	50	1	10	50	1	10	50
0.7	Guanylurea	94	109	97	4	3	5	a	117	116	a	2	6	107	103	90	9	9	5
0.8	Metformin	95	105	95	6	5	2	a	a	105	a	a	3	94	105	95	7	5	5
1.2	Sulfanilamide	b	109	107	b	9	4	b	104	105	b	11	3	b	102	104	b	12	9
1.7	Cotinine	118	111	103	5	4	5	102	106	104	1	10	6	117	106	110	4	6	6
2.0	Amidotrizoic acid	85	101	95	14	2	5	89	113	107	9	3	6	84	96	101	14	8	5
2.2	Amoxicillin	116	109	110	b	1	5	93	115	103	11	7	5	b	96	102	b	11	3
2.3	Sotalol	106	107	97	2	2	1	112	113	109	2	2	4	103	109	98	2	4	5
2.4	Paracetamol	b	110	105	b	8	6	a	a	a	a	a	a	b	111	104	b	4	3
2.5	Salbutamol	99	104	94	7	5	8	106	109	100	4	3	5	105	98	95	1	11	1
2.5	Ranitidine	b	105	124	b	4	8	b	104	111	b	5	9	b	103	128	2	6	5
2.5	Atenolol	98	102	92	10	3	8	a	101	101	a	6	6	93	107	91	3	10	4
2.6	Sulfadiazine	93	96	94	5	2	19	104	106	105	8	5	5	106	97	93	17	5	4
2.9	3-Methoxy Paracetamol	107	101	94	9	4	4	a	84	89	4	4	3	108	97	98	12	3	4
3.0	3-Desmethyl Trimethoprim	88	94	88	5	1	8	85	86	91	7	5	6	88	91	90	11	5	8
3.1	α-Hydroxy Trimethoprim	91	91	84	6	0	12	101	98	97	5	5	5	91	92	84	10	7	7
3.3	Clopidol	a	100	98	b	1	12	a	107	107	b	5	8	a	104	93	b	7	11
3.3	Gabapentin	95	94	93	7	2	14	a	97	105	2	2	4	107	95	89	b	b	7
3.6	Trimethoprim	95	101	100	2	3	6	102	109	104	3	3	4	94	101	100	8	7	5
3.6	Caffeine	a	107	109	a	8	14	a	a	108	a	a	9	b	117	113	b	9	4
3.7	Ofloxacin	162	160	58	5	2	5	130	144	82	5	4	5	165	153	61	5	12	9
3.9	Ciprofloxacin	83	119	47	11	2	5	76	97	62	10	3	2	90	117	49	25	12	10

4.0	Lidocaine	90	95	86	3	6	8	103	106	97	3	4	3	91	98	82	5	8	7
4.1	Sulfamethoxazole	93	95	90	7	4	10	96	98	100	4	7	3	94	91	86	9	6	1
4.5	Desmethylvenlafaxine	108	112	101	1	4	3	114	110	107	0	2	4	110	109	103	6	6	3
4.7	Acebutolol	102	110	99	3	4	6	106	110	100	9	2	2	105	108	99	5	4	0
4.7	Lamotrigine	101	96	89	9	6	6	102	111	95	12	8	1	97	100	90	4	5	8
4.8	Primidone	107	104	95	7	3	1	103	111	106	10	8	5	107	101	97	9	3	4
4.8	Metoprolol	111	105	102	14	11	3	115	109	99	10	5	10	119	103	97	3	2	5
4.9	Fluconazole	95	95	97	4	6	15	100	96	103	4	1	4	102	96	90	8	5	3
5.4	Ifosfamide	119	117	106	5	3	7	105	103	101	3	1	4	124	112	107	5	4	3
5.5	4-Hydroxy Omeprazole	102	96	92	4	5	6	97	103	97	3	4	1	103	98	89	3	8	4
5.9	Chlorpheniramine	141	100	76	4	5	5	121	135	82	6	12	10	140	100	77	8	4	4
5.9	Carbamazepine-10,11-epoxide	116	105	98	8	3	5	102	105	97	1	5	0	115	107	96	10	7	3
5.9	Venlafaxine	106	115	107	10	5	6	105	108	97	6	2	2	109	113	106	5	3	4
5.9	Bisoprolol	100	108	97	5	5	6	98	104	96	16	5	3	102	104	99	1	7	1
6.1	Propranolol	114	110	104	9	2	4	97	110	96	6	5	4	115	109	104	10	7	3
6.2	Citalopram	90	118	104	2	4	4	102	105	97	23	13	1	94	116	102	1	2	3
6.2	Desmethylcitalopram	103	113	102	6	7	8	120	124	111	24	11	5	98	116	106	3	1	3
6.5	Omeprazole	b	131	97	b	20	31	b	109	103	b	49	19	b	102	109	b	11	30
6.8	Hydroxyibuprofen	a	108	101	a	2	5	a	106	93	a	2	5	a	105	104	a	8	7
6.9	Carbamazepine	107	107	101	3	8	8	103	104	96	2	7	1	112	105	99	8	8	6
7.1	Mebendazole	172	218	192	4	5	4	12	199	199	10	3	2	185	210	196	7	10	2
7.3	Fexofenadine	112	113	103	2	3	8	a	112	102	6	5	1	114	110	105	7	8	7
7.4	Erythromycin	224	46	b	5	4	4	107	78	b	32	28	8	228	45	b	3	5	4
7.5	Lansoprazole	152	152	75	105	49	27	b	107	53	b	27	33	b	b	96	b	b	18
7.6	Oxazepam	121	111	96	10	1	11	116	109	98	3	4	11	114	110	103	11	13	12

RT	Analyte	Influent						Effluent						River						Sludge					
7.6	Lorazepam	122	102	94	14	10	6	111	111	102	19	11	9	120	106	93	19	12	16
7.7	Climbazole	170	169	149	1	2	6	161	141	133	3	3	6	213	156	121	15	9	7
7.7	Fluoxetine	97	88	90	8	6	9	91	99	100	29	11	19	98	91	86	6	5	1
7.8	Temazepam	122	105	96	8	12	6	118	104	103	5	1	10	112	108	102	10	7	12
7.8	Ketoprofen	118	105	96	5	6	9	116	108	103	12	6	13	117	102	100	15	5	15
7.9	Cetirizine	a	235	222	a	3	6	a	206	185	a	2	5	352	242	214	9	1	6
8.1	Clarithromycin	107	116	100	1	2	6	125	105	103	29	2	6	106	116	100	7	2	5
8.1	Norethisterone	103	111	104	11	11	7	106	106	99	5	5	6	125	110	98	12	8	8
8.1	Bezafibrate	110	100	94	5	8	8	101	102	98	8	5	2	114	102	89	10	7	5
8.2	Crotamiton	147	154	138	6	3	10	142	187	146	31	26	12	140	173	132	15	17	7
8.2	Clotrimazole	99	98	91	1	3	8	103	108	103	3	8	6	100	97	92	9	5	5
8.2	Warfarin	114	106	95	5	8	7	115	109	98	3	2	2	114	107	93	7	10	7
9.0	Atorvastatin	113	101	91	2	3	1	139	131	117	2	1	3	135	129	116	4	3	4
9.4	Miconazole	157	178	174	4	10	13	47	52	41	5	3	13	37	104	104	8	9	18
5.6	Estriol	120	109	91	16	1	4	127	114	92	8	5	5	116	110	95	6	1	5
6.0	Naproxen	a	107	109	a	12	12	b	122	87	b	5	8	b	121	96	b	11	3
7.1	Diclofenac	b	102	115	b	6	11	b	121	95	b	10	11	b	109	106	b	12	3
7.4	17β-Estradiol	109	100	96	6	9	7	115	106	96	22	7	6	111	103	89	7	3	5
7.5	Estrone	122	110	95	4	2	2	100	106	98	9	7	8	105	102	94	5	2	5
7.5	17α-Ethinylestradiol	115	115	99	4	9	5	83	104	107	b	8	8	117	104	93	1	4	3
7.5	Ibuprofen	b	a	106	b	9	6	b	124	98	b	2	14	b	121	110	b	9	6
8.7	Gemfibrozil	116	94	104	13	8	10	a	114	88	4	13	4	99	105	93	15	13	3

a) concentration in sample higher than spiked levels, b) concentration above or below MQL

Table S12: Method accuracy and precision (both in %) for liquid samples analysed after SPE and sludge, spiked at three concentrations. Concentrations were 0.01, 0.1 and 0.5 µg L^{-1} in influent and effluent, 0.005, 0.05, and 0.25 µg L^{-1} in river water, and 50, 250, and 500 ng g^{-1} in the sludge (n = 3).

RT	Analyte	Influent	Effluent	River	Sludge

/min		Accuracy			Precision			Accuracy			Precision			Accuracy			Precision			Accuracy			Precision		
		1	10	50	1	10	50	1	10	50	1	10	50	1	10	50	1	10	50	10	50	100	1	10	50
0.7	Guanylurea	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
0.8	Metformin	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
1.2	Sulfanilamide	b	98	108	b	5	5	b	73[b]	134[b]	b	19	17	99	82	85	b	8	4	a	a	a	a	a	a
1.7	Cotinine	118	97	98	6	3	2	c	100[b]	74[b]	c	6	1	113	96	105	4	6	8	100	102	88	6	1	4
2.0	Amidotrizoic acid	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
2.2	Amoxicillin	b	119	77	b	22	16	b	117	92	b	8	10	b	b	150	b	b	1	a	a	a	a	a	a
2.3	Sotalol	106	95	96	19	3	4	108	106	105	3	9	4	99	96	101	7	5	0.3	78	80	76	5	4	1
2.4	Paracetamol	c	c	c	c	c	c	c	c	c	c	c	c	b	117	99	b	12	0.2	c	c	c	c	c	c
2.5	Salbutamol	93	94	90	9	1	4	101	98	93	7	1	5	91	92	94	8	3	4	107	97	87	14	10	5
2.5	Ranitidine	b	88	112	b	11	8	c	98	116	c	4	3	b	92	108	b	18	13	84	97	106	12	12	11
2.5	Atenolol	86	106	99	4	3	6	c	82	97	c	9	8	98	93	101	8	7	10	a	107	89	a	8	4
2.6	Sulfadiazine	101	96	99	9	9	5	c	110	111	c	13	14	107	97	93	11	3	7	66	100	111	14	29	10
2.9	3-Methoxy Paracetamol	c	98	97	1	1	4	c	c	123	c	c	5	93	89	94	6	6	7	84	86	94	4	9	5
3.0	3-Desmethyl Trimethoprim	114	104	103	4	2	7	c	124	104	c	5	1	102	113	107	9	13	4	112	98	104	7	12	18
3.1	α-Hydroxy Trimethoprim	135	94	94	5	16	9	107	108	115	2	3	10	96	99	93	18	2	2	127	107	86	5	11	16
3.3	Clopidol	b	100	97	b	17	5	b	106	109	b	5	12	b	96	97	b	8	2	120	113	105	9	14	4
3.3	Gabapentin	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
3.6	Trimethoprim	85	111	103	4	7	5	c	124	101	c	5	9	60	120	106	4	22	3	84	82	83	16	19	4
3.6	Caffeine	c	c	c	c	c	c	c	c	c	c	c	c	76	108	98	6	10	1	c	c	c	c	c	c
3.7	Ofloxacin	115	101	136	16	16	3	78	117	60	23	18	14	b	106	133	b	13	33	a	a	a	a	a	a
3.9	Ciprofloxacin	b	80	78	b	7	5	b	105	65	b	14	11	b	81	78	b	13	34	167	152	97	35	2	8
4.0	Lidocaine	93	98	91	2	0	4	c	99	117	c	6	16	88	94	102	5	5	9	102	97	61	5	8	12
4.1	Sulfamethoxazole	106	99	105	1	5	4	118	103	100	1	3	11	106	105	100	5	10	2	88	91	126	16	24	4
4.5	Desmethylvenlafaxine	99	105	106	5	2	10	c	119	98	c	5	5	101	104	104	9	3	2	96	102	112	9	3	5

4.7	Acebutolol	90	104	96	3	3	5	99	102	94	2	1	2	96	99	95	1	3	6	103	107	88	1	4	7
4.7	Lamotrigine	106	92	88	8	13	2	121	88	100	12	7	18	100	89	98	2	9	6	c	101	92	c	7	12
4.8	Metoprolol	99	105	105	12	1	5	153	106	101	13	7	7	117	95	98	3	4	0	89	93	91	1	8	13
4.8	Primidone	102	102	103	4	7	3	111	103	104	7	5	11	105	100	101	13	5	1	90	94	86	5	6	1
4.9	Fluconazole	100	92	106	16	8	4	100	105	107	7	3	9	105	100	95	5	4	1	110	112	110	1	4	3
5.4	Ifosfamide	98	99	102	9	0	1	99	87	84	4	5	6	112	94	94	13	2	3	112	122	146	7	5	15
5.5	4-Hydroxy Omeprazole	c	c	c	c	c	c	b	87	100	b	6	15	99	93	99	10	2	4	116	91	92	12	6	8
5.9	Chlorpheniramine	c	c	96	c	c	5	c	109	104	c	5	1	116	72	122	4	6	6	88	163	101	2	2	24
5.9	Carbamazepine-10,11-epoxide	118	100	95	20	3	2	108	92	100	9	8	23	116	97	100	11	5	10	75	83	83	4	6	5
5.9	Venlafaxine	119	103	107	8	5	5	c	104	107	c	2	4	92	113	123	7	1	4	c	119	104	c	4	1
5.9	Bisoprolol	101	103	102	2	6	4	c	104	98	c	3	3	103	103	100	3	5	1	92	91	91	1	2	2
6.1	Propranolol	116	112	105	6	2	2	98	112	98	10	11	7	b	111	106	b	20	8	c	81	88	c	3	5
6.2	Citalopram	c	c	70	c	c	2	c	91	76	c	7	1	91	102	100	14	7	10	c	118	101	c	3	5
6.2	Desmethylcitalopram	c	106	112	c	0	3	c	117	104	c	8	2	b	97	105	b	3	0	c	c	110	c	c	12
6.5	Omeprazole	a	a	a	a	a	a	b	141	127	b	12	13	b	127	83	b	19	18	a	a	a	a	a	a
6.8	Hydroxyibuprofen	c	c	c	c	c	c	c	c	c	c	c	c	b	100	97	b	4	18	c	105	68	c	6	6
6.9	Carbamazepine	111	110	106	4	1	2	112	103	99	0.5	3	9	110	107	109	5	6	6	102	97	91	3	3	5
7.1	Mebendazole	b	172	200	b	6	4	b	170	246	b	1	5	b	193	223	b	2	11	c	115	108	c	8	4
7.3	Fexofenadine	c	105	106	c	2	6	c	c	c	c	c	c	99	108	102	19	8	2	c	c	c	c	c	c
7.4	Erythromycin	63	50	58	5	2	10	171	43	30	28	7	11	238	51	b	22	21	b	86	87	75	12	6	5
7.5	Lansoprazole	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a	a
7.6	Oxazepam	178	104	103	7	6	9	c	111	113	c	10	10	130	99	90	12	11	13	118	93	87	3	5	13
7.6	Lorazepam	b	115	111	b	1	6	b	115	104	b	17	8	b	105	100	b	6	11	98	88	58	4	1	17
7.7	Climbazole	b	77	125	b	1	1	b	101	122	b	1	4	b	114	120	b	24	32	54	99	116	9	11	8
7.7	Fluoxetine	101	97	96	17	9	33	92	107	100	20	8	21	a	a	a	a	a	a	97	76	109	18	26	17
7.8	Temazepam	129	97	97	3	1	3	110	110	104	9	18	9	124	102	97	19	9	8	129	134	107	6	12	17

7.8	Ketoprofen	114	104	101	5	1	3	110	124	101	4	15	9	124	105	110	14	8	15	114	115	115	12	12	4
7.9	Cetirizine	237	162	164	5	3	5	c	c	c	c	c	c	225	195	193	12	8	4	c	119	86	c	15	8
8.1	Clarithromycin	86	93	101	5	10	9	89	98	91	2	10	4	94	103	86	4	4	1	81	110	74	12	8	3
8.1	Norethisterone	b	104	109	b	6	4	b	115	92	b	17	3	112	101	110	21	8	7	138	100	90	8	4	5
8.1	Bezafibrate	97	99	90	13	3	6	b	109	93	b	9	4	110	92	101	4	3	15	63	87	89	4	3	1
8.2	Clotrimazole	b	116	126	b	14	10	151	150	160	11	7	5	b	148	130	b	30	11	b	108	101	b	12	5
8.2	Crotamiton	92	99	99	2	4	7	c	c	c	c	c	c	120	95	93	13	11	7	83	115	122	10	18	11
8.2	Warfarin	129	106	103	6	1	7	142	99	82	3	9	7	112	98	104	3	7	8	106	122	125	12	7	7
9.0	Atorvastatin	74	135	138	16	5	6	c	c	c	c	c	c	90	144	143	20	3	1	c	126	120	c	33	6
9.4	Miconazole	89	59	59	8	4	28	96	115	159	18	20	26	a	a	a	5	6	27	c	125	98	c	16	26
5.6	Estriol	97	97	104	8	6	4	c	88	89	c	11	2	102	101	98	6	8	14	94	80	94	2	7	18
6.0	Naproxen	b	106	110	b	11	3	b	c	c	b	c	c	98	99	92	7	7	10	c	98	86	c	12	5
7.1	Diclofenac	b	94	109	b	7	3	c	c	98	c	c	16	94	123	104	13	11	14	c	c	92	c	c	16
7.4	17β-Estradiol	96	98	97	10	7	5	111	109	91	13	9	4	118	98	99	b	5	10	110	84	83	18	4	11
7.5	Estrone	75	94	100	7	1	4	c	100	87	c	2	1	102	101	98	11	12	10	104	84	71	6	5	4
7.5	17α-Ethinylestradiol	b	103	94	b	5	7	b	101	91	b	0	7	b	89	109	b	13	11	107	85	86	11	3	14
7.5	Ibuprofen	c	c	c	c	c	c	c	c	c	c	c	c	b	75	101	b	11	10	c	c	c	c	c	c
8.7	Gemfibrozil	101	105	116	16	9	3	91	109	104	21	43	16	120	117	106	7	9	16	60	86	73	11	17	20

a) method not suitable, b) concentration above or below MQL, c) concentration in sample higher than spiked levels

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