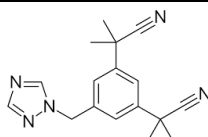
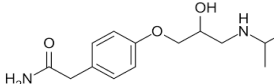
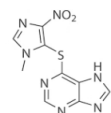
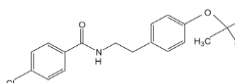
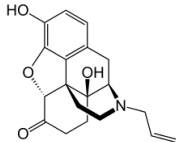
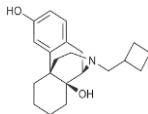
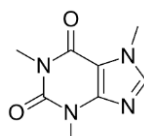
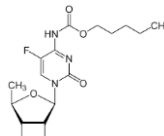
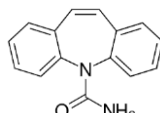
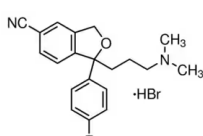
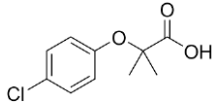
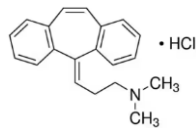
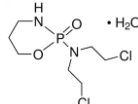
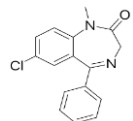
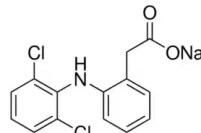
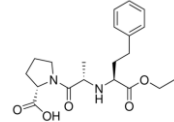
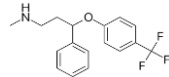
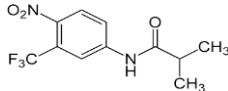
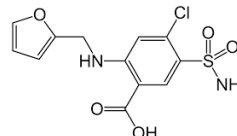
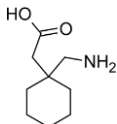
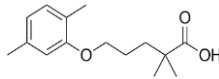
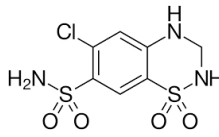
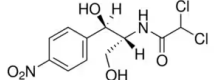
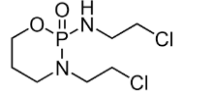
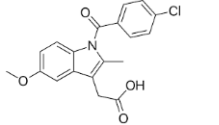
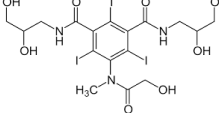
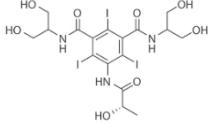
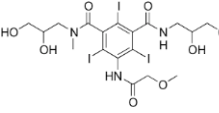
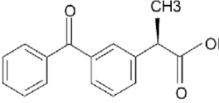
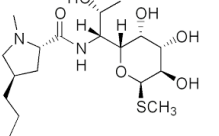
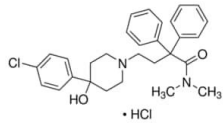
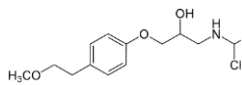
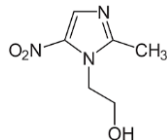
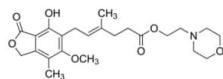
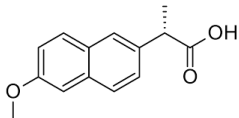
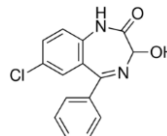
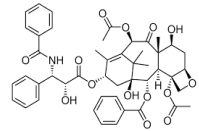
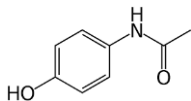
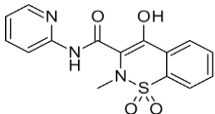
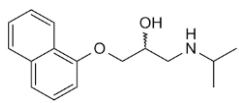


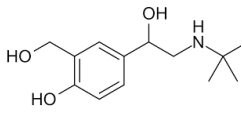
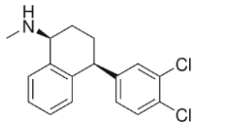
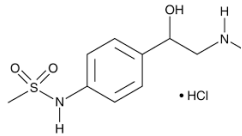
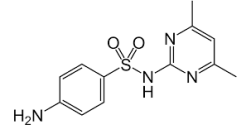
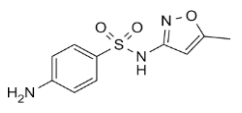
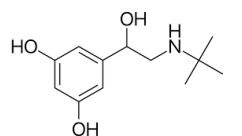
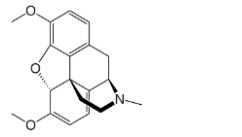
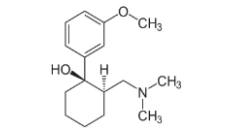
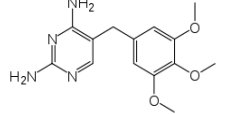
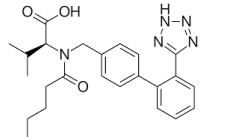
Table S1. List of analytical standards of drugs included in the validation and their characteristics - CAS number, summary formula, relative molecular weight and structure.

	Analyt	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
1	Anastrozole	120511-73-1	C ₁₇ H ₁₉ N ₅ (293.4)		Merck
2	Atenolol	29122-68-7	C ₁₄ H ₂₂ N ₂ O ₃ (266.3)		Merck
3	Azathioprine	446-86-6	C ₉ H ₇ N ₇ O ₂ S (277.3)		Sigma - Aldrich
4	Bezafibrate	41859-67-0	C ₁₉ H ₂₀ ClNO ₄ (361.8)		Neochema
5	Buprenorphine	52485-79-7	C ₂₉ H ₄₁ NO ₄ (467.6)		Chromservis
6	Butorphanol tartrate	200-659-6	C ₂₁ H ₂₉ NO ₂ (327.5)		Merck
7	Caffeine	58-08-2	C ₈ H ₁₀ N ₄ O ₂ (194.2)		Neochema
8	Capecitabine	154361-50-9	C ₁₅ H ₂₂ FN ₃ O ₆ (359.4)		Merck
9	Carbamazepine	298-46-4	C ₁₅ H ₁₂ N ₂ O (236.3)		Neochema
10	Citalopram hydrobromide	59729-33-8	C ₂₀ H ₂₁ FN ₂ O · HBr (323.1)		Neochema

	Analyt	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
11	Clofibric acid	882-09-7	$C_{10}H_{11}ClO_3$ (214.7)		Neochema
12	Cyclobenzaprine hydrochloride	6202-23-9	$C_{20}H_{21}N \cdot HCl$ (311.9)		Chromservis
13	Cyclophosphamide monohydrate	50-18-0	$C_7H_{15}Cl_2N_2O_2P \cdot H_2O$ (279.1)		Neochema
14	Diazepam	439-14-5	$C_{16}H_{13}ClN_2O$ (284.7)		Chromservis
15	Diclofenac sodium	15307-79-6	$C_{14}H_{11}Cl_2NO_2$ (296.2)		Neochema
16	Enalapril maleate	76095-16-4	$C_{20}H_{28}N_2O_5 \cdot C_4H_4O_4$ (492.5)		Neochema
17	Fluoxetine hydrochloride	59333-67-4	$C_{17}H_{18}F_3NO$ (345.8)		Neochema
18	Flutamide	13311-84-7	$C_{11}H_{11}F_3N_2O_3$ (276.2)		Merck
19	Furosemide	54-31-9	$C_{12}H_{11}ClN_2O_5S$ (308.7)		Neochema
20	Gabapentin	60142-96-3	$C_9H_{17}NO_2$ (171.2)		Neochema

	Analyt	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
21	Gemfibrozil	25812-30-0	C ₁₅ H ₂₂ O ₃ (250.3)		Neochema
22	Hydrochlorothiazide	58-93-5	C ₇ H ₈ ClN ₃ O ₄ S ₂ (297.7)		Neochema
23	Chloramphenicol	56-75-7	C ₁₁ H ₁₂ Cl ₂ N ₂ O ₅ (297.7)		Neochema
24	Ifosfamide	3778-73-2	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P (261.1)		Neochema
25	Indomethacin	53-86-1	C ₁₉ H ₁₆ ClNO ₄ (357.8)		Neochema
26	Iomeprol	78649-41-9	C ₁₇ H ₂₂ I ₃ N ₃ O ₈ (777.1)		Neochema
27	Iopamidol	60166-93-0	C ₁₇ H ₂₂ I ₃ N ₃ O ₈ (777.1)		Neochema
28	Iopromide	73334-07-3	C ₁₈ H ₂₄ I ₃ N ₃ O ₈ (791.1)		Neochema
29	Ketoprofen	22071-15-4	C ₁₆ H ₁₄ O ₃ (254.3)		Neochema
30	Lincomycin hydrochloride	154-21-2	C ₁₈ H ₃₄ N ₂ O ₆ S (406.5)		Neochema

	Analyt	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
31	Loperamide hydrochloride	34552-83-5	$C_{29}H_{33}ClN_2O_2 \cdot HCl$ (477.0)		Chromservis
32	Metoprolol tartrate	37350-58-6	$C_{15}H_{25}NO_3$ $\cdot 1/2 C_4H_6O_6$ (267.4)		Neochemia
33	Metronidazole	443-48-1	$C_6H_9N_3O_3$ (171.1)		Neochemia
34	Mycophenolate Mofetil	128794-94-5	$C_{23}H_{31}NO_7$ (433.5)		Merck
35	Naproxen	22204-53-1	$C_{14}H_{14}O_3$ (230.3)		Neochemia
36	Oxazepam	604-75-1	$C_{15}H_{11}ClN_2O_2$ (286.7)		Chromservis
37	Paclitaxel	33069-62-4	$C_{47}H_{51}NO_{14}$ (853.9)		Chromservis
38	Paracetamol (Acetaminophen)	103-90-2	$C_8H_9NO_2$ (151.2)		Neochemia
39	Piroxicam	36322-90-4	$C_{15}H_{13}N_3O_4S$ (331.4)		Neochemia
40	Propranolol hydrochloride	525-66-6	$C_{16}H_{22}ClNO_2 \cdot HCl$ (259.3)		Neochemia

			Summary formula (Relative molecular weight)	Structure	Supplier
Analyt	CAS				
41	Salbutamol	18559-94-9	$C_{13}H_{21}NO_3$ (239.3)		Neochema
42	Sertraline hydrochloride	79617-96-2	$C_{17}H_{17}Cl_2N \cdot HCl$ (306.2)		Merck
43	Sotalol hydrochloride	959-24-0	$C_{12}H_{20}N_2O_3S \cdot HCl$ (308.8)		Neochema
44	Sulfamethazine	57-68-1	$C_{12}H_{14}N_4O_2S$ (278.3)		Neochema
45	Sulfamethoxazole	723-46-6	$C_{10}H_{11}N_3O_3S$ (253.3)		Neochema
46	Terbutaline	23031-25-6	$C_{12}H_{19}NO_3$ (225.3)		Neochema
47	Thebaine	115-37-7	$C_{19}H_{21}NO_3$ (311.4)		TEVA
48	Tramadol hydrochloride	36282-47-0	$C_{16}H_{25}NO_2 \cdot HCl$ (263.4)		Neochema
49	Trimethoprim	738-70-5	$C_{14}H_{18}N_4O_3$ (290.3)		Neochema
50	Valsartan	137862-53-4	$C_{24}H_{29}N_5O_3$ (435.5)		Neochema

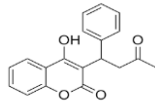
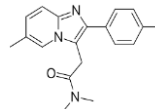
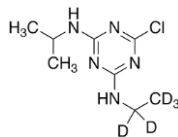
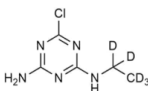
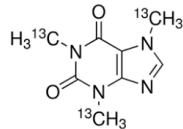
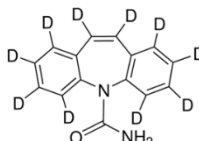
	Analyt	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
51	Warfarin	81-81-2	C ₁₉ H ₁₆ O ₄ (308.3)		Neochema
52	Zolpidem hemitartrate	99294-93-6	C ₁₉ H ₂₁ N ₃ O (307.4)		Chromservis

Table S2. List of ISTDs included in the validation and their characteristics - ISTD CAS number, summary formula, relative molecular weight and structure.

	Name	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
1	Atrazine D5	163165-75-1	C ₈ H ₁₄ ClN ₅ (220.7)		Chromservis
2	Atrazine-desisopropyl D5	1189961-78-1	C ₅ H ₈ ClN ₅ (178.63)		Chromservis
3	Caffeine-13C	78072-66-9	¹³ C ₃ C ₅ H ₁₀ N ₄ O ₂ (197.17)		Neochema
4	Carbamazepine D10	132183-78-9	C ₁₅ D ₁₀ H ₂ N ₂ O (246.33)		Neochema

	Name	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
5	Carbendazim D4	291765-95-2	$C_9H_9N_3O_2$ (195.21)		HPST
6	Citalopram D6 hydrobromide	1190003-26-9	$C_{20}H_{15}D_6FN_2O$ ·HBr (330.43)		Chromservis
7	Diclofenac D4	153466-65-0	$C_{14}H_7D_4Cl_2NO_2$ (300.17)		Neochema
8	Metolachlor D6	1219803-97-0	$C_{15}H_{16}D_6ClNO_2$ (289.83)		Chromservis
9	Naproxen 13C D3	1216704-11-8	$C_{13}^{13}CH_{11}D_3O_3$ (234.27)		Chromservis
10	Norethindrone D6	-	$C_{20}H_{20}D_6O_2$ (304.46)		Chromservis
11	Phosalone D10	-	$C_{12}H_5ClD_{10}NO_4PS$ 2 (377.87)		Chromservis
12	Sulfamethoxazole D4	1020719-86-1	$C_{10}H_7D_4N_3O_3S$ (257.30)		Neochema

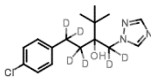
	Name	CAS	Summary formula (Relative molecular weight)	Structure	Supplier
13	Tebuconazole D6	-	C ₁₆ H ₁₆ ClN ₃ OD ₆ (313.86)		Chromservis

Table S3. Parameters of the MS/MS method (MRM transitions of analytes. collision energy and retention time of analytes) - transitions marked in bold are used as quantification (* designation of precursor ions containing 2 isotopes of chlorine atoms).

Analyte	Ionization	Precursor ions (<i>m/z</i>)	Product ions (<i>m/z</i>)	Cone voltage (V)	Collision energy (V)	Retention time (tr)
Anastrozole	ESI+	294.1	225.0 /114.8	30	20/52	4.24
Atenolol	ESI+	267.0	145.0 /190.0	30	23/16	2.55
Azathioprine	ESI+	278.0	141.8 /232.0	30	11/13	2.92
Bezafibrate	ESI+	262.0	139.0 /121.0	30	25/29	4.70
Buprenorphine	ESI+	468.3	396.1 /414.2	30	39/32	3.83
Butorphanol	ESI+	328.0	124.0 /282.0	30	26/29	3.47
Caffeine	ESI+	195.0	138.0 /110.0	30	17/23	2.89
Capecitabine	ESI+	360.0	173.8 /244.0	30	19/10	3.94
Carbamazepine	ESI+	237.0	194.0 /179.0	35	20/35	4.16
Citalopram	ESI+	325.2	109.0 /262.2	30	24/19	3.72
Clofibric acid	ESI-	213.0	127.0 /85.0	30	15/11	4.59
Cyclobenzaprine	ESI+	276.0	216.0 /231.0	30	24/16	3.93
Cyclophosphamide	ESI+	261.0	140.0 /106.0	30	22/18	3.70
Diazepam	ESI+	285.0	154.0 /193.0	30	26/30	4.94
Diclofenac	ESI+	294.0/296.0*	250.0 /252.0	30	11/11	5.21

Analyte	Ionization	Precursor ions (<i>m/z</i>)	Product ions (<i>m/z</i>)	Cone voltage (V)	Collision energy (V)	Retention time (tr)
Enalapril	ESI-	377.1	234.0/91.0	30	20/55	3.66
Fluoxetine	ESI+	310.1	148.0/44.0	30	8/7	4.05
Flutamide	ESI-	275.0	202.0/205.0	30	23/22	5.09
Furosemide	ESI-	329.0	205.0/285.0	30	22/14	4.06
Gabapentin	ESI+	172.2	154.3/137.3	25	15/18	2.72
Gemfibrozil	ESI-	249.0	121.0/127.0	30	15/10	5.47
Hydrochlorothiazide	ESI-	296.0	269.0/205.0	30	19/22	2.88
Chloramphenicol	ESI-	321.0	152.1/257.1	30	18/12	3.73
Ifosfamide	ESI+	261.0	92.0/154.0	30	25/21	3.64
Indomethacin	ESI+	358.0	139.0/174.0	30	22/11	5.20
Iomeprol	ESI+	777.8	405.0/531.8	30	38/30	2.46
Iopamidol	ESI+	777.8	387.0/313.8	30	39/52	1.93
Iopromide	ESI+	791.8	300.0/572.8	30	56/23	2.65
Ketoprofen	ESI+	255.1	209.0/105.0	30	15/23	4.67
Lincomycin	ESI+	407.0	126.0/359.0	35	20/18	2.83
Loperamide	ESI+	477.2	210.1/266.1	30	45/12	4.29
Metoprolol	ESI+	268.2	116.0/72.0	30	18/22	3.25
Metronidazole	ESI+	172.0	128.0/82.0	30	15/21	2.71
Mycophenolate Mofetil	ESI+	434.0	114.0/195.0	30	24/33	3.82
Naproxen	ESI+	231.0	185.0/170.0	30	14/29	4.63
Oxazepam	ESI+	287.0	241.0/269.0	30	23/15	4.30
Paclitaxel	ESI+	876.4	308.1/591.3	30	27/23	5.08
Paracetamol (Acetaminophen)	ESI+	152.0	110.0/65.0	30	15/30	2.68

Analyte	Ionization	Precursor ions (<i>m/z</i>)	Product ions (<i>m/z</i>)	Cone voltage (V)	Collision energy (V)	Retention time (tr)
Piroxicam	ESI+	332.0	95.0/121.0	30	18/25	4.33
Propranolol	ESI+	260.0	116.0/183.0	30	16/16	3.65
Salbutamol	ESI+	240.0	148.0/166.0	30	20/12	2.52
Sertraline	ESI+	306.0	159.0/275.0	30	23/11	4.04
Sotalol	ESI+	273.0	133.0/213.0	30	27/17	2.52
Sulfamethazine	ESI+	279.0	124.0/186.0	30	20/18	3.26
Sulfamethoxazole	ESI+	254.0	156.0/92.0	30	16/26	3.58
Terbutaline	ESI+	226.1	152.0/107.0	30	16/26	2.47
Thebaine	ESI+	312.0	58.0/266.0	30	30/40	3.29
Tramadol	ESI+	264.0	58.0/246.0	30	15/10	3.26
Trimethoprim	ESI+	291.0	230.0/123.0	39	24/27	2.90
Valsartan	ESI+	436.0	207.0/235.0	30	28/22	4.72
Warfarin	ESI+	309.0	163.0/251.0	30	14/22	4.91
Zolpidem	ESI+	308.0	235.0/263.0	30	33/27	3.44
Atrazine D5	ESI+	221.0/223.0*	179.0/181.0	35	18/18	4.53
Atrazine-desisopropyl D5	ESI+	179.0	101.0/137.0	35	18/16	3.10
Caffeine-13C	ESI+	198.0	140.0/112.0	30	19/22	2.89
Carbamazepine D10	ESI+	247.0	204.0/201.0	30	21/22	4.14
Carbendazim D4	ESI+	196.0	164.0/136.0	35	20/28	2.90
Citalopram D6	ESI+	331.3	109.1/262.2	30	26/19	3.78
Diclofenac D4	ESI-	298.0/300.0*	254.0/256.0	30	12/12	5.20
Phosalon D10	ESI+	378.0	182.0/111.0	35	16/38	5.77
Metolachlor D6	ESI+	290.0	258.0/182.0	35	16/25	5.39

Analyte	Ionization	Precursor ions (<i>m/z</i>)	Product ions (<i>m/z</i>)	Cone voltage (V)	Collision energy (V)	Retention time (tr)
Naproxen 13C D3	ESI+	235.0	189.0/170.0	30	15/25	4.62
Noreethindrone D6	ESI+	305.3	113.0/237.2	30	30/21	4.71
Sulfamethoxazole D4	ESI+	258.0	160.0/96.0	30	16/26	3.57
Tebuconazole D6	ESI+	314.0	71.8/124.8	30	21/38	5.24

Table S4. List of ISTDs and assigned analytes in MQ and drinking matrices.

ISTD – MQ and drinking water	Analyte
Atrazine D5	Anastrozole Bezafibrate Capecitabine Cyclophosphamide Diazepam Enalapril Flutamide Indomethacin Oxazepam Piroxicam Sulfamethazine
Atrazine-desisopropyl D5	Lincomycin Paracetamol (Acetaminophen)
Caffeine-13C	Caffeine Iopamidol Iopromide
Carbamazepine D10	Carbamazepine Fluoxetine Valsartan
Carbendazim D4	Azathioprine Cyklobenzaprine Gabapentin Chloramphenikol

ISTD – MQ and drinking water	Analyte
	Ifosfamide
	Metronidazole
	Trimethoprim
	Zolpidem
Citalopram D6	Atenolol
	Buprenorphine
	Butorphanol
	Citalopram
	Iomeprol
	Loperamide
	Metoprolol
	Salbutamol
	Sotalol
	Terbutaline
	Thebaine
	Tramadol
Diclofenac D4	Diclofenac
Metolachlor D6	Gemfibrozil
Naproxen 13C D3	Clofibric acid
Noreethindrone D6	Naproxen
	Paclitaxel
	Propranolol
	Sertraline
Phosalone D10	Furosemide
	Ketoprofen
Sulfamethoxazole D4	Mycophenolate mofetil
	Sulfamethoxazole
Tebuconazole D6	Hydrochlorothiazide
	Warfarin

Table S5. Overview of linear range, coefficient of determination (R²) values and working range for individual analytes in drinking water.

Analyte	Linear range [ng L ⁻¹]	Coefficient of determination (R ²)	Working range for drinking waters [ng L ⁻¹]
Anastrozole	2.5 – 500	0.9998	5.0 – 500
Atenolol	2.5 – 500	0.9997	10.0 – 500
Azathioprine	2.5 – 500	0.9997	10.0 – 500
Bezafibrate	2.5 – 1000	0.9999	10.0 – 1000
Buprenorphine	2.5 – 1000	0.9994	5.0 – 1000
Butorphanol	2.5 – 1000	0.9997	25.0 – 500
Caffeine	50.0 – 1000	0.9988	250.0 – 1000
Capecitabine	5.0 – 1000	0.9992	250.0 – 1000
Carbamazepine	2.5 – 1000	1.0000	5.0 – 1000
Citalopram	2.5 – 1000	0.9993	25.0 – 1000
Clofibric acid	50.0 – 1000	0.9996	250.0 – 1000
Cyclobenzaprine	50.0 – 1000	0.9997	100.0 – 1000
Cyclophosphamide	2.5 – 1000	0.9999	10.0 – 1000
Diazepam	2.5 – 1000	0.9999	2.5 – 1000
Diclofenac	5.0 – 1000	0.9996	50.0 – 1000
Enalapril	2.5 – 1000	0.9999	10.0 – 1000
Fluoxetine	50.0 – 1000	0.9993	250.0 – 1000
Flutamide	2.5 – 1000	0.9999	10.0 – 1000
Furosemide	5.0 – 1000	0.9995	25.0 – 1000
Gabapentin	50.0 – 1000	0.9997	50.0 – 1000
Gemfibrozil	5.0 – 1000	0.9997	25.0 – 1000
Hydrochlorothiazide	2.5 – 500	0.9997	25.0 – 500
Chloramfenikol	2.5 – 1000	0.9992	25.0 – 1000
Ifosfamide	2.5 – 1000	0.9999	10.0 – 1000
Indomethacin	2.5 – 1000	0.9999	10.0 – 1000
Iomeprol	50.0 – 1000	0.9994	500.0 – 1000
Iopamidol	2.5 – 1000	0.9991	25.0 – 1000
Iopromide	2.5 – 500	0.9991	25.0 – 500
Ketoprofen	2.5 – 1000	0.9998	10.0 – 1000
Lincomycin	2.5 – 1000	0.9999	10.0 – 1000
Loperamide	50.0 – 1000	0.9997	250.0 – 1000
Metoprolol	2.5 – 1000	0.9996	10.0 – 1000
Metronidazole	2.5 – 500	0.9999	2.5 – 500
Mycophenolate Mofetil	2.5 – 1000	0.9998	25.0 – 1000
Naproxen	50.0 – 1000	0.9993	75.0 – 1000/
Oxazepam	2.5 – 1000	0.9999	5.0 – 1000
Paclitaxel	5.0 – 1000	0.9995	250.0 – 1000
Paracetamol	2.5 – 500	0.9998	25.0 – 500
Piroxicam	2.5 – 1000	1.0000	5.0 – 1000
Propranolol	2.5 – 1000	0.9998	10.0 – 1000

Analyte	Linear range [ng L ⁻¹]	Coefficient of determination (R ²)	Working range for drinking waters [ng L ⁻¹]
Salbutamol	2.5 – 500	0.9997	25.0 – 500
Sertraline	50.0 – 1000	0.9990	250.0 – 1000
Sotalol	2.5 – 500	0.9996	10.0 – 500
Sulfamethazine	2.5 – 1000	0.9999	5.0 – 1000
Sulfamethoxazole	2.5 – 1000	0.9999	10.0 – 1000
Terbutaline	2.5 – 500	0.9997	25.0 – 500
Thebaine	2.5 – 1000	0.9998	25.0 – 1000
Tramadol	2.5 – 1000	0.9998	25.0 – 1000
Trimethoprim	2.5 – 1000	0.9999	25.0 – 1000
Valsartan	2.5 – 1000	0.9999	25.0 – 1000
Warfarin	2.5 – 1000	0.9999	10.0 – 1000
Zolpidem	2.5 – 500	0.9998	10.0 – 500

Table S6. Summary of repeatability results expressed as RSD (%). average of measured concentrations of a given analyte at one concentration level and standard deviation of individual analytes in MQ water.

Analyte	MQ water					
	L1 (0.01 ng mL ⁻¹)			L2 (0.1 ng mL ⁻¹)		
	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]
Anastrozole	9.57	0.26	2.69	94.09	2.56	2.72
Atenolol	11.47	0.88	7.67	113.00	4.05	3.58
Azathioprine	9.87	0.48	4.86	94.84	2.02	2.13
Bezafibrate	8.88	0.86	9.67	82.09	6.82	8.31
Buprenorphine	12.04	0.40	3.34	113.34	6.63	5.85
Butorphanol	11.92	1.12	9.42	115.00	7.19	6.25
Caffeine	n.d.*	-	-	95.94	15.60	17.15
Capecitabine	n.d.*	-	-	88.04	17.02	19.34
Carbamazepine	9.54	0.36	3.80	95.47	1.75	1.83
Citalopram	13.39	1.37	10.23	112.12	5.22	4.66
Clofibric acid	n.d.*	-	-	66.05	12.59	19.07
Cyclobenzaprine	n.d.*	-	-	67.31	7.70	11.44
Cyclophosphamide	9.26	0.56	6.05	95.57	2.51	2.63
Diazepam	9.79	0.19	1.96	93.73	1.90	2.03
Diclofenac	n.d.*	-	-	77.64	10.55	13.59
Enalapril	9.89	0.46	4.62	98.87	1.53	1.55
Fluoxetine	n.d.*	-	-	93.57	17.08	18.26
Flutamide	8.69	0.55	6.31	80.21	9.53	11.88
Furosemide	8.14	1.47	18.00	68.79	11.83	17.20
Gabapentin	n.d.*	-	-	88.59	2.97	3.36
Gemfibrozil	10.59	1.05	9.88	90.92	5.25	5.77
Hydrochlorothiazide	n.d.*	-	-	97.86	6.27	6.41

Analyte	MQ water					
	L1 (0.01 ng mL ⁻¹)			L2 (0.1 ng mL ⁻¹)		
	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]
Chloramfenikol	11.42	1.39	12.14	92.78	4.56	4.92
Ifosfamide	10.02	0.62	6.16	95.11	2.32	2.44
Indomethacin	8.44	0.70	8.28	73.56	8.58	11.66
Iomeprol	n.d.*	-	-	87.95	25.87	16.38
Iopamidol	9.96	0.92	9.26	103.09	0.92	0.89
Iopromide	8.13	1.09	13.46	105.72	5.11	4.83
Ketoprofen	7.79	0.58	7.48	76.60	7.72	10.07
Lincomycin	10.28	0.64	6.24	100.96	1.68	1.67
Loperamide	n.d.*	-	-	145.68	19.76	13.56
Metoprolol	11.55	0.90	7.77	103.46	2.72	2.63
Metronidazole	9.90	0.19	1.88	98.19	0.74	0.75
Mycophenolate Mofetil	8.10	1.50	18.52	86.08	4.92	5.72
Naproxen	n.d.*	-	-	79.33	6.37	8.03
Oxazepam	9.56	0.32	3.30	94.31	2.40	2.54
Paclitaxel	n.d.*	-	-	74.46	12.44	19.29
Paracetamol	9.25	1.20	12.96	92.01	1.32	1.43
Piroxicam	9.93	0.31	3.09	97.59	1.10	1.12
Propranolol	9.42	0.63	6.65	82.26	10.54	16.94
Salbutamol	11.96	0.93	7.81	113.13	3.82	3.38
Sertraline	n.d.*	-	-	73.65	14.35	19.49
Sotalol	10.97	0.81	7.37	107.08	3.48	3.25
Sulfamethazine	9.68	0.24	2.49	97.16	1.85	1.91
Sulfamethoxazole	9.46	0.55	5.78	97.58	1.44	1.48
Terbutaline	11.93	1.37	11.46	117.22	6.27	5.35
Thebaine	11.92	1.38	11.61	106.99	5.53	5.17
Tramadol	11.54	1.09	9.44	105.59	3.67	3.48
Trimethoprim	8.04	1.19	14.81	77.05	8.88	11.52
Valsartan	9.09	1.27	14.00	82.81	7.58	9.15
Warfarin	8.04	0.51	6.36	80.45	3.35	4.16
Zolpidem	9.29	0.68	7.32	88.92	4.02	4.52

n.d.* - detection limit of the analyte is higher than the lower concentration level of the spike L1 = 0.01 µg L⁻¹

Table S7. Summary of repeatability results expressed as RSD (%). average of measured concentrations of a given analyte at one concentration level and standard deviation of individual analytes in drinking water.

Analyte	Drinking water					
	L1 (0.01 ng mL ⁻¹)			L2 (0.1 ng mL ⁻¹)		
	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]
Anastrozole	9.47	0.35	3.66	94.30	1.65	1.75

Analyte	Drinking water					
	L1 (0.01 ng mL ⁻¹)			L2 (0.1 ng mL ⁻¹)		
	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]
Atenolol	10.75	0.48	4.43	101.98	1.67	1.64
Azathioprine	9.39	0.38	4.09	91.88	2.35	2.56
Bezafibrate	8.27	0.79	9.57	91.29	6.00	6.57
Buprenorphine	8.93	1.03	11.53	90.03	5.83	6.48
Butorphanol	9.47	0.32	3.36	94.51	0.99	1.05
Caffeine	n.d.*	-	-	66.84	5.50	8.24
Capecitabine	n.d.*	-	-	220.97*	15.88	7.19
Carbamazepine	10.01	0.30	3.01	95.98	0.96	1.00
Citalopram	9.71	0.65	6.65	96.71	4.37	4.52
Clofibric acid	n.d.*	-	-	72.59	9.94	13.69
Cyclobenzaprine	n.d.*	-	-	113.73	2.64	2.32
Cyclophosphamide	9.11	0.51	5.61	95.43	1.84	1.92
Diazepam	9.48	0.18	1.91	96.55	1.13	1.17
Diclofenac	n.d.*	-	-	82.51	6.30	7.63
Enalapril	10.87	0.22	2.03	112.76	1.24	1.10
Fluoxetine	n.d.*	-	-	117.24	4.19	3.58
Flutamide	8.09	0.99	12.18	85.38	6.96	8.15
Furosemide	9.42	0.93	9.90	78.48	9.72	12.39
Gabapentin	n.d.*	-	-	104.98	4.19	3.99
Gemfibrozil	8.86	1.54	17.37	89.48	5.16	5.77
Hydrochlorothiazide	n.d.*	-	-	101.70	8.25	8.11
Chloramfenikol	10.40	1.59	15.33	93.80	4.58	4.88
Ifosfamide	9.80	0.51	5.17	94.23	1.40	1.48
Indomethacin	8.01	1.00	12.43	84.73	6.74	7.96
Iomeprol	n.d.*	-	-	255.86*	45.18	17.66
Iopamidol	7.04	0.45	6.37	97.52	4.41	4.52
Iopromide	7.58	1.23	16.24	118.59	6.36	5.37
Ketoprofen	8.74	0.34	3.87	89.44	4.37	4.89
Lincomycin	9.66	0.27	2.82	98.26	2.10	2.13
Loperamide	n.d.*	-	-	134.31*	1.98	1.48
Metoprolol	9.56	0.74	7.69	97.64	2.62	2.69
Metronidazole	9.28	0.16	1.70	96.58	0.72	0.74
Mycophenolate Mofetil	9.19	0.95	10.34	88.63	3.86	4.35
Naproxen	n.d.*	-	-	88.65	9.70	10.94
Oxazepam	9.18	0.54	5.93	94.50	2.08	2.20
Paclitaxel	n.d.*	-	-	73.22	7.83	10.69
Paracetamol	9.44	0.70	7.45	99.41	5.00	5.03
Piroxicam	9.28	0.38	4.11	96.09	3.29	3.43
Propranolol	9.69	0.68	7.01	99.35	3.50	3.52
Salbutamol	10.04	0.12	1.21	104.25	2.20	2.11
Sertraline	n.d.*	-	-	116.22	1.66	1.43
Sotalol	9.64	0.28	2.93	99.98	1.47	1.47

Analyte	Drinking water					
	L1 (0.01 ng mL ⁻¹)			L2 (0.1 ng mL ⁻¹)		
	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]	Average [ng L ⁻¹]	SD [ng L ⁻¹]	RSD [%]
Sulfamethazine	9.75	0.42	4.34	94.80	1.19	1.25
Sulfamethoxazole	9.48	0.42	4.42	93.47	1.69	1.81
Terbutaline	9.32	0.39	4.18	99.91	2.00	2.00
Thebaine	9.19	0.73	7.94	87.18	4.11	4.72
Tramadol	9.40	0.60	6.40	92.89	3.24	3.49
Trimethoprim	8.96	0.51	5.65	92.89	3.78	4.07
Valsartan	7.95	1.06	13.36	94.91	6.68	7.04
Warfarin	9.25	0.68	7.34	89.21	2.20	2.46
Zolpidem	9.03	0.35	3.93	94.05	1.36	1.45

*n.d.** - detection limit of the analyte is higher than the lower concentration level of the spike L1 = 0.01 µg L⁻¹

* The given analytes were determined in raw validation samples at levels that were many times higher than the level of fortification. For these analytes, RSD (%) values were calculated from concentrations determined by repeated spike analysis.

Table S8. Method accuracy results expressed as recovery for MQ and drinking water.

Analyte	Recovery [%]			
	MQ water		Drinking water	
	L1	L2	L1	L2
Anastrozole	100.1	102.4	100.3	98.9
Atenolol	84.0	96.7	107.3	104.9
Azathioprine	104.9	103.1	96.9	94.1
Bezafibrate	92.9	89.4	87.6	95.8
Buprenorphine	88.1	97.0	89.2	92.6
Butorphanol	87.2	98.4	94.6	97.2
Caffeine	n.d.*	91.7	n.d.*	70.1
Capecitabine	n.d.*	95.8	n.d.*	231.8
Carbamazepine	97.7	99.5	101.4	97.3
Citalopram	98.0	95.9	96.9	99.4
Clofibric acid	n.d.*	84.9	n.d.*	75.7
Cyclobenzaprine	n.d.*	73.1	n.d.*	116.5
Cyclophosphamide	96.9	104.0	96.5	100.1
Diazepam	102.4	102.0	99.2	101.3
Diclofenac	n.d.*	97.0	n.d.*	86.5
Enalapril	103.5	107.6	115.2	118.3
Fluoxetine	n.d.*	97.5	n.d.*	118.9
Flutamide	91.0	87.3	85.7	89.6
Furosemide	90.2	81.6	112.5	94.1
Gabapentin	n.d.*	96.3	116.9	107.5
Gemfibrozil	108.9	97.3	92.2	93.5

Analyte	Recovery [%]			
	MQ water		Drinking water	
	L1	L2	L1	L2
Hydrochlorothiazide	n.d.*	104.9	n.d.*	109.0
Chloramfenikol	121.3	100.8	107.3	96.0
Ifosfamide	106.5	103.4	101.1	96.5
Indomethacin	88.3	80.1	84.8	88.9
Iomeprol	n.d.*	135.1	n.d.*	263.1
Iopamidol	103.4	104.0	74.0	102.3
Iopromide	84.4	106.6	79.7	124.4
Ketoprofen	86.3	90.8	104.4	107.3
Lincomycin	105.2	105.3	101.8	102.1
Loperamide	n.d.*	124.6	n.d.*	138.1
Metoprolol	84.5	88.5	95.4	100.4
Metronidazole	105.2	106.7	95.7	98.9
Mycophenolate Mofetil	83.3	88.7	96.1	92.8
Naproxen	n.d.*	98.4	n.d.*	94.2
Oxazepam	100.0	102.7	97.2	99.1
Paclitaxel	n.d.*	82.9	n.d.*	76.3
Paracetamol	94.6	95.9	99.4	103.3
Piroxicam	103.9	106.2	98.3	100.8
Propranolol	14.7	80.1	88.8	103.6
Salbutamol	87.5	96.8	100.2	107.2
Sertraline	n.d.*	94.7	n.d.*	121.2
Sotalol	80.3	91.6	96.2	102.8
Sulfamethazine	101.3	105.8	103.3	99.4
Sulfamethoxazole	97.2	100.6	99.1	97.9
Terbutaline	87.3	100.3	93.0	102.7
Thebaine	87.2	91.5	91.7	89.6
Tramadol	84.5	90.3	93.8	95.5
Trimethoprim	85.5	83.7	92.4	95.1
Valsartan	93.1	86.3	80.6	96.2
Warfarin	81.7	86.3	96.1	95.6
Zolpidem	98.7	96.6	93.2	96.3