Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.
This journal is © The Royal Society of Chemistry 2022

Spatiotemporal profiling of Chemicals of Emerging Concern in a megacity: A case study of Lagos, Nigeria

Idera Fabunmi[a,b,c], Kathryn Proctor[b], Temilola Oluseyi[a*], Aderonke Oyeyiola[a], Kehinde Olayinka[a], Barbara Kasprzyk-Hordern[b]

[a]Department of Chemistry, University of Lagos, Lagos, Nigeria
[b]Department of Chemistry, University of Bath, Bath BA2 7AY, UK
[c]Nigerian Institute for Oceanography and Marine Research, Lagos, Nigeria
*Corresponding author: toluseyi@unilag.edu.ng

The supplementary material contains eleven tables:

Table S1. Physiochemical properties of target analytes

Figure S1. Sample collection points for wastewater and surface water

Table S2. Instrument details including chromatographic retention time and mass spectrometry parameters used in the determination of target analytes

Table S3. Instrument performance data of target analytes

Table S4. Absolute and corrected recoveries in matrices sampled

Table S5. Mean concentrations (ng L^{-1}) of target compounds in influent and effluent samples

Table S6. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP1

Table S7. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP2

Table S8. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP3

Table S9. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP4

Table S10. Concentrations (ng L^{-1}) of target compounds in influent samples at SDP1

Table S11. Concentrations (ng L^{-1}) of target compounds in influent samples at SDP2

Table S12. Percentage intra and inter-site variance of target compounds in influent samples

Table S13. Maximum Environmental Concentrations (MECs), Predicted No-Effect Concentrations (PNECs) and Risk Quotients (RQs) for target compounds

Table S1. Physiochemical properties of target analytes

Micropollutant class	Micropollutant	CAS No.	Molecular Formula	Molecular Weight (g mol^{-1})	Water Solubility (mg L^{-1})[i]	Log Kow[ii]	Log Koc[iii]	Log Dow[iv]	Henry's Law Constant (atm m^{3}mol^{-1})[v]	Vapour Pressure (Torr)[vi]	pKa (Most acidic)[vii]	pKa (Most basic)[viii]
Anaesthetic and metabolite	Ketamine	6740-88-1	$C_{13}H_{16}ClNO$	237.73	$3.87x10^3$	3.12	2.283	3.18	$1.38x10^{-8}$	$1.76x10^{-5}$	-	6.46±0.20
	Norketamine	35211-10-0	$C_{15}H_{11}ClN_{2O}$	233.70	-	-	-	2.71	$1.78x10^{-10}$	$1.26x10^{-5}$	-	6.25±0.20
Analgesics and metabolites	Morphine	57-27-2	$C_{17}H_{19}NO_3$	285.35	$2.64x10^4$	0.72	1.163	-0.37	$1.33x10^{-16}$	$7.06x10^{-10}$	9.48±0.40	8.25±0.40
	Dihydromorphine	509-60-4	$C_{17}H_{21}NO_3$	287.36	$2.38x10^4$	0.93	1.185	-0.26	$1.51x10^{-16}$	$7.65x10^{-10}$	9.56±0.40	8.44±0.40
	Normorphine	466-97-7	$C_{16}H_{17}NO_3$	271.32	$2.56x10^5$	0.50	0.599	-2.05	$6.07x10^{-17}$	$2.99x10^{-10}$	9.17±0.40	9.54±0.40
	Methadone	76-99-3	$C_{21}H_{27}NO$	309.46	48.5	4.17	3.229	3.39	$4.97x10^{-10}$	$2.20x10^{-7}$	-	9.50±0.50
	Codeine	76-57-3	$C_{18}H_{21}NO_3$	299.37	$1.22x10^4$	1.28	1.218	-0.23	$7.58x10^{-14}$	$2.47x10^{-9}$	13.40±0.20	8.23±0.40
	Dihydrocodeine	125-28-0	$C_{18}H_{23}NO_3$	301.39	$6.53x10^3$	1.49	1.384	-0.11	$8.61x10^{-14}$	$2.48x10^{-9}$	14.22±0.2	8.43±0.40
	Norcodeine	467-15-2	$C_{17}H_{19}NO_3$	285.35	$3.92x10^4$	1.07	0.964	-2.28	$3.45x10^{-14}$	$1.51x10^{-9}$	13.34±0.20	9.28±0.40
	Tramadol	27203-92-5	$C_{16}H_{25}NO_2$	263.38	$1.15x10^3$	3.01	1.959	0.72	$1.54x10^{-11}$	$1.02x10^{-6}$	14.47±0.40	9.61±0.28
	N-desmethyltramadol	75377-45-6	$C_{15}H_{23}NO_2$	249.35	-	-	-	-0.27	-	$9.16x10^{-6}$	14.46±0.40	10.56±0.10
	O-desmethyltramadol	185453-02-5	$C_{15}H_{23}NO_2$	249.35	-	-	-	0.38	-	$3.14x10^{-7}$	10.00±0.10	9.61±0.28
Antibacterial/antibiotics	Clarithromycin	81103-11-9	$C_{38}H_{69}NO_{13}$	747.97	0.3	3.18	1.371	2.31	$1.73x10^{-29}$	$5.06x10^{-30}$	13.08±0.70	8.16±0.70
	Azithromycin	83905-01-5	$C_{38}H_{72}N_2O_{12}$	749.00	0.1	3.24	1.676	-2.48	$5.30x10^{-29}$	$2.51x10^{-31}$	13.28±0.70	8.59±0.70
	Trimethoprim	738-70-5	$C_{14}H_{18}N_4O_3$	290.32	$2.33x10^3$	0.73	1.896	1.13	$2.39x10^{-14}$	$3.74x10^{-11}$	-	7.04±0.10
	Sulfamethoxazole	723-46-6	$C_{10}H_{11}N_3O_3S$	253.28	$3.94x10^3$	0.48	1.536	-0.03	$9.56x10^{-13}$	$1.87x10^{-9}$	5.81±0.50	1.39±0.10
Anti-cancer	Azathioprine	446-86-6	$C_9H_7N_7O_2S$	277.26	272.0	-0.09	2.395	1.21	$2.64x10^{-15}$	$5.94x10^{-11}$	-	7.47±0.20
	Methotrexate	59-05-2	$C_{20}H_{22}N_8O_5$	454.45	$2.60x10^3$	-1.28	-0.387	-7.06	$1.54x10^{-31}$	-	3.47±0.10	5.56±0.10
	Tamoxifen	10540-29-1	$C_{26}H_{29}NO$	317.53	0.2	6.30	4.400	5.07	$4.49x10^{-10}$	$1.85x10^{-9}$	-	8.69±0.28
	Ifosfamide	3778-73-2	$C_7H_{15}Cl_2N_2O_2P$	261.09	$3.78x10^3$	0.97	1.439	0.10	$1.36x10^{-11}$	$1.15x10^{-4}$	-	1.44±0.20
Anti-depressants and metabolites	Fluoxetine	54910-89-3	$C_{17}H_{18}F_3NO$	309.33	60.3	4.65	3.050	1.92	$8.90x10^{-8}$	$1.88x10^{-6}$	-	10.05±0.10
	Norfluoxetine	83891-03-6	$C_{16}H_{16}F_3NO$	295.30	-	-	-	1.54	-	$5.21x10^{-6}$	-	9.05±0.13
	Sertraline	79617-96-2	$C_{17}H_{17}Cl_2N$	306.24	3.5	5.29	3.808	3.11	$5.10x10^{-8}$	$3.85x10^{-7}$	-	9.47±0.40
	Citalopram	59729-33-8	$C_{20}H_{21}FN_2O$	324.40	31.1	3.74	3.230	1.50	$2.69x10^{-11}$	$1.53x10^{-7}$	-	9.57±0.28
	Desmethylcitalopram	62498-67-3	$C_{19}H_{19}FN_2O$	310.37	-	-	-	0.14	-	$1.40x10^{-7}$	-	10.50±0.10
	Venlafaxine	93413-69-5	$C_{17}H_{27}N_1O_2$	277.41	266.7	3.28	2.318	1.32	$2.87x10^{-11}$	$4.92x10^{-7}$	14.84±0.20	9.26±0.28
Anti-epileptic and metabolites	Carbamazepine	298-46-4	$C_{15}H_{12}N_2O$	236.28	17.7	2.25	2.227	2.77	$1.08x10^{-10}$	$5.78x10^{-7}$	13.94±0.20	-0.49±0.20
	Carbamazepine10,11-epoxide	36507-30-9	$C_{15}H_{12}N_2O_2$	252.27	-	-	-	1.97	-	$2.69x10^{-6}$	13.91±0.20	-0.50±0.20
	10,11 dihydro 10 hydroxycarbamazepine	29331-92-8	$C_{15}H_{14}N_2O_2$	254.28				1.73	-	$3.33x10^{-8}$	13.75±0.20	-0.53±0.40
Anti-psychotic	Quetiapine	111974-69-7	$C_{21}H_{25}N_3O_2S$	384.52	0.6	3.17	2.111	2.67	$7.45x10^{-18}$	$3.22x10^{-13}$	14.41±0.10	6.74±0.10
Antihistamine	Cetirizine	83881-51-0	$C_{21}H_{25}ClN_2O_3$	388.90	1.1	-0.61	0.875	0.69	$4.19x10^{-17}$	$1.39x10^{-12}$	3.46±0.10	6.71±0.10
Beta-blocker	Atenolol	29122-68-7	$C_{14}H_{22}N_2O_3$	266.34	685.0	-0.03	0.611	-1.71	$1.37x10^{-18}$	$3.82x10^{-11}$	13.88±0.20	9.43±0.10
	Metoprolol	51384-51-1	$C_{15}H_{25}NO_3$	267.37	$4.77x10^3$	1.69	1.475	-0.38	$1.40x10^{-13}$	$4.52x10^{-7}$	13.89±0.20	9.43±0.10
	Propranolol	525-66-6	$C_{16}H_{21}NO_2$	259.35	228.0	2.60	2.451	0.45	$7.98x10^{-13}$	$2.48x10^{-8}$	13.84±0.20	9.50±0.30
Calcium channel blocker	Diltiazem	42399-41-7	$C_{22}H_{26}N_2O_4S$	414.52	12.3	2.79	2.296	1.97	$8.61x10^{-17}$	$4.27x10^{-14}$	-	8.94±0.28
Cough suppressant	Pholcodine	509-67-1	$C_{23}H_{30}N_2O_4$	398.51	$1.01x10^4$	0.59	0.731	-0.48	$3.42x10^{-19}$	$3.44x10^{-14}$	13.40±0.20	8.22±0.40

Table S1. (continued)

Micropollutant class	Micropollutant	CAS No.	Molecular Formula	Molecular Weight (g mol^{-1})	Water Solubility (mg L^{-1})[i]	Log Kow[ii]	Log Koc[iii]	Log Dow[iv]	Henry's Law Constant (atm m^{3}mol^{-1})[v]	Vapour Pressure (Torr)[vi]	pKa (Most acidic)[vii]	pKa (Most basic)[viii]
Anti-diabetes	Metformin	657-24-9	$C_4H_{11}N_5$	129.17	$1.00x10^6$	-2.64	-0.666	-6.45	$7.64x10^{-16}$	1.33	-	12.27±0.10
	Gliclazide	21187-98-4	$C_{15}H_{21}N_3O_3S$	323.41	138.4	2.12	2.205	0.79	$7.95x10^{-13}$	-	6.07±0.10	3.89±0.20
Drug precursor and metabolite	Ephedrine/ pseudoephedrine	299-42-3	$C_{10}H_{15}NO$	165.24	$7.15x10^4$	0.68	1.095	-1.13	$8.65x10^{-11}$	$8.65x10^{-3}$	13.96±0.20	9.38±0.10
	Norephedrine	492-39-7	$C_9H_{13}NO$	151.21	$1.49x10^5$	0.22	0.951	-1.40	$3.94x10^{-11}$	$1.10x10^{-3}$	12.07±0.45	8.47±0.10
H_2 receptor agonists	Ranitidine	66357-35-5	$C_{13}H_{22}N_4O_3S$	314.41	$2.47x10^4$	0.29	1.141	-1.56	$3.42x10^{-15}$	$7.66x10^{-8}$	-	8.35±0.28
	Cimetidine	51481-61-9	$C_{10}H_{16}N_6S$	252.34	$1.05x10^4$	0.57	1.850	-0.30	$9.55x10^{-16}$	$3.13x10^{-9}$	14.13±0.10	7.07±0.61
Nicotine and metabolites	Nicotine	54-11-5	$C_{10}H_{14}N_2$	162.24	$1.00x10^6$	1.00	1.683	-2.34	$3.00x10^{-9}$	$3.03x10^{-2}$	-	8.00±0.50
	Caffeine	58-08-2	$C_8H_{10}N_4O_2$	194.19	$2.63x10^3$	0.16	0.980	-0.55	$3.58x10^{-11}$	$3.72x10^{-7}$	-	0.52±0.70
	Cotinine	486-56-6	$C_{10}H_{12}N_2O$	176.22	$9.99x10^5$	0.34	1.093	0.21	$3.33x10^{-12}$	$4.21x10^{-4}$	-	4.72±0.12
	1,7 dimethylxantine	611-59-6	$C_7H_8N_4O_2$	180.17	$4.14x10^3$	-0.39	0.919	0.24	$1.75x10^{-12}$	-	8.50±0.50	0.21±0.70
Hypertension	Lisinopril	76547-98-3	$C_{21}H_{31}N_3O_5$	405.50	8.6	-0.94	-0.516	-3.23	$1.89x10^{-22}$	$1.14x10^{-18}$	2.18±0.10	10.50±0.10
	Temazepam	846-50-4	$C_{16}H_{13}ClN_2O_2$	300.75	163.9	2.15	1.678	2.79	$1.13x10^{-8}$	$6.33x10^{-13}$	11.66±0.40	1.58±0.50
Anti-inflammatory	Acetaminophen	103-90-2	$C_8H_9NO_2$	151.17	$3.04x10^4$	0.27	1.321	0.90	$6.42x10^{-13}$	$1.43x10^{-6}$	9.86±0.13	1.72±0.50
Stimulants and metabolites	Heroin	561-27-3	$C_{21}H_{23}NO_5$	369.42	$2.15x10^3$	1.80	1.658	-0.06	$6.15x10^{-13}$	$7.38x10^{-10}$	-	7.93±0.40
	Amphetamine	300-62-9	$C_9H_{13}N_1$	135.21	$2.80x10^4$	1.76	1.877	-1.23	$1.08x10^{-6}$	0.31	-	9.94±0.10
	Methamphetamine	537-46-2	$C_{10}H_{15}N$	149.24	$1.33x10^4$	2.22	2.027	-1.01	$2.37x10^{-6}$	0.15	-	10.38±0.10
	MDMA	42542-10-9	$C_{11}H_{15}NO_2$	193.25	$7.03x10^3$	2.28	2.183	-1.38	$2.75x10^{-9}$	$3.17x10^{-3}$	-	10.32±0.10
	MDA	101-77-9	$C_{13}H_{14}N_2$	198.27	$1.96x10^3$	2.18	1.761	-1.61	$1.58x10^{-11}$	$1.52x10^{-6}$	-	5.32±0.25
	6-acetylmorphine	2784-73-8	$C_{19}H_{21}NO_4$	327.37	-	-	-	-0.22	-	$1.83x10^{-9}$	9.41±0.40	8.03±0.40
	Cocaine	50-36-2	$C_{17}H_{21}NO_4$	303.36	$1.30x10^3$	2.17	2.001	0.92	$4.24x10^{-11}$	$1.87x10^{-6}$	-	8.97±0.60
	Benzoylecgonine	519-09-5	$C_{16}H_{19}NO_4$	289.33	$1.61x10^3$	-1.32	-0.705	-0.60	$1.03x10^{-13}$	$1.32x10^{-8}$	3.35±0.40	10.83±0.40
	Anhydroecgonine methylester	43021-26-7	$C_{10}H_{15}NO_2$	181.23	-	-	-	0.21	-	$2.19x10^{-2}$	-	7.97±0.40
	Cocaethylene	529-38-4	$C_{18}H_{23}NO_4$	317.38	-	-	-	1.35	-	$6.80x10^{-7}$	-	9.04±0.60
	Mephedrone	1189805-46-6	$C_{11}H_{15}NO$	177.24	-	-	-	1.47	-	$3.84x10^{-3}$	-	7.41±0.10
UV filter	3-benzophenone	131-57-7	$C_{14}H_{12}O_3$	228.25	68.6	3.52	3.440	3.06	$1.50x10^{-8}$	$5.26x10^{-6}$	7.56±0.35	-
Veterinary	Tylosin	1401-69-0	$C_{46}H_{77}NO_{17}$	916.12	0.5	1.05	0.205	2.14	$5.77x10^{-38}$	0.00	13.06±0.70	7.39±0.70
X-ray contrast media	Iopromide	73334-07-3	$C_{18}H_{24}I_3N_3O_8$	791.12	23.8	-2.49	-1.672	-0.44	$1.00x10^{-28}$	$5.00x10^{-30}$	10.62±0.70	-2.60±0.70

[i] As calculated by EPI Suite at 25°C [1]
[ii] As calculated by EPI Suite (KOWWIN v1.68 estimate) [1]
[iii] As calculated by EPI Suite based on Log Know [1]
[iv] As calculated by Marvin Beans at pH 7.5 [1]
[v] As calculated by EPI Suite based on Bond SAR method [1]
[vi] As stated on Scifinder calculated using Advanced Chemistry Development (ACD/Labs) Software v11.02 (© 1994-2015 ACD/Labs) [1]
[vii] As stated on Scifinder calculated using Advanced Chemistry Development (ACD/Labs) Software v11.02 (© 1994-2015 ACD/Labs) at 25°C [1]

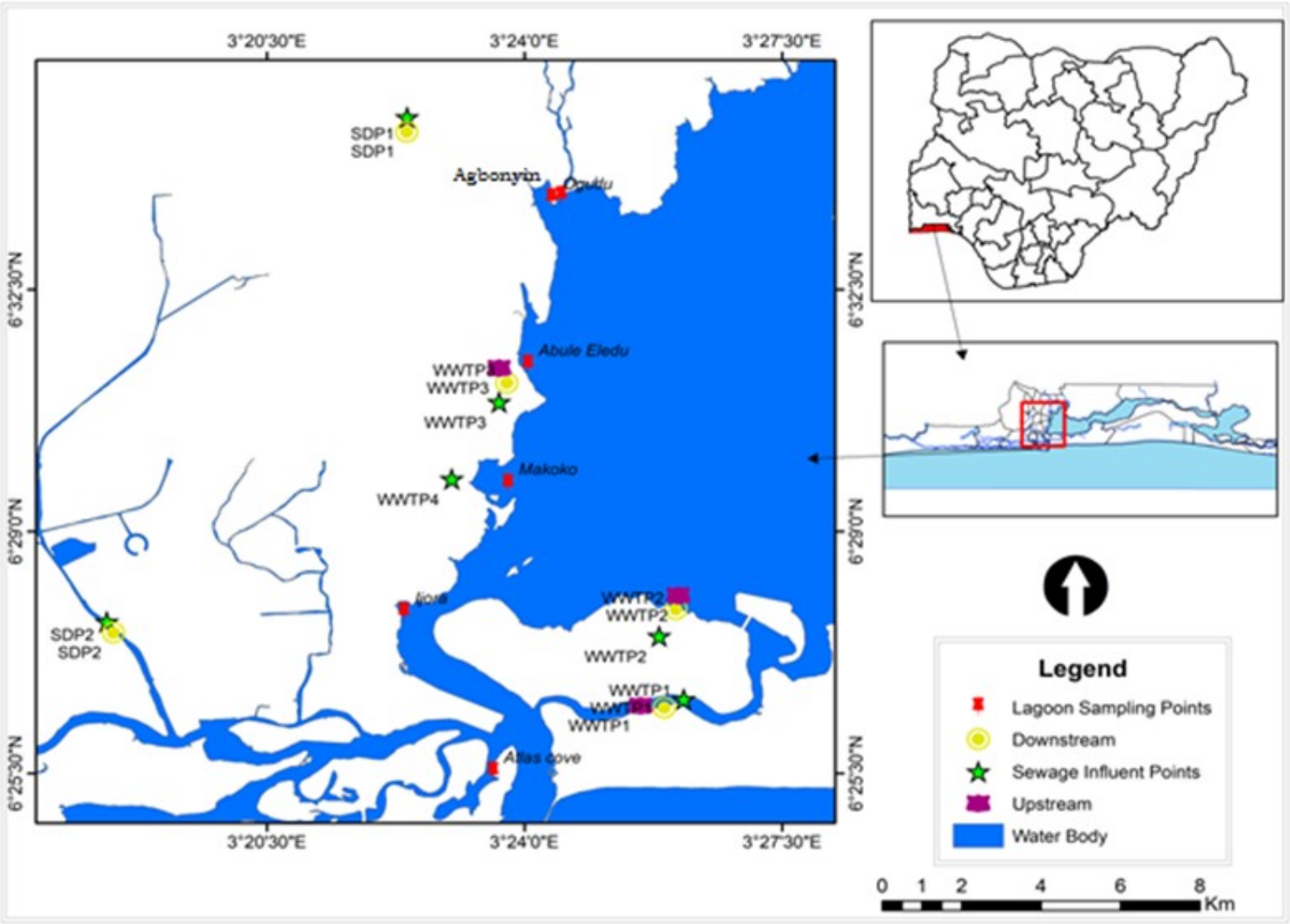

Figure S1. Sample collection points for wastewater and surface water

Table S2. Instrument details including chromatographic retention time and mass spectrometry parameters used in the determination of target analytes

Micropollutant class	Micropollutant	t_R (min)	Precursor ion (m/z)	Product ion 1 (m/z)	CV (V)	CE (eV)	Product ion 2 (m/z)	CV (V)	CE (eV)	Ion ratio[a]	Internal Standard
Anaesthetic and metabolite	Ketamine	10.59	238.1	125.0	31	27	220.1	31	15	2.93 ± 0.04	Ketamine-d_4
	Norketamine	11.08	224.0	207.1	23	12	125.0	23	27	1.00 ± 0.02	Norketamine-d_4
Analgesics and metabolites	Morphine	3.46	286.2	165.1	53	38	152.1	53	56	0.98 ± 0.04	Morphine-d_3
	Dihydromorphine	3.30	288.2	185.0	28	42	213.0	28	32	2.82 ± 0.14	Morphine-d_3
	Normorphine	3.41	272.1	165.0	45	43	152.1	45	49	1.16 ± 0.05	Morphine-d_3
	Methadone	17.59	310.2	265.1	31	15	105.1	31	28	1.50 ± 0.05	Methadone-d_9
	Codeine	6.05	300.2	215.1	49	25	152.1	49	57	1.17 ± 0.04	Codeine-d6
	Dihydrocodeine	5.47	302.1	199.1	53	33	128.1	53	60	1.91 ± 0.05	Codeine-d6
	Norcodeine	6.45	286.1	165.1	46	40	268.2	46	20	1.11 ± 0.04	Codeine-d6
	Tramadol	10.97	264.0	58.0	28	45	120.7	28	46	270 ± 21.4	Metoprolol-d_7
	N-desmethyltramadol	11.88	250.1	44.0	25	12	232.1	25	8	38.6 ± 0.06	Cocaine-d_3
	O-desmethyltramadol	8.29	250.2	58.0	30	18	232.1	30	10	181 ± 6.40	Cotinine-d_3
Antibacterial/antibiotics	Clarithromycin	18.87	748.5	158.1	40	31	590.4	40	20	3.71 ± 0.03	Methadone-d_9
	Azithromycin	13.95	749.5	116.1	60	54	83.1	0	60	0.95 ± 0.02	EDDP-d_3
	Trimethoprim	8.43	291.2	230.2	26	26	123.1	26	36	1.07 ± 0.03	Methamphetamine-d_5
	Sulfamethoxazole	9.56	254.1	92.2	36	30	156.1	36	20	1.44 ± 0.03	Benzoylecgonine-d_8
Anti-cancer	Azathioprine	7.75	278.0	142.0	28	13	85.0	28	20	5.49 ± 0.17	Cotinine-d_3
	Methotrexate	7.89	455.1	308.1	40	20	175.1	40	35	1.93 ± 0.50	Amphetamine-d_5
	Tamoxifen	22.39	372.2	72.0	50	25	129.0	50	28	30.6 ± 0.91	Tamoxifen $^{13}C_2$ ^{15}N
	Ifosfamide	12.69	261.0	92.0	40	28	154.0	40	22	1.89 ± 0.03	Metoprolol-d_7
Anti-depressants and metabolites	Fluoxetine	18.35	310.2	44.1	34	10	148.1	34	10	14.9 ± 0.54	Fluoxetine-d_5
	Norfluoxetine	18.42	296.1	134.1	18	6	-	-	-	-	Fluoxetine-d_5
	Sertraline	19.22	306.0	159.0	23	27	275.0	23	10	1.26 ± 0.02	Sertraline-d_3
	Citalopram	15.06	325.1	262.1	46	18	109.9	46	26	21.8 ± 3.45	Citalopram-d_6
	Desmethylcitalopram	15.17	311.4	109.0	46	27	262.0	46	18	3.58 ± 0.11	Citalopram-d_6
	Venlafaxine	14.14	278.2	58.1	27	40	260.1	27	12	1.78 ± 0.02	Metoprolol-d_7
Anti-epileptic and metabolites	Carbamazepine	16.15	237.0	194.1	40	20	179.1	40	38	10.6 ± 0.15	Carbamazepine $^{13}C_6$
	Carbamazepine10,11-epoxide	13.47	253.1	180.1	39	25	210.1	39	12	1.96 ± 0.04	Carbamazepine $^{13}C_6$
	10,11 dihydro 10 hydroxycarbamazepine	13.49	255.1	194.1	20	20	179.1	20	40	9.75 ± 0.29	Carbamazepine $^{13}C_6$
Anti-psychotic	Quetiapine	17.87	384.1	253.1	50	21	221.1	50	40	1.97 ± 0.04	Quetiapine-d_8
Antihistamine	Cetirizine	18.68	389.1	201.0	32	21	166.0	32	40	2.51 ± 0.05	Temazepam-d_5
Beta-blocker	Atenolol	4.32	267.3	145.1	38	30	190.1	38	16	1.61 ± 0.07	Atenolol-d_7
	Metoprolol	11.17	268.3	116.1	42	20	121.1	42	22	2.36 ± 0.04	Metoprolol-d_7
	Propranolol	15.14	260.2	183.1	42	18	116.1	42	16	1.88 ± 0.09	Propranolol-d_7
Calcium channel blocker	Diltiazem	16.72	415.0	178.0	40	25	310.1	40	25	23.4 ± 1.30	Carbamazepine $^{13}C_6$
Cough suppressant	Pholcodine	3.70	399.2	381.2	55	25	100.1	55	37	3.00 ± 0.43	Atenolol-d_7

Table S2. (continued)

Micropollutant class	Micropollutant	t_R (min)	Precursor ion (m/z)	Product ion 1 (m/z)	CV (V)	CE (eV)	Product ion 2 (m/z)	CV (V)	CE (eV)	Ion ratio[a]	Internal Standard
Anti-diabetes	Metformin	2.84	130.0	60.0	30	15	71.0	30	20	1.89 ± 0.02	Metformin-d_6
	Gliclazide	17.80	324.1	127.0	41	20	110.0	41	20	0.98 ± 0.04	Quetiapine-d_8
Drug precursor and metabolite	Ephedrine/pseudoephedrine	7.22	166.1	148.1	23	12	133.1	23	21	6.58 ± 0.12	1S,2R-(+) Ephedrine-d_3
	Norephedrine	6.34	152.2	134.1	23	10	117.1	23	16	2.99 ± 0.06	1S,2R-(+) Ephedrine-d_3
H_2 receptor agonists	Ranitidine	4.62	315.9	176.0	26	17	123.9	26	24	8.44 ± 0.50	Atenolol-d_7
	Cimetidine	5.32	252.9	159.4	22	16	211.2	22	10	9.02 ± 0.40	Acetaminophen-d_4
Nicotine and metabolites	Nicotine	3.34	163.1	130.0	37	20	117.0	37	20	1.37 ± 0.02	Atenolol-d_7
	Caffeine	8.29	195.1	138.0	38	15	110.0	38	23	2.56 ± 0.05	Cotinine-d_3
	Cotinine	7.22	177.1	80.0	34	21	98.1	34	22	2.91 ± 0.05	Cotinine-d_3
	1,7 dimethylxantine	6.78	181.0	124.1	54	21	-	-	-	-	Cotinine-d_3
Hypertension	Lisinopril	7.14	406.2	84.0	38	27	246.1	38	22	9.42 ± 0.30	Amphetamine-d_5
	Temazepam	18.16	301.1	255.1	37	21	283.1	37	14	2.21 ± 0.05	Temazepam-d_5
Anti-inflammatory	Acetaminophen	5.11	151.9	110.0	26	16	92.9	26	24	5.54 ± 0.13	Acetaminophen-d_4
Stimulants and metabolites	Heroin	10.85	370.2	165.1	51	50	268.1	51	29	1.41 ± 0.02	Heroin-d_9
	Amphetamine	8.39	136.2	91.1	18	16	119.1	18	8	1.20 ± 0.04	Amphetamine-d_5
	Methamphetamine	8.51	150.2	91.1	24	19	119.1	24	10	1.73 ± 0.03	Methamphetamine-d_5
	MDMA	8.62	194.1	163.1	24	13	105.1	24	24	2.34 ± 0.03	MDMA-d_5
	MDA	8.59	180.0	163.1	21	11	105.1	21	22	2.73 ± 0.06	MDA-d_5
	6-acetylmorphine	7.65	328.1	165.1	52	39	211.1	52	26	1.46 ± 0.04	Cotinine-d_3
	Cocaine	11.32	304.2	182.1	40	20	82.1	40	31	2.75 ± 0.09	Cocaine-d_3
	Benzoylecgonine	9.68	290.2	168.1	38	19	105.1	38	30	1.95 ± 0.03	Benzoylecgonine-d_8
	Anhydroecgonine methylester	3.45	182.1	118.0	39	23	122.1	37	20	1.23 ± 0.03	Atenolol-d_7
	Cocaethylene	12.91	318.2	196.2	38	20	82.1	38	30	1.90 ± 0.05	Cocaethylene-d_3
	Mephedrone	9.79	178.1	160.1	10	12	145.0	10	22	1.55 ± 0.06	Mephedrone-d_3
UV filter	3-benzophenone	21.23	229.0	151.0	35	18	105.0	35	20	1.58 ± 0.04	Methadone-d_9
Veterinary	Tylosin	17.25	916.5	174.2	80	45	101.0	80	56	1.88 ± 0.07	Methadone-d_9
X-ray contrast media	Iopromide	4.89	792.0	573.0	46	25	558.9	46	32	1.45 ± 0.06	Acetaminophen-d_4

t_R, retention time; CV, cone voltage; CE, collision energy

[a]MRM ratio: Product ion 1/Product ion 2 ratio average over the entire calibration range

Table S3. Instrument performance data of target analytes

Micropollutant class	Micropollutant	Corresponding	Linearity		$IDL_{S/N}$	$IQL_{S/N}$	Intra-day instrument performance[a]		Inter-day instrument performance[a]	
		Internal standard	Range (ng mL^{-1})	r2	(ng mL^{-1})	(ng mL^{-1})	Precision (%)	Accuracy (%)	Precision (%)	Accuracy (%)
Anaesthetic and metabolite	Ketamine	Ketamine D4	0.05-500	0.999	0.01	0.05	1.3	93.6	1.8	92.5
	Norketamine	Norketamine D4	0.10-500	0.999	0.03	0.1	3.2	94	1.8	94.1
Analgesics and metabolites	Morphine	Morphine D3	1.00-500	0.997	0.3	1	2.5	97.5	2.9	99.1
	Dihydromorphine	Morphine-D3	0.05-500	0.998	0.01	0.05	2.7	108.5	4.4	106
	Normorphine	Morphine-D3	1.00-500	0.997	0.3	1	2.2	99.8	1.5	101
	Methadone	Methadone D9	0.05-400	0.998	0.01	0.05	1.4	100.2	1.5	98.7
	Codeine	Codeine D6	0.50-500	0.999	0.1	0.5	4	95.1	2	93.5
	Dihydrocodeine	Codeine D6	0.10-500	0.999	0.03	0.1	2.1	94.6	1.6	94.2
	Norcodeine	Codeine D6	1.00-500	0.999	0.3	1	4.8	98.6	2.8	98.5
	Tramadol	Metoprolol D7	1.00-500	0.999	0.01	1	1.9	98.4	1.6	100.1
	N-desmethyltramadol	Cocaine-D3	0.50-500	0.999	0.01	0.5	2.2	94.4	2.5	92.5
	O-desmethyltramadol	MDA-D5	1.00-400	0.997	0.01	1	4.9	98.5	3.3	95.3
Antibacterial/ antibiotics	Clarithromycin	Methadone D9	0.06-500	1	0.01	0.06	2.4	101.8	2.6	99.8
	Azithromycin	EDDP D3	0.11-500	0.999	0.03	0.11	2.1	98.5	3.8	95
	Trimethoprim	Methamphetamine D5	0.10-500	0.999	0.03	0.1	2.2	99.5	3	96.9
	Sulfamethoxazole	Benzoylecgonine D8	0.10-500	0.999	0.03	0.1	2.4	96	3.5	95.1
Anti-cancer	Azathioprine	Cotinine D3	0.10-500	0.998	0.03	0.1	13.9	97.4	7.6	97.5
	Methotrexate	Amphetamine D5	0.92-500	0.996	0.28	0.92	4.1	112.2	8.7	108
	Tamoxifen	Tamoxifen 13C2 15N	0.03-1000	0.998	0.01	0.03	2.4	96.8	4	96
	Ifosfamide	Metoprolol D7	0.05-500	0.999	0.01	0.05	2.7	95.3	2.4	93.6
Anti-depressants and metabolites	Fluoxetine	Fluoxetine D5	0.05-1000	0.999	0.01	0.05	1.8	98.3	1.7	96.8
	Norfluoxetine	Fluoxetine D5	0.05-500	0.998	0.01	0.05	3.1	103.1	1.5	102.7
	Sertraline	Sertraline D3	0.05-500	1	0.01	0.05	1.7	95.7	1.6	95.3
	Citalopram	Citalopram D6	0.50-500	0.999	0.05	0.5	2.6	101.8	0.7	101.2
	Desmethylcitalopram	Citalopram D6	0.05-500	0.999	0.01	0.05	3	103.4	1.8	103
	Venlafaxine	Metoprolol D7	0.04-500	1	0.01	0.04	1.7	90.5	2.5	91.2
Anti-epileptic and metabolites	Carbamazepine	Carbamazepine 13C6	0.05-500	1	0.01	0.05	1.6	92.7	2	91.7
	Carbamazepine10,11-epoxide	Carbamazepine 13C6	0.10-500	0.998	0.03	0.1	2.1	89.9	1.6	88.9
	10,11-Dihydro-10-hydroxycarbamazepine	Carbamazepine 13C6	0.50-500	0.999	0.05	0.5	5.6	93.8	2.8	92.2
Anti-psychotic	Quetiapine	Quetiapine D8	0.05-500	0.999	0.01	0.05	1.2	96.4	1.4	95.3
Antihistamine	Cetirizine	Temazepam D5	0.08-500	1	0.02	0.08	1.3	100.8	1.3	100.5
Beta-blocker	Atenolol	Atenolol D5	0.10-500	1	0.03	0.1	2.3	96.8	2.1	95.3
	Metoprolol	Metoprolol D7	0.05-500	0.999	0.01	0.05	2	96.1	1.3	96.8
	Propranolol	Propranolol D7	0.09-500	0.999	0.03	0.09	1	106.2	2	105.4
Calcium channel blocker	Diltiazem	Carbamazepine 13C6	0.10-500	0.999	0.01	0.1	2.3	93.6	2.3	92.7
Cough suppressant	Pholcodine	Atenolol D7	1.14-500	0.994	0.35	1.14	3.3	99.2	4.7	99.5

Table S3. (continued)

Micro-pollutant class	Micro-pollutant	Corresponding	Linearity		$IDL_{S/N}$	$IQL_{S/N}$	Intra-day instrument performance[a]		Inter-day instrument performance[a]	
		Internal standard	Range (ng mL^{-1})	r2	(ng mL^{-1})	(ng mL^{-1})	Precision (%)	Accuracy (%)	Precision (%)	Accuracy (%)
	Gliclazide	Carbamazepine 13C6	0.05-500	0.998	0.01	0.05	2.8	95.3	2.1	93.2
Drug precursor and metabolite	Ephedrine/pseudoephedrine	1S,2R-(+) Ephedrine D3	0.10-500	1	0.03	0.1	3.4	97.3	4.1	94
	Norephedrine	1S,2R-(+) Ephedrine D3	0.50-500	0.999	0.01	0.5	5.1	95.2	4.3	96.3
H_2 receptor agonists	Ranitidine	Cotinine D3	5.17-500	0.998	1.03	5.17	9.7	97.5	2.5	100.1
	Cimetidine	Codeine D6	0.52-500	0.998	0.1	0.52	9	99.3	4.2	104.1
Nicotine and metabolites	Nicotine	Codeine D6	1.00-500	0.996	0.3	1	2.4	98.4	1.2	98.3
	Caffeine	Cotinine D3	0.50-500	0.999	0.1	0.5	2.8	100.4	1.7	99.6
	Cotinine	Cotinine D3	0.05-500	0.999	0.01	0.05	1.5	98.8	1.5	98.4
	1,7 dimethylxantine	Cotinine D3	1.00-500	0.999	0.3	1	9.9	94.9	6	94.3
Hypertension	Lisinopril	Amphetamine D5	0.93-400	0.995	0.3	1	7.2	95.2	2.2	97.2
	Temazepam	Temazepam D5	0.05-500	0.999	0.01	0.05	1.6	97.9	1	97
Anti-inflammatory	Acetaminophen	Acetaminophen D4	0.54-500	0.999	0.11	0.54	2.6	99	1.6	97.4
Stimulants and metabolites	Heroin	Heroin D9	0.50-500	0.999	0.1	0.5	1.8	99.3	1.9	98.2
	Amphetamine	Amphetamine D5	0.10-500	0.999	0.03	0.1	1.6	100.7	4.4	100.8
	Methamphetamine	Methamphetamine D5	0.10-500	0.999	0.03	0.1	1.3	101.1	2.2	101
	MDMA	MDMA D5	0.05-500	1	0.01	0.05	1.7	99.8	1.3	99.2
	MDA	MDA D5	0.10-500	0.999	0.03	0.1	0.7	100	1.1	98.4
	6-acetylmorphine	Cotinine D3	0.10-500	0.998	0.03	0.1	5.1	100.1	6.1	95.3
	Cocaine	Cocaine D3	0.05-500	1	0.01	0.05	1.5	99	2.2	97.2
	Benzoylecgonine	Benzoylecgonine D8	0.05-500	0.998	0.01	0.05	0.9	103.2	2.4	103.4
	Anhydroecgonine methylester	Acetaminophen D4	0.50-500	0.997	0.1	0.5	2.4	98.7	2.3	101.1
	Cocaethylene	Cocaethylene D3	0.05-500	1	0.01	0.05	1.7	94.7	2.8	95.1
	Mephedrone	Mephedrone D3	0.05-500	0.998	0.01	0.05	2.9	85.7	1.8	87.1
UV filter	3-benzophenone	Methadone D9	0.05-400	0.99	0.01	0.05	4.5	86.8	3.2	84.9
Veterinary	Tylosin	Methadone D9	0.56-500	0.997	0.11	0.56	4	100.2	2.2	99.5
X-ray contrast media	Iopromide	Atenolol D7	5.79-500	0.99	1.16	5.79	12	105.4	5	101.2

[a]Instrument performance was determined at concentration 10, 100, 500 ng mL^{-1}

IDL, Instrument detection limit; IQL, Instrument quantification limit; S/N, signal to noise ratio

Table S4. Absolute and corrected recoveries in matrices sampled

Micropollutant class	Micropollutants	Influent		Effluent		Surface water	
		Absolute Recovery (%)	Corrected Recovery (%)	Absolute Recovery (%)	Corrected Recovery (%)	Absolute Recovery (%)	Corrected Recovery (%)
Anaesthetic and metabolite	Ketamine	41.7	111.6	53.8	115.6	68.2	107.7
	Norketamine	42.2	98.9	53.9	108.6	65.7	103.2
Analgesics and metabolites	Morphine	34.2	93.9	47.8	109.8	57.1	112.5
	Dihydromorphine	19.9	95.7	31.4	96.2	45.4	92.8
	Normorphine	30.3	109.5	38.6	106.5	42.8	87.3
	Methadone	49.6	109	47.9	111.7	46.5	119.2
	Codeine	39	94.8	68.4	102.8	67.5	93.1
	Dihydrocodeine	34.7	85.7	54.8	118.6	66.4	98.5
	Norcodeine	35.5	95.7	36.4	87.5	52.5	90.6
	Tramadol	33.3	69.5	47	88.3	60.9	104.8
	N-desmethyltramadol	17.9	81.3	33.4	98.8	42.2	69.1
	O-desmethyltramadol	31.8	87.3	36	93.9	58.6	108.1
Antibacterial/antibiotics	Clarithromycin	33.2	80.9	40.1	97.2	31	77.6
	Azithromycin	22.2	101.1	24.5	67	21.9	86.9
	Trimethoprim	41.4	109.6	59.8	123.7	59.2	118
	Sulfamethoxazole	42.1	102.8	64	111	78.9	108.4
Anti-cancer	Azathioprine	72	109.5	81.5	83.8	88.9	66.4
	Methotrexate	39.1	98.8	30.7	114.1	22.6	95.7
	Tamoxifen	9.5	85.2	8.7	98.4	0.2	112.8
	Ifosfamide	33.4	89.2	41.9	80.2	62.9	90.8
Anti-depressants and metabolites	Fluoxetine	19.8	110.7	7.1	111.1	4.4	112.3
	Norfluoxetine	23.6	94.8	7.9	91.7	3	74.4
	Sertraline	13.4	91.5	8.3	105	3.1	108
	Citalopram	40.3	119.9	35.5	124.1	41.1	115
	Desmethylcitalopram	32.5	93.1	27.5	110.9	36.2	89.5
	Venlafaxine	23.8	70.2	36.3	89.5	58.8	96.8
Anti-epileptic and metabolites	Carbamazepine	37.4	88.3	55.5	102.5	68.2	101.7
	Carbamazepine 10,11-epoxide	56.7	143.7	55	126.9	94.8	136.1
	10,11-Dihydro -10-hydroxycarbamazepine	50.3	152.2	59.5	120.6	74.1	125.1
Anti-psychotic	Quetiapine	37.8	72.6	46.8	95.1	51.6	87.2
Antihistamine	Cetirizine	48.6	77.3	78.8	114.3	47.9	77.3
Beta-blocker	Atenolol	42.8	88.6	54.6	109.7	76	115.1
	Metoprolol	36.2	97.4	53.1	104.3	71.8	107.8
	Propranolol	38.7	105	36.1	102.7	45.4	107.2
Calcium channel blocker	Diltiazem	36.3	118.1	30.1	82.3	43.7	82.9
Cough suppressant	Pholcodine	13.7	42	43.1	102	76.9	119.6
Anti-diabetes	Metformin	36.7	78.7	53	96	55.2	93.3
	Gliclazide	46.4	80.1	61.8	108.4	32.9	69.5
Drug precursor and metabolite	Ephedrine/pseudoephedrine	23	92.8	18.7	88.6	25.4	67.8
	Norephedrine	26.9	85.4	28.9	100.9	28.4	78.2
H_2 receptor agonists	Ranitidine	70.1	97.8	46.4	106.8	65	88.6
	Cimetidine	20.6	123.7	33.4	106.2	32.7	95.3
Nicotine and metabolites	Nicotine	98.5	77.3	55.7	83.9	45.3	54.9
	Caffeine	82.9	96.6	89.8	131.7	137	122.8
	Cotinine	37.4	85.2	47.3	101.5	72	105.9
	1,7-dimethylxanthine	89.3	79.6	26.6	110.6	47.5	75.5
Hypertension	Lisinopril	28.6	102.3	21.9	88.5	21.4	93.7
	Temazepam	54.5	107.3	72.5	113.9	66.3	115.3
Anti-inflammatory	Acetaminophen	77.8	77.8	44.8	116.4	44.4	140.5
Stimulants and metabolites	Heroin	23.9	105.3	29.1	103	54.1	100.9
	Amphetamine	24.5	91.7	27.4	107.8	22.5	98.7
	Methamphetamine	31.9	102.1	42.5	97.1	47.7	97.6
	MDMA	29.4	118.5	37	112.9	50	100.9
	MDA	30.7	99.4	30.3	99.1	28.7	99.6
	6-acetylmorphine	33.9	103.6	40	85.4	52.9	72.6
	Cocaine	21.7	97.4	44.9	105.2	71.4	106.9
	Benzoylecgonine	46.5	106.3	55.1	116.4	74.2	126.2
	Anhydroecgonine methylester	33.9	91.3	50.2	109.5	53.6	79.5
	Cocaethylene	7.6	109.9	48.1	107.4	71.3	105.9
	Mephedrone	18.2	94.8	22.8	103.7	22.8	97.3
UV filter	3-benzophenone	27	58.5	51.9	89.4	33	74.4
Veterinary	Tylosin	34.3	98.3	50.3	110	43.8	100.4
X-ray contrast media	Iopromide	47.2	138.5	82.1	123.7	97	143

Table S5. Mean concentrations (ng L^{-1}) of target compounds in influent and effluent samples

Micropollutant class	Micropollutants	Influent (ng L^{-1})						Effluent (ng L^{-1})			
		WWTP1	WWTP2	WWTP3	WWTP4	SDP1	SDP2	WWTP1	WWTP2	WWTP3	WWTP4
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	195.9 ± 271.0	<MQL	23.5 ± 52.8	<MQL	227.7 ± 450.3	62.9 ± 119.0	<MQL	<MQL	<MQL	<MQL
	Dihydromorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	7.4± 13.9	31.7 ± 12.8	35.8 ± 5.2	20.8 ± 8.8
	Normorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	3.9 ± 10.2	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	73.7 ± 111.3	<MQL	8.4 ± 10.7	<MQL	<MQL	<MQL	<MQL	<MQL	0.2 ± 0.7	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	193.5 ± 192.6	168.5 ± 186.1	382.8 ± 182.9	31.7 ± 13.0	60.3 ± 72.8	86.1 ± 94.3	75.7 ± 92.3	342.0 ± 207.1	26.3 ± 65.4	60.6 ± 43.6
	N-desmethyltramadol	107.1 ± 62.1	30.4 ± 42.7	346.5 ± 178.7	11.4 ± 19.1	115.2 ± 117.1	344.4 ± 255.6	32.9 ± 44.0	61.8 ± 39.4	13.5 ± 35.6	149.5 ± 266.9
	O-desmethyltramadol	348.9 ± 148.0	469.3 ± 676.3	1259.2 ± 914.4	72.5 ± 47.0	<MQL	<MQL	125.7 ± 142.6	503.6 ± 206.4	295.3 ± 742.7	352.3 ± 655.2
Antibacterial/ antibiotics	Clarithromycin	7.0 ± 5.2	<MQL	10.4 ± 11.0	<MQL	34.2 ± 61.8	53.9 ± 95.7	<MQL	<MQL	<MQL	<MQL
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	219.3 ± 134.5	211.5 ± 456.0	71.6 ± 74.4	<MQL	774.8 ± 467.9	<MQL	82.5 ± 104.9	524.4 ± 424.3	3.1 ± 8.1	33.3 ± 86.3
	Sulfamethoxazole	594.1 ± 710.6	639.8 ± 1123.9	900.7 ± 1095.8	31.6 ± 13.9	987.2 ± 1361.5	1049.5 ± 1039.6	298.6 ± 729.3	162.2 ± 227.1	22.0 ± 21.1	51.7 ± 42.6
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	<MQL	22.2 ± 12.2	<MQL	24.4 ± 12.2	<MQL	2.3 ± 6.1	2.2 ± 5.9	<MQL	6.6 ± 17.5	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	<MQL	12.5 ± 21.9	22.7 ± 55.0	<MQL	1.2 ± 3.0	<MQL	<MQL	<MQL	14.7 ± 23.0
	Norfluoxetine	3.4 ± 3.2	<MQL	5.2 ± 2.3	<MQL	15.7 ± 26.2	<MQL	<MQL	<MQL	<MQL	<MQL
	Sertraline	<MQL	1.8 ± 4.7	<MQL	<MQL	<MQL	100.8 ± 266.7	<MQL	197.8 ± 198.3	<MQL	<MQL
	Citalopram	<MQL	<MQL	7.0 ± 18.5	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	0.2 ± 0.4	<MQL	<MQL
Anti-epileptic and metabolites	Carbamazepine	14.9 ± 23.7	<MQL	824.8 ± 317.3	15.8 ± 35.1	535.8 ± 728.1	484.9 ± 518.7	2.6 ± 4.0	4.3 ± 7.8	58.1 ± 152.7	97.3 ± 180.1
	Carbamazepine 10,11 epoxide	145.6 ± 241.1	<MQL	296.9 ± 164.4	5.3 ± 8.7	983.4 ± 1311.5	1594.4 ± 2743.1	16.4 ± 22.5	15.2 ± 10.5	20.8 ± 52.2	22.8 ± 30.5
	10,11 dihydro 10 hydroxycarbamazepine	80.0 ± 190.6	5.8 ± 15.3	<MQL	<MQL	140.2 ± 371.0	<MQL	82.6 ± 112.2	36.6 ± 60.7	<MQL	<MQL
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	146.7 ± 122.0	16.6 ± 43.9	17.2 ± 13.5	95.1 ± 118.2	<MQL	247.9 ± 446.1	468.1 ± 459.7	<MQL	6.7 ± 17.2	<MQL
	Metoprolol	36.3 ± 27.1	5.6 ± 11.8	10.4 ± 20.1	0.5 ± 1.4	<MQL	7.8 ± 20.7	6.3 ± 9.4	12.8 ± 7.6	0.1 ± 0.2	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	4.4 ± 11.5	3.7 ± 9.9	<MQL	<MQL	<MQL	<MQL
Calcium channel blocker	Diltiazem	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	178.2 ± 322.8	<MQL	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S5 (continued)

Micropollutant class	Micropollutants	Influent (ng L^{-1})						Effluent (ng L^{-1})			
		WWTP1	WWTP2	WWTP3	WWTP4	SDP1	SDP2	WWTP1	WWTP2	WWTP3	WWTP4
Anti-diabetes	Metformin	1224.9 ± 1189.3	186.3 ± 385.4	79.9 ± 80.4	438.7 ± 539.8	9.9 ± 26.2	36.3 ± 60.0	12.9 ± 25.9	247.0 ± 197.7	7.4 ± 11.4	317.2 ± 196.2
	Gliclazide	16.2 ± 18.0	<MQL	80.2 ± 194.3	<MQL	3.3 ± 8.7	122.8 ± 261.6	147.2 ± 364.2	<MQL	10.6 ± 13.3	<MQL
Drug precursor and metabolite	Ephedrine/pseudoephedrine	31.9 ± 40.0	<MQL	36.8 ± 42.0	<MQL	259.0 ± 502.4	<MQL	<MQL	15.7 ± 14.5	<MQL	7.0 ± 13.1
	Norephedrine	<MQL	241.9 ± 529.5	<MQL	87.0 ± 62.6	<MQL	229.9 ± 253.3	2.7 ± 6.9	225.3 ± 174.4	22.8 ± 30.7	126.2 ± 101.0
H_2 receptor agonists	Ranitidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	25.4 ± 48.2	<MQL	95.2 ± 219.6	<MQL
	Cimetidine	36.0 ± 50.1	<MQL	156.4 ± 139.1	<MQL	1419.1 ± 1568.7	1430.6 ± 1788.0	0.5 ± 1.3	<MQL	2.3 ± 6.0	7.3 ± 19.4
Nicotine and metabolites	Nicotine	240.8 ± 373.9	<MQL	73.4 ± 18.1	<MQL	288.2 ± 392.3	<MQL	37.6 ± 20.7	<MQL	35.9 ± 8.9	<MQL
	Caffeine	2154.1 ± 2917.0	<MQL	777.1 ± 368.5	<MQL	571.8 ± 614.8	<MQL	<MQL	<MQL	<MQL	<MQL
	Cotinine	497.5 ± 451.1	277.4 ± 446.4	61.3 ± 30.6	72.4 ± 34.2	587.4 ± 1041.3	1281.9 ± 2084.7	2.6 ± 4.6	126.7 ± 87.7	5.6 ± 12.3	95.1 ± 51.2
	1,7 dimethylxantine	1448.5 ± 2737.9	1534.7 ± 2280.2	1066.0 ± 1145.3	3373.9 ± 3277.6	<MQL	877.4 ± 926.1	128.0 ± 338.7	2545.8 ± 2537.6	75.1 ± 292.9	2409.0 ± 2612.8
Hypertension	Lisinopril	49.0 ± 23.9	15.2 ± 23.5	32.1 ± 34.7	128.2 ± 45.2	695.1 ± 848.4	238.3 ± 170.5	2.9 ± 7.7	<MQL	13.9 ± 18.4	91.7 ± 35.8
	Temazepam	<MQL	<MQL	<MQL	<MQL	<MQL	59.5 ± 56.7	<MQL	<MQL	<MQL	<MQL
Anti-inflammatory	Acetaminophen	35.1 ± 93.0	518.1 ± 1263.1	55.7 ± 58.7	965.2 ± 1566.2	528.2 ± 475.9	291.2 ± 167.2	12.6 ± 24.3	<MQL	33.7 ± 24.1	1334.4 ± 3455.1
Stimulants and metabolites	Heroin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Amphetamine	<MQL	35.9 ± 16.4	<MQL	113.8 ± 102.3	<MQL	110.8 ± 98.0	8.6 ± 12.0	935.4 ± 1628.4	25.0 ± 32.8	83.8 ± 65.4
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	0.6 ± 1.7	0.2 ± 0.6	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	<MQL	<MQL	<MQL	21.9 ± 30.6	<MQL	<MQL	<MQL	<MQL	<MQL	33.6 ± 71.6
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	594.9 ± 538.1	<MQL	75.5 ± 199.9	476.5 ± 457.8	67.1 ± 177.6	<MQL	35.4 ± 63.0	1.7 ± 3.3	<MQL	508.2 ± 659.7
	Anhydroecgonine methylester	5.4 ± 10.2	<MQL	5.0 ± 13.2	<MQL	<MQL	<MQL	11.7 ± 16.3	<MQL	5.7 ± 9.8	<MQL
	Cocaethylene	<MQL	184.8 ± 488.9	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	<MQL	<MQL	<MQL	32.9 ± 40.4	<MQL	102.6 ± 166.5	<MQL	<MQL	<MQL	2.2 ± 5.9
UV filter	3-benzophenone	92.0 ± 36.5	164.9 ± 13.0	74.0 ± 14.1	185.1 ± 64.4	59.6 ± 33.9	135.1 ± 60.2	54.2 ± 56.4	176.8 ± 35.1	158.1 ± 25.1	182.1 ± 74.5
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S6. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP1

Micropollutant class	Micropollutants	WWTP1 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	696.0	<MQL	118.0	<MQL	<MQL	<MQL	0.5	<MQL	445.5	<MQL	<MQL	<MQL	111.5	<MQL
	Dihydromorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	36.0	<MQL	<MQL	<MQL	15.7
	Normorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	312.0	<MQL	95.0	<MQL	<MQL	<MQL	<MQL	<MQL	53.0	<MQL	<MQL	<MQL	56.0	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	343.9	<MQL	397.2	148.5	>MQL	<MQL	>MQL	84.7	439.8	243.0	88.5	<MQL	85.0	53.5
	N-desmethyltramadol	77.1	<MQL	126.6	73.1	113.2	<MQL	200.3	51.3	159.7	106.0	50.3	<MQL	22.6	<MQL
	O-desmethyltramadol	385.6	<MQL	529.1	174.4	181.9	<MQL	382.7	159.1	446.6	390.8	403.8	<MQL	112.2	155.3
Antibacterial/ antibiotics	Clarithromycin	18.6	<MQL	5.8	<MQL	4.7	<MQL	4.7	<MQL	4.1	<MQL	6.7	<MQL	4.7	<MQL
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	409.0	<MQL	273.0	63.5	324.5	<MQL	200.5	214.5	230.0	53.0	41.5	<MQL	56.5	246.5
	Sulfamethoxazole	1,458.2	<MQL	1,763.2	56.4	280.6	<MQL	221.5	37.3	>MQL	44.9	363.6	<MQL	71.5	1,951.6
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	15.5	<MQL	<MQL	<MQL	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norfluoxetine	5.9	<MQL	5.9	<MQL	5.9	<MQL	<MQL	<MQL	<MQL	<MQL	6.1	<MQL	<MQL	<MQL
	Sertraline	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Citalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-epileptic and metabolites	Carbamazepine	8.7	<MQL	<MQL	4.1	<MQL	<MQL	<MQL	3.6	36.0	10.8	59.6	<MQL	<MQL	<MQL
	Carbamazepine 10,11 epoxide	73.5	<MQL	<MQL	30.5	<MQL	<MQL	<MQL	26.0	26.0	57.5	275.5	<MQL	644.5	1.0
	10,11 dihydro 10 hydroxycarbamazepine	>MQL	<MQL	<MQL	156.5	39.5	<MQL	1.5	141.0	511.0	281.0	>MQL	<MQL	8.0	<MQL
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	397.0	476.9	194.0	1,418.1	92.5	299.5	103.5	336.7	144.2	18.6	50.3	144.7	45.2	582.4
	Metoprolol	62.3	<MQL	23.1	13.2	25.1	<MQL	40.1	6.6	82.2	24.4	11.2	<MQL	10.2	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Calcium channel blocker	Diltiazem	<MQL	878.7	<MQL	247.4	<MQL	2.4	<MQL	<MQL	<MQL	<MQL	<MQL	119.1	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S6. (continued)

Micropollutant class	Micropollutants	WWTP1 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anti-diabetes	Metformin	3,351.0	<MQL	1,395.5	6.9	843.2	<MQL	2,061.7	71.2	923.0	6.9	<MQL	<MQL	<MQL	5.6
	Gliclazide	41.7	972.5	<MQL	25.3	37.1	<MQL	<MQL	<MQL	<MQL	<MQL	22.9	<MQL	11.7	32.6
Drug precursor and metabolite	Ehedrine/pseudoephedrine	93.1	<MQL	73.1	<MQL	3.0	<MQL	<MQL	<MQL	52.2	<MQL	<MQL	<MQL	2.2	<MQL
	Norephedrine	<MQL	<MQL	<MQL	18.4	<MQL	<MQL	<MQL	<MQL	<MQL	0.7	<MQL	<MQL	<MQL	<MQL
H_2 receptor agonists	Ranitidine	<MQL	<MQL	<MQL	<MQL	<MQL	22.8	<MQL	7.2	<MQL	15.0	<MQL	<MQL	<MQL	132.9
	Cimetidine	44.4	<MQL	145.5	<MQL	18.7	<MQL	8.6	<MQL	19.9	3.5	15.3	<MQL	<MQL	<MQL
Nicotine and metabolites	Nicotine	1,065.5	56.0	285.0	<MQL	51.0	40.5	35.0	38.5	101.0	37.0	34.5	64.0	113.5	27.0
	Caffeine	5,516.9	<MQL	>MQL	<MQL	>MQL	<MQL	2,859.6	<MQL	>MQL	<MQL	<MQL	<MQL	6,702.2	<MQL
	Cotinine	756.0	<MQL	938.5	<MQL	898.5	<MQL	8.0	8.0	831.5	10.5	<MQL	<MQL	50.0	<MQL
	1,7 dimethylxantine	>MQL	<MQL	7,493.7	<MQL	1,254.7	<MQL	<MQL	<MQL	>MQL	896.2	<MQL	<MQL	1,391.3	<MQL
Hypertension	Lisinopril	52.6	<MQL	<MQL	<MQL	44.2	<MQL	77.1	<MQL	52.6	20.4	60.8	<MQL	55.4	<MQL
	Temazepam	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-inflammatory	Acetaminophen	246.0	<MQL	<MQL	19.0	<MQL	<MQL	<MQL	4.0	<MQL	65.5	<MQL	<MQL	<MQL	<MQL
Stimulants and metabolites	Heroin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Amphetamine	<MQL	<MQL	<MQL	2.5	<MQL	<MQL	<MQL	23.5	<MQL	28.0	<MQL	<MQL	<MQL	6.0
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	4.5	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	1,283.7	<MQL	438.7	92.8	453.4	<MQL	<MQL	<MQL	1,326.3	154.7	22.4	<MQL	639.7	<MQL
	Anhydroecgonine methylester	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	20.0	26.5	20.0	11.5	42.0
	Cocaethylene	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
UV filter	3-benzophenone	92.9	<MQL	67.2	71.2	168.7	<MQL	100.0	91.9	82.3	144.9	64.1	<MQL	68.7	71.7
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S7. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP2

Micropollutant class	Micropollutants	WWTP2 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Dihydromorphine	<MQL	27.1	<MQL	37.9	<MQL	38.6	<MQL	35.8	<MQL	49.2	<MQL	23.7	<MQL	9.6
	Normorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	<MQL	>MQL	222.4	451.2	159.0	542.4	547.2	449.6	16.9	193.8	68.5	482.5	165.7	148.8
	N-desmethyltramadol	<MQL	29.6	24.1	49.0	29.9	99.5	122.4	131.9	<MQL	44.5	6.5	24.4	29.9	53.7
	O-desmethyltramadol	606.3	766.8	>MQL	366.2	230.8	616.7	1,934.0	616.4	29.5	211.5	186.6	639.3	297.7	308.4
Antibacterial/ antibiotics	Clarithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	<MQL	141.0	>MQL	263.5	1,239.0	876.0	95.0	1,043.5	>MQL	377.5	127.5	957.5	19.0	11.5
	Sulfamethoxazole	1,632.6	659.1	>MQL	111.9	57.5	131.8	>MQL	148.9	>MQL	83.8	2,788.5	>MQL	>MQL	>MQL
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	31.1	<MQL	<MQL	<MQL	31.1	<MQL	31.1	<MQL	15.5	<MQL	31.1	<MQL	15.5	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norfluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Sertraline	<MQL	24.0	<MQL	557.0	12.5	222.5	<MQL	295.5	<MQL	246.0	<MQL	39.5	<MQL	<MQL
	Citalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	1.2
Anti-epileptic and metabolites	Carbamazepine	<MQL	2.1	<MQL	<MQL	<MQL	1.5	<MQL	21.6	<MQL	0.5	<MQL	<MQL	<MQL	4.1
	Carbamazepine 10,11 epoxide	<MQL	14.5	<MQL	8.5	<MQL	17.5	<MQL	13.5	<MQL	<MQL	<MQL	18.0	<MQL	34.5
	10,11 dihydro 10 hydroxycarbamazepine	40.5	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	6.5	<MQL	137.0	<MQL	112.5
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	116.1	<MQL	<MQL	<MQL
	Metoprolol	<MQL	19.3	3.1	20.3	32.0	13.7	<MQL	19.3	4.1	6.6	<MQL	10.7	<MQL	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Calcium channel blocker	Diltiazem	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S7. (continued)

Micropollutant class	Micropollutants	WWTP2 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anti-diabetes	Metformin	200.2	202.8	9.9	142.4	3.0	333.6	18.6	547.6	1,045.5	431.1	6.9	20.7	20.3	50.5
	Gliclazide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Drug precursor and metabolite	Ephedrine/pseudoephedrine	<MQL	11.5	<MQL	11.8	<MQL	29.1	<MQL	39.3	<MQL	17.9	<MQL	<MQL	<MQL	<MQL
	Norephedrine	1,439.2	72.0	10.9	318.8	21.8	184.3	55.6	192.8	120.8	576.1	<MQL	137.5	44.7	95.6
H_2 receptor agonists	Ranitidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cimetidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Nicotine and metabolites	Nicotine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Caffeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cotinine	914.5	75.0	25.0	154.5	<MQL	210.5	6.5	234.0	946.0	167.0	<MQL	0.5	50.0	45.5
	1,7 dimethylxantine	>MQL	670.4	1,625.9	4,678.6	388.5	469.0	2,521.3	310.3	>MQL	822.8	<MQL	6,329.0	6,207.4	4,540.4
Hypertension	Lisinopril	<MQL	<MQL	<MQL	<MQL	63.2	<MQL	<MQL	<MQL	21.4	<MQL	21.7	<MQL	<MQL	<MQL
	Temazepam	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-inflammatory	Acetaminophen	3,380.5	<MQL	134.0	<MQL	<MQL	<MQL	50.0	<MQL	62.5	<MQL	<MQL	<MQL	<MQL	<MQL
Stimulants and metabolites	Heroin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Amphetamine	>MQL	4,515.5	42.5	191.0	46.5	79.0	37.5	190.0	37.5	265.0	48.0	1,219.5	39.0	87.5
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	1.5	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	3.4	<MQL	8.6
	Anhydroecgonine methylester	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaethylene	1,293.5	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
UV filter	3-benzophenone	158.1	166.7	142.9	156.6	170.2	175.7	177.3	247.5	179.8	193.9	168.7	147.5	157.1	149.5
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S8. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP3

Micropollutant class	Micropollutants	WWTP3 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	142.5	<MQL	<MQL	<MQL	8.0	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	14.0	<MQL
	Dihydromorphine	<MQL	36.0	<MQL	34.6	<MQL	37.2	<MQL	38.1	<MQL	42.4	<MQL	25.3	<MQL	37.0
	Normorphine	<MQL	27.0	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	19.0	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	1.5	24.0	<MQL	15.5	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	435.8	2.7	324.8	2.9	553.1	174.5	572.4	<MQL	504.8	1.6	168.0	0.9	121.0	1.1
	N-desmethyltramadol	409.5	<MQL	365.5	<MQL	520.7	94.3	592.1	<MQL	270.7	<MQL	127.6	<MQL	139.3	<MQL
	O-desmethyltramadol	>MQL	<MQL	1,841.8	<MQL	2,282.0	1,978.0	>MQL	<MQL	1,827.9	89.4	1,627.4	<MQL	1,235.5	<MQL
Antibacterial/ antibiotics	Clarithromycin	34.0	<MQL	5.8	<MQL	5.2	<MQL	4.1	<MQL	4.1	<MQL	14.2	<MQL	5.5	<MQL
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	207.5	<MQL	79.5	<MQL	124.5	21.5	55.5	<MQL	34.0	<MQL	<MQL	<MQL	<MQL	<MQL
	Sulfamethoxazole	>MQL	9.8	342.9	8.4	>MQL	69.0	217.6	18.5	2,870.6	16.0	1,854.6	15.4	1,019.4	16.5
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	<MQL	46.2	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	52.6	<MQL	34.7	<MQL
	Norfluoxetine	6.6	<MQL	6.1	<MQL	5.9	<MQL	5.9	<MQL	<MQL	<MQL	5.9	<MQL	6.1	<MQL
	Sertraline	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Citalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	49.0	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-epileptic and metabolites	Carbamazepine	565.9	<MQL	950.4	1.0	1,178.1	404.5	1,181.7	1.5	931.4	<MQL	593.7	<MQL	372.7	<MQL
	Carbamazepine 10,11 epoxide	516.5	<MQL	493.0	<MQL	269.0	139.0	229.0	4.0	60.5	1.5	328.0	<MQL	182.0	1.0
	10,11 dihydro 10 hydroxycarbamazepine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	18.6	<MQL	17.6	<MQL	12.1	<MQL	<MQL	45.7	4.0	1.5	36.7	<MQL	31.7	<MQL
	Metoprolol	<MQL	<MQL	19.8	<MQL	<MQL	<MQL	<MQL	<MQL	52.8	0.5	<MQL	<MQL	<MQL	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Calcium channel blocker	Diltiazem	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S8. (continued)

Micropollutant class	Micropollutants	WWTP3 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anti-diabetes	Metformin	167.9	3.9	46.2	5.2	215.8	32.4	69.5	7.8	30.6	2.6	0.9	<MQL	28.1	<MQL
	Gliclazide	<MQL	<MQL	<MQL	24.8	520.2	<MQL	<MQL	24.8	<MQL	24.8	20.8	<MQL	20.3	<MQL
Drug precursor and metabolite	Ephedrine/pseudoephedrine	58.2	<MQL	<MQL	<MQL	76.6	<MQL	101.9	<MQL	20.9	<MQL	<MQL	<MQL	<MQL	<MQL
	Norephedrine	<MQL	<MQL	<MQL	18.1	<MQL	88.7	<MQL	<MQL	<MQL	24.2	<MQL	7.5	<MQL	21.2
H_2 receptor agonists	Ranitidine	<MQL	8.2	<MQL	10.9	<MQL	593.0	<MQL	22.8	<MQL	16.5	<MQL	7.2	<MQL	7.8
	Cimetidine	279.4	<MQL	85.5	<MQL	44.6	15.9	51.3	<MQL	412.5	<MQL	148.0	<MQL	73.7	<MQL
Nicotine and metabolites	Nicotine	82.5	36.5	51.5	35.5	82.0	43.5	91.5	17.5	91.0	35.5	68.0	44.0	47.5	39.0
	Caffeine	794.9	<MQL	557.6	<MQL	898.9	<MQL	434.0	<MQL	809.0	<MQL	445.2	<MQL	1,500.0	<MQL
	Cotinine	87.0	<MQL	77.0	<MQL	48.0	33.0	52.5	0.5	108.5	5.5	28.5	<MQL	27.5	<MQL
	1,7 dimethylxantine	>MQL	<MQL	1,332.9	<MQL	1,321.9	503.5	1,793.3	<MQL	3,014.1	22.5	<MQL	<MQL	<MQL	<MQL
Hypertension	Lisinopril	<MQL	<MQL	15.6	<MQL	67.6	36.3	91.4	<MQL	28.5	40.8	21.4	20.4	<MQL	<MQL
	Temazepam	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-inflammatory	Acetaminophen	>MQL	27.0	51.0	36.5	132.5	72.5	82.0	8.5	124.5	7.0	<MQL	57.0	<MQL	27.5
Stimulants and metabolites	Heroin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Amphetamine	<MQL	<MQL	<MQL	9.5	<MQL	95.0	<MQL	14.5	<MQL	15.0	<MQL	5.5	<MQL	35.5
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	528.8	<MQL
	Anhydroecgonine methylester	35.0	20.0	<MQL	<MQL	<MQL	20.0	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaethylene	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
UV filter	3-benzophenone	97.0	142.4	57.6	142.9	84.8	154.0	74.2	213.6	64.6	158.6	61.1	148.0	78.8	147.5
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S9. Concentrations (ng L^{-1}) of target compounds in influent and effluent samples at WWTP4

Micropollutant class	Micropollutants	WWTP4 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Dihydromorphine	<MQL	39.8	<MQL	20.1	<MQL	19.4	<MQL	19.2	<MQL	14.8	<MQL	18.3	<MQL	13.6
	Normorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	29.7	151.4	41.2	47.4	27.2	42.8	55.3	72.4	31.1	53.3	18.0	42.0	19.6	14.7
	N-desmethyltramadol	5.7	30.4	12.7	2.7	<MQL	244.1	3.5	23.9	53.7	722.7	4.5	22.9	<MQL	<MQL
	O-desmethyltramadol	32.1	143.8	160.5	41.7	41.9	103.0	112.8	85.0	55.3	198.7	42.5	1,833.4	62.5	60.5
Antibacterial/antibiotics	Clarithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	<MQL	<MQL	<MQL	<MQL	<MQL	4.0	<MQL	<MQL	<MQL	229.0	<MQL	<MQL	<MQL	<MQL
	Sulfamethoxazole	41.8	60.8	15.1	17.9	31.4	<MQL	42.1	46.8	16.3	112.1	23.6	101.2	50.7	22.7
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	31.1	<MQL	31.1	<MQL	15.5	<MQL	31.1	<MQL	<MQL	<MQL	31.1	<MQL	31.1	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	8.6	4.7	56.2	7.3	<MQL	<MQL	<MQL	<MQL	<MQL	147.2	37.8	<MQL	<MQL
	Norfluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Sertraline	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Citalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-epileptic and metabolites	Carbamazepine	1.0	5.1	13.9	2.1	0.5	66.8	0.5	<MQL	94.6	<MQL	<MQL	493.4	<MQL	113.6
	Carbamazepine 10,11 epoxide	<MQL	8.5	10.0	8.0	<MQL	25.5	<MQL	<MQL	23.0	7.5	4.0	89.0	<MQL	21.0
	10,11 dihydro 10 hydroxycarbamazepine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	<MQL	<MQL	<MQL	<MQL	166.8	<MQL	230.2	<MQL	<MQL	<MQL	257.3	<MQL	11.1	<MQL
	Metoprolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	3.6	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Calcium channel blocker	Diltiazem	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S9. (continued)

Micropollutant class	Micropollutants	WWTP4 (ng L^{-1})													
		Wednesday		Thursday		Friday		Saturday		Sunday		Monday		Tuesday	
		Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent	Influent	Effluent
Anti-diabetes	Metformin	302.5	159.7	1,417.1	279.6	413.8	396.1	20.7	313.3	9.1	568.7	907.9	503.1	<MQL	<MQL
	Gliclazide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Drug precursor and metabolite	Ephedrine/pseudoephedrine	<MQL	34.3	<MQL	13.7	<MQL	1.1	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norephedrine	52.9	324.9	187.0	29.0	125.3	78.8	49.1	48.8	32.1	137.2	137.5	88.7	24.9	175.8
H_2 receptor agonists	Ranitidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cimetidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	51.3	<MQL	<MQL
Nicotine and metabolites	Nicotine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Caffeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cotinine	31.0	86.0	49.5	32.0	115.5	152.0	112.5	91.5	43.0	175.5	92.0	61.0	63.5	67.5
	1,7 dimethylxantine	>MQL	>MQL	>MQL	6,624.3	4,523.8	582.8	7,835.6	5,278.0	373.5	906.5	6,647.2	2,888.5	4,237.2	582.8
Hypertension	Lisinopril	193.9	72.0	159.3	151.5	127.7	92.1	80.8	112.4	60.8	51.9	133.4	108.0	141.3	53.7
	Temazepam	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-inflammatory	Acetaminophen	3,847.0	9,169.5	147.5	36.5	153.0	44.0	52.5	76.5	28.5	14.0	2,528.0	<MQL	<MQL	<MQL
	Amphetamine	135.5	221.0	312.5	32.0	159.0	74.0	8.5	29.5	35.0	98.0	82.0	78.0	64.0	54.0
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	30.0	194.0	77.0	10.5	46.0	30.5	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	<MQL	167.0	145.2	104.5	389.1	199.8	730.1	1,841.6	142.8	<MQL	1,326.0	327.5	602.3	917.3
	Anhydroecgonine methylester	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaethylene	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	45.5	<MQL	10.5	<MQL	83.0	<MQL	<MQL	<MQL	<MQL	<MQL	91.0	<MQL	<MQL	15.5
UV filter	3-benzophenone	161.6	73.7	143.9	153.0	185.8	242.9	171.2	309.1	151.5	166.7	327.8	162.6	154.0	166.7
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S10. Concentrations (ng L^{-1}) of target compounds in influent samples at SDP1

Micropollutant class	Micropollutants	SDP1 (ng L^{-1})						
		Wednesday	Thursday	Friday	Saturday	Sunday	Monday	Tuesday
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	<MQL	<MQL	209.0	155.5	1,229.5	<MQL	<MQL
	Dihydromorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Normorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	160.1	>MQL	>MQL	24.1	<MQL	155.8	82.3
	N-desmethyltramadol	146.0	>MQL	320.9	34.1	<MQL	112.9	192.1
	O-desmethyltramadol	>MQL	>MQL	>MQL	>MQL	>MQL	>MQL	>MQL
Antibacterial/antibiotics	Clarithromycin	<MQL	<MQL	<MQL	4.1	169.9	27.6	37.5
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	738.5	1042.5	412	580	1670.5	259	721
	Sulfamethoxazole	19.1	178.3	>MQL	404.3	398.4	3,202.6	2,708.0
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norfluoxetine	<MQL	8.3	<MQL	<MQL	33.3	<MQL	68.3
	Sertraline	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Citalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-epileptic and metabolites	Carbamazepine	454.9	>MQL	2,121.8	138.8	256.0	173.7	605.5
	Carbamazepine 10,11 epoxide	825.0	3,850.5	>MQL	234.5	339.0	622.0	1,012.5
	10,11 dihydro 10 hydroxycarbamazepine	<MQL	<MQL	<MQL	<MQL	<MQL	981.5	<MQL
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Metoprolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	30.5
Calcium channel blocker	Diltiazem	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-diabetes	Metformin	69.5	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Gliclazide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	22.9
Drug precursor and metabolite	Ephedrine/pseudoephedrine	<MQL	355.4	67.0	10.2	1,361.1	<MQL	19.2
	Norephedrine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
H_2 receptor agonists	Ranitidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cimetidine	>MQL	>MQL	2,953.4	799.8	>MQL	2,643.5	3,537.2
Nicotine and metabolites	Nicotine	36.5	194.5	1,091.0	507.0	>MQL	80.5	108.0
	Caffeine	122.2	1,852.5	667.1	581.5	<MQL	282.3	497.2
	Cotinine	<MQL	241.0	2,817.0	960.0	>MQL	21.0	72.5
	1,7 dimethylxantine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Hypertension	Lisinopril	<MQL	2,282.7	1,279.1	<MQL	<MQL	604.5	699.3
	Temazepam	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-inflammatory	Acetaminophen	134.0	911.0	252.0	370.0	1,440.5	210.5	379.5
Stimulants and metabolites	Heroin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Amphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	<MQL	<MQL	<MQL	<MQL	<MQL	470.0	<MQL
	Anhydroecgonine methylester	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaethylene	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
UV filter	3-benzophenone	74.7	32.8	106.1	70.2	<MQL	67.2	66.2
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S11. Concentrations (ng L^{-1}) of target compounds in influent samples at SDP2

Micropollutant class	Micropollutants	SDP2 (ng L^{-1})						
		Wednesday	Thursday	Friday	Saturday	Sunday	Monday	Tuesday
Anaesthetic and metabolite	Ketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norketamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Analgesics and metabolites	Morphine	<MQL	<MQL	309.0	131.0	<MQL	<MQL	<MQL
	Dihydromorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Normorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methadone	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Codeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Dihydrocodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norcodeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tramadol	>MQL	44.5	153.4	76.2	43.6	267.8	17.2
	N-desmethyltramadol	221.4	462.0	373.2	145.5	190.3	859.0	159.5
	O-desmethyltramadol	>MQL	>MQL	>MQL	>MQL	>MQL	>MQL	>MQL
Antibacterial/antibiotics	Clarithromycin	4.1	<MQL	<MQL	<MQL	243.3	126.6	2.9
	Azithromycin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Trimethoprim	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Sulfamethoxazole	2,612.1	2,046.1	1,436.9	1,048.3	130.4	<MQL	72.9
Anti-cancer	Azathioprine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Methotrexate	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Tamoxifen	16.0	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Ifosfamide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-depressants and metabolites	Fluoxetine	<MQL	<MQL	<MQL	8.0	<MQL	<MQL	<MQL
	Norfluoxetine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Sertraline	705.5	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Citalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Desmethylcitalopram	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Venlafaxine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-epileptic and metabolites	Carbamazepine	389.1	1,613.5	>MQL	258.5	298.6	391.7	442.6
	Carbamazepine 10,11 epoxide	330.5	2,982.0	7,339.0	200.5	126.0	31.5	151.5
	10,11 dihydro 10 hydroxycarbamazepine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-psychotic	Quetiapine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Antihistamine	Cetirizine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Beta-blocker	Atenolol	>MQL	<MQL	1,197.5	419.6	118.1	<MQL	<MQL
	Metoprolol	<MQL	<MQL	54.8	<MQL	<MQL	<MQL	<MQL
	Propranolol	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	26.1
Calcium channel blocker	Diltiazem	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Cough suppressant	Pholcodine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
Anti-diabetes	Metformin	132.9	114.4	<MQL	<MQL	6.5	<MQL	<MQL
	Gliclazide	700.5	<MQL	<MQL	<MQL	159.0	<MQL	<MQL
Drug precursor and metabolite	Ephedrine/pseudoephedrine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Norephedrine	24.2	520.1	603.8	311.3	<MQL	150.2	<MQL
H_2 receptor agonists	Ranitidine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cimetidine	3,119.0	3,508.7	>MQL	>MQL	>MQL	3,386.6	>MQL
Nicotine and metabolites	Nicotine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Caffeine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cotinine	530.0	16.5	5,664.5	2,251.5	333.5	177.5	<MQL
	1,7 dimethylxantine	853.6	2,297.9	1,329.0	1,661.4	<MQL	<MQL	<MQL
Hypertension	Lisinopril	121.9	138.3	547.9	295.9	192.9	334.2	37.4
	Temazepam	<MQL	<MQL	109.0	90.5	93.0	<MQL	124.0
Anti-inflammatory	Acetaminophen	551.0	337.0	365.5	298.0	203.5	283.5	<MQL
Stimulants and metabolites	Heroin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Amphetamine	94.5	179.0	284.5	132.5	28.0	<MQL	57.0
	Methamphetamine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDMA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	MDA	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	6-acetylmorphine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Benzoylecgonine	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Anhydroecgonine methylester	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Cocaethylene	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
	Mephedrone	54.5	<MQL	423.0	241.0	<MQL	<MQL	<MQL
UV filter	3-benzophenone	>MQL	145.4	157.6	170.7	164.6	158.1	149.0
Veterinary	Tylosin	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL
X-ray contrast media	Iopromide	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL	<MQL

Table S12. Percentage intra and inter-site variance of target compounds in influent samples

Micropollutant class	Micropollutants	%Intra-site variance						%Inter-site variance		
		WWTP1	WWTP2	WWTP3	WWTP4	SDP1	SDP2	STDev	Mean	Variance
Anaesthetic and metabolite	Ketamine	-	-	-	-	-	-	-	-	-
	Norketamine	-	-	-	-	-	-	-	-	-
Analgesics and metabolites	Morphine	138	-	225	-	198	189	101	125	81
	Dihydromorphine	-	-	-	-	-	-	-	-	-
	Normorphine	-	-	-	-	-	-	-	-	-
	Methadone	-	-	-	-	-	-	-	-	-
	Codeine	151	-	128	-	-	-	72	47	156
	Dihydrocodeine	-	-	-	-	-	-	-	-	-
	Norcodeine	-	-	-	-	-	-	-	-	-
	Tramadol	100	110	48	41	121	110	35	88	39
	N-desmethyltramadol	58	140	52	167	102	74	47	99	47
	O-desmethyltramadol	42	144	73	65	-	-	44	81	54
Antibacterial/antibiotics	Clarithromycin	74	-	105	-	181	178	81	90	90
	Azithromycin	-	-	-	-	-	-	-	-	-
	Trimethoprim	61	216	104	-	60	-	80	74	109
	Sulfamethoxazole	120	176	122	44	138	99	44	116	38
Anti-cancer	Azathioprine	-	-	-	-	-	-	-	-	-
	Methotrexate	-	-	-	-	-	-	-	-	-
	Tamoxifen	-	55	-	50	-	265	103	62	167
	Ifosfamide	-	-	-	-	-	-	-	-	-
Anti-depressants and metabolites	Fluoxetine	-	-	176	242	-	265	128	114	113
	Norfluoxetine	94	-	44	-	167	-	68	51	134
	Sertraline	-	265	-	-	-	265	137	88	155
	Citalopram	-	-	265	-	-	-	-	44	-
	Desmethylcitalopram	-	-	-	-	-	-	-	-	-
	Venlafaxine	-	-	-	-	-	-	-	-	-
Anti-epileptic and metabolites	Carbamazepine	159	-	38	222	136	107	81	111	73
	Carbamazepine 10,11 epoxide	166	-	55	164	133	172	71	115	62
	10,11 dihydro 10 hydroxycarbamazepine	238	265	-	-	265	-	140	128	110
Anti-psychotic	Quetiapine	-	-	-	-	-	-	-	-	-
Antihistamine	Cetirizine	-	-	-	-	-	-	-	-	-
Beta-blocker	Atenolol	83	265	78	124	-	180	92	122	75
	Metoprolol	75	210	194	265	-	265	108	168	64
	Propranolol	-	-	-	-	265	265	137	88	155
Calcium channel blocker	Diltiazem	-	-	-	-	-	-	-	-	-
Cough suppressant	Pholcodine	-	-	-	-	-	-	-	-	-
Anti-diabetes	Metformin	97	207	101	123	265	165	66	160	42
	Gliclazide	111	-	242	-	265	213	119	139	86
Drug precursor and metabolite	Ephedrine/pseudoephedrine	125	-	114	-	194	-	84	72	116
	Norephedrine	-	219	-	72	-	110	88	67	131
H_2 receptor agonists	Ranitidine	-	-	-	-	-	-	-	-	-
	Cimetidine	139	-	89	-	111	125	62	77	80
Nicotine and metabolites	Nicotine	155	-	25	-	136	-	71	105	67
	Caffeine	135	-	47	-	108	-	45	97	46
	Cotinine	91	161	50	47	177	163	59	115	52
	1,7 dimethylxantine	189	149	107	97	-	106	63	108	59
Hypertension	Lisinopril	49	155	108	35	122	72	46	90	51
	Temazepam	-	-	-	-	-	95	-	16	-
Anti-inflammatory	Acetaminophen	265	244	105	162	90	57	85	154	55
Stimulants and metabolites	Heroin	-	-	-	-	-	-	-	-	-
	Amphetamine	-	46	-	90	-	88	44	37	118
	Methamphetamine	-	-	-	-	-	-	-	-	-
	MDMA	265	265	-	-	-	-	137	88	155
	MDA	-	-	-	140	-	-	-	23	-
	6-acetylmorphine	-	-	-	-	-	-	-	-	-
	Cocaine	-	-	-	-	-	-	-	-	-
	Benzoylecgonine	90	-	265	96	265	-	120	119	101
	Anhydroecgonine methylester	188	-	265	-	-	-	119	76	158
	Cocaethylene	-	265	-	-	-	-	-	44	-
	Mephedrone	-	-	-	123	-	162	75	48	157
UV filter	3-benzophenone	40	8	19	35	57	45	18	34	52
Veterinary	Tylosin	-	-	-	-	-	-	-	-	-
X-ray contrast media	Iopromide	-	-	-	-	-	-	-	-	-

Table S13. Maximum Environmental Concentrations (MECs), Predicted No-Effect Concentrations (PNECs) and Risk Quotients (RQs) for target compounds

Micropollutant class	Micropollutants	PNEC (µg L^{-1})	Effluent		Surface Water	
			MEC (ng L^{-1})	RQ	MEC (ng L^{-1})	RQ
Anaesthetic and metabolite	Ketamine	-	<MQL	-	<MQL	-
	Norketamine	-	<MQL	-	<MQL	-
Analgesics and metabolites	Morphine	-	<MQL	-	<MQL	-
	Dihydromorphine	-	49.2	-	33.9	-
	Normorphine	-	27	-	110.5	-
	Methadone	-	<MQL	-	<MQL	-
	Codeine	1.280[a]	1.5	0.001	27.3	0.021
	Dihydrocodeine	-	<MQL	-	<MQL	-
	Norcodeine	-	<MQL	-	<MQL	-
	Tramadol	-	542.4	-	274	-
	N-desmethyltramadol	-	722.7	-	108.7	-
	O-desmethyltramadol	-	1978	-	1056.9	-
Antibacterial/antibiotics	Clarithromycin	0.050[b]	<MQL	-	<MQL	-
	Azithromycin	-	<MQL	-	<MQL	-
	Trimethoprim	4.800[a]	1043.5	0.217	57.5	0.012
	Sulfamethoxazole	0.146[b]	1,951.60	13.367	1685.2	11.542
Anti-cancer	Azathioprine	-	<MQL	-	<MQL	-
	Methotrexate	-	<MQL	-	<MQL	-
	Tamoxifen	0.200[c]	46.2	0.231	22.9	0.115
	Ifosfamide	-	<MQL	-	<MQL	-
Anti-depressants and metabolites	Fluoxetine	4.650[d]	56.2	0.012	49	0.011
	Norfluoxetine	-	<MQL	-	<MQL	-
	Sertraline	-	557	-	0.3	-
	Citalopram	-	<MQL	-	<MQL	-
	Desmethylcitalopram	-	<MQL	-	<MQL	-
	Venlafaxine	-	1.2	-	<MQL	-
Anti-epileptic and metabolites	Carbamazepine	0.395[a]	493.4	1.249	29.8	0.075
	Carbamazepine 10,11 epoxide	-	139	-	31.8	-
	10,11 dihydro 10 hydroxycarbamazepine	-	281	-	<MQL	-
Anti-psychotic	Quetiapine	-	<MQL	-	<MQL	-
Antihistamine	Cetirizine	-	<MQL	-	<MQL	-
Beta-blocker	Atenolol	0.445[a]	1418.1	3.187	80.4	0.181
	Metoprolol	7.300[a]	24.4	0.003	<MQL	-
	Propranolol	0.094[a]	<MQL	-	<MQL	-
Calcium channel blocker	Diltiazem	8.200[b]	878.7	0.107	<MQL	-
Cough suppressant	Pholcodine	-	<MQL	-	<MQL	-
Anti-diabetes	Metformin	-	568.7	-	8.6	-
	Gliclazide	1.335[d]	972.5	0.728	24.6	0.018
Drug precursor and metabolite	Ephedrine/pseudoephedrine	-	39.3	-	9.9	-
	Norephedrine	-	576.1	-	45.4	-
H_2 receptor agonists	Ranitidine	6.600[a]	593	0.09	139.9	0.021
	Cimetidine	271.300[b]	51.3	0.0002	160.7	0.001
Nicotine and metabolites	Nicotine	-	64	-	24.3	-
	Caffeine	-	<MQL	-	<MQL	-
	Cotinine	-	234	-	26.5	-
	1,7 dimethylxantine	-	6,624.30	-	465.6	-
Hypertension	Lisinopril	-	151.5	-	10.2	-
	Temazepam	-	<MQL	-	<MQL	-
Anti-inflammatory	Acetaminophen	0.253[a]	9169.5	36.243	9.8	0.039
Stimulants and metabolites	Heroin	-	<MQL	-	<MQL	-
	Amphetamine	-	4515.5	-	26.8	-
	Methamphetamine	-	<MQL	-	1.8	-
	MDMA	-	<MQL	-	<MQL	-
	MDA	-	194	-	<MQL	-
	6-acetylmorphine	-	<MQL	-	<MQL	-
	Cocaine	-	<MQL	-	<MQL	-
	Benzoylecgonine	-	1841.6	-	<MQL	-
	Anhydroecgonine methylester	-	42	-	20	-
	Cocaethylene	-	<MQL	-	<MQL	-
	Mephedrone	-	15.5	-	<MQL	-
UV filter	3-benzophenone	-	309.1	-	<MQL	-
Veterinary	Tylosin	-	<MQL	-	<MQL	-
X-ray contrast media	Iopromide	-	<MQL	-	<MQL	-

References

1 K. Proctor, B. Petrie, R. Barden, T. Arnot and B. Kasprzyk-hordern, *Anal. Bioanal. Chem.*, 2019, **411**, 7061–7086.