

Supplementary Material

A thorough analysis of the occurrence, removal and environmental risks of organic micropollutants in a full-scale hybrid membrane bioreactor fed by hospital wastewater

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1. Materials and methods

Text S1. Description of the wastewater treatment plant under investigation.

The wastewater treatment plant (WWTP) under study treats the effluent produced in the local large hospital and the urban wastewater of the surrounding area (Figure 1 in the manuscript). The hospital includes 900 beds and several departments (anesthetics, dermatology, endocrinology, forensics, gastroenterology, genetics, geriatrics, gynecology, hematology, infectious disease, neurology, nuclear medicine, oncology, pediatrics, traumatology and surgery) and a large set of medical services (clinical analysis, dialysis, pharmacology and radiology). It opened in 2012 when it was relocated from the center of the city (Ferrara) to the outskirts. The hospital wastewater (HWW) is directly discharged into a separate sewer pipe, and once it reaches the WWTP, it is cotreated with the wastewater coming from the catchment area, which includes households and small businesses. The sewer also collects rainwater that can strongly increase the influent flow rate to the plant. This second contribution is called urban wastewater (UWW).

The core treatment of the WWTP is an MBR equipped with submerged hollow fiber UF membranes (Koch Separation Solution, 8 modules, 500 m²/module, nominal pore size of 0.05 μm, maximum permeate flux of 25 L/(m²·h¹), leading to a maximum hourly flow rate of 100 m³/h according to the nominal surface flow rate of the installed membranes (Figure 1). In particular, the WWTP consists of a pre-treatment (screening and degritting), the MBR, which includes P removal (100 m³), denitrification (250 m³), nitrification (350 m³) and membrane filtration (72 m³), followed by a tertiary treatment. The average hydraulic retention time (HRT) is 24 hours. The sludge recycled in the MBR (denitrification tank) is approximately 2100 m³/d. The excess sludge, which is withdrawn from the denitrification tank, accounts for between 0 – 43.6 m³/d (average of 16.3 m³/d) depending on the food/microorganism ratio and the bioreactor performance. The mixed liquor concentration in the nitrification tank is on average 6.7 ± 1.3 g/L with an organic loading rate of 0.039 gBOD₅/(gVSS·d), which is characteristic of an extended aeration plant. The sludge retention time (SRT) is between 24 and 40 days (on average 27 days). The average operating temperature is 23 °C and the pH of the final effluent is 7.1. Oxygen concentration in the nitrification tank is maintained at 1.5 ± 0.3 mg/L. Further details of the plant are available in Verlicchi et al., (2010).

The tertiary treatment consists of UV disinfection (irradiation of 100 mJ/cm², exposure time of about 4 – 7 s) of the permeate before its release into a canal belonging to the local surface water network which is used for irrigation: The final WWTP effluent (average flow of 0.011 m³/s) is therefore indirectly reused for irrigation, and is diluted by approximately 50% once it is discharged into the water body (average flow of 0.01 m³/s).

The WWTP also includes an accumulation tank (180 m³) that dampens the variations in the influent flow rate due to rain events and guarantees a correct and safe working of the treatment train, in particular the membranes. The accumulation tank is installed before the pre-treatments and stores any excess wastewater arriving at the WWTP. Then, the collected wastewater is gradually sent back to the UWW line. In this way, the effect of intense rain events is controlled and mitigated, and a very stable influent flow rate is guaranteed. However, the climatic conditions during the monitoring and experimental periods of this study were predominantly stable, with very few, light rain events.

Text S2. Experimental procedure to maintain the PAC concentration stable inside the MBR.

The PAC concentration was maintained stable IN THE BIOREACTOR by periodical and controlled additions of fresh PAC following this procedure. On the first day of the second (0.1PAC) and the third (0.2PAC) campaigns, a fixed amount of PAC (70 and 150 kg, respectively) was dispersed into the MBR tanks by means of 10 kg-water soluble bags until the desired PAC concentration was reached. Then, PAC additions were made to counterbalance PAC losses associated with the excess sludge withdrawn from the regularly-monitored MBR. By doing so, the PAC concentration varied by less than 10% from the nominal concentration. Average PAC concentrations were therefore 0.10 ± 0.01 g/L for 0.1PAC campaign and 0.20 ± 0.02 g/L for 0.2PAC campaign. The daily amount of PAC lost (wasted) from the system (PAC_w , kg/d) was estimated according to eq. 1:

$$PAC_w = PAC_{MBR} \cdot WAS \quad \text{eq. 1}$$

where PAC_{MBR} is the PAC concentration inside the MBR (kg/m^3) and WAS the daily volume flow rate of the excess sludge removed from the system (m^3/d). A mass balance of the PAC was carried out every day in order to calculate the residual concentration of PAC inside the MBR (PAC_{MBR}) after the withdrawal of excess sludge containing the PAC. This updated value of PAC_{MBR} was compared with the lower limit of acceptability of the specific campaign (0.09 g/L or 0.018 g/L) thus monitoring its decrement. In this way, it was clear in which day fresh PAC had to be added in order to maintain its concentration within the desired interval. The amount added corresponds to the PAC quantity necessary to increase its concentration inside the MBR up to the maximum value (upper limit of acceptability) of 0.11 g/L or 0.22 g/L depending on the campaign. In order to guarantee a rapid mixing and a homogenous PAC concentration in the MBR, the aeration was stopped in the nitrification before PAC addition and immediately switched on soon afterwards. Moreover, samples of the permeate were taken at least one day later. Due to technical reasons and time restrictions, it was not possible to prepare a solution (slurry) with the fresh PAC to be fed to the MBR when necessary.

2. Analyzed contaminants

Table S1. Main physicochemical properties and Predicted No-Effect Concentration (PNEC) in freshwater of the target OMPs analyzed. The compound classes were attributed according to the Anatomic Therapeutic Chemical (ATC) classification. The transformation products are written in *italics*. Data on (predicted) physicochemical properties were obtained from CAS Scifinderⁿ (<https://scifinder.cas.org>) and the PNEC values from the NORMAN database (<https://www.norman-network.com/nds/ecotox/>). The charge was obtained from pK_a values by calculating the molecular/ionic species at pH 7 (see **text S1**).

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge pH = 7
Analgesics/anti-inflammatories	<i>4-Acetylaminoantipyrine</i>	83-15-8	-	C13H15N3O2	100	245.28	12.84±0.20	1.07±0.65	-0.88	-0.88	-0.88	-0.885±0.282	neutral
Analgesics/anti-inflammatories	<i>4-FormylAminoAntipyrine</i>	1672-58-8	-	C12H13N3O2	1000	231.25	12.72±0.20	1.07±0.65	-0.06	-0.06	-0.06	-0.055±0.268	neutral
Analgesics/anti-inflammatories	<i>6-Acetylmorphine</i>	2784-73-8	-	C19H21NO4	5.19	327.38	9.41±0.40	8.03±0.40	-0.3	0.62	1.27	1.562±0.520	cationic
Analgesics/anti-inflammatories	Acetaminophen	103-90-2	N02BE01	C8H9NO2	134	151.16	9.86±0.13	1.72±0.50	0.48	0.47	0.47	0.475±0.210	neutral
Analgesics/anti-inflammatories	<i>Acetylcodeine</i>	6703-27-1	-	C20H23NO4	1.1	341.4	-	8.02±0.40	0.1	1.03	1.77	2.084±0.539	cationic
Analgesics/anti-inflammatories	Acetylsalicylic acid	50-78-2	N02BA01	C9H8O4	18.5	180.16	3.48±0.10	-	-1.03	-1.6	-1.73	1.399±0.226	anion
Analgesics/anti-inflammatories	Alfentanil	71195-58-9	N01AH02	C21H32N6O3	0.18	416.52	-	7.82±0.20	0.67	1.55	2.04	2.160±0.606	cationic
Analgesics/anti-inflammatories	Aminopyrine	58-15-1	N02BB03	C13H17N3O	17.6	231.29	-	4.50±0.65	0.84	0.85	0.85	0.854±0.283	neutral
Analgesics/anti-inflammatories	Betamethasone 17,21-dipropionate	5593-20-4	A07EA04	C28H37FO7	2.89	504.59	12.87±0.70	-	3.67	3.67	3.67	3.666±0.659	neutral
Analgesics/anti-inflammatories	Buprenorphine	52485-79-7	N02AE01	C29H41NO4	0.23	467.64	9.47±0.60	8.31±0.60	0.57	1.49	2.32	2.826±0.595	cationic
Analgesics/anti-inflammatories	<i>Buprenorphine glucuronide</i>	101224-22-0	-	C35H49NO10	0.14	643.77	2.77±0.70	8.29±0.60	-2.1	-2.12	-2.26	0.397±0.712	zwitterionic

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{ow}$ pH = 6	$\log D_{ow}$ pH = 7	$\log D_{ow}$ pH = 8	$\log K_{ow}$	Charge pH = 7
Analgesics/anti-inflammatories	Carisoprodol	78-44-4	M03BA02	C12H24N2O4	12.5	260.33	12.49±0.46	-1.40±0.70	2.1	2.1	2.1	2.099±0.348	neutral
Analgesics/anti-inflammatories	Codeine	76-57-3	R05DA04	C18H21NO3	7.19	299.36	13.40±0.20	8.23±0.40	-0.83	0.1	0.93	1.394±0.550	cationic
Analgesics/anti-inflammatories	Dextromethorphan	125-71-3	R05DA09	C18H25NO	3.20	271.4	-	9.13±0.20	1.08	1.8	2.74	3.893±0.412	cationic
Analgesics/anti-inflammatories	Dextropropoxyphene	469-62-5	N02AC04	C22H29NO2	0.45	339.47	-	9.19±0.28	1.25	1.95	2.88	4.097±0.349	cationic
Analgesics/anti-inflammatories	Diclofenac	15307-79-6	M01AB05	C14H11Cl2NO2	0.05	296.15	4.18±0.10	-2.26±0.50	2.72	1.77	1.06	4.548±0.572	anion
Analgesics/anti-inflammatories	Etodolac	41340-25-4	M01AB08	C17H21NO3	1.43	287.35	4.31±0.10	-1.96±0.40	1.75	0.79	0.02	3.424±0.421	anion
Analgesics/anti-inflammatories	Fentanyl	437-38-7	N01AH01	C22H28N2O	0.17	336.47	-	8.92±0.20	1.33	2.23	3.11	3.683±0.357	cationic
Analgesics/anti-inflammatories	Hydrocodone	125-29-1	R05DA03	C18H21NO3	3.46	299.36	-	8.52±0.20	0.15	1.05	1.94	2.567±0.536	cationic
Analgesics/anti-inflammatories	Hydromorphone	466-99-9	N02AA03	C17H19NO3	3.64	285.34	9.34±0.20	8.53±0.20	-0.19	0.72	1.53	2.127±0.518	cationic
Analgesics/anti-inflammatories	Ibuprofen	15687-27-1	M01AE01	C13H18O2	0.01	206.28	4.41±0.10	-	1.91	0.94	0.14	3.502±0.227	anion
Analgesics/anti-inflammatories	Ketoprofen	22071-15-4	M01AE03	C16H14O3	2.1	254.28	4.23±0.10	-	1.14	0.19	-0.55	2.911±0.331	anion
Analgesics/anti-inflammatories	Lidocaine	137-58-6	N01BB02	C14H22N2O	4.67	234.34	14.23±0.70	7.96±0.10	0.44	1.36	2	2.196±0.368	cationic
Analgesics/anti-inflammatories	Meloxicam	71125-38-7	M01AC06	C14H13N3O4S2	0.7	351.4	4.50±1.00	3.18±0.10	1.15	0.17	-0.78	2.662±0.848	anion
Analgesics/anti-inflammatories	Morphine	57-27-2	N02AA01	C17H19NO3	5.38	285.34	9.48±0.40	8.25±0.40	-1.23	-0.3	0.45	0.872±0.532	cationic
Analgesics/anti-inflammatories	<i>Morphine-6-β-D-glucuronide</i>	20290-10-2	-	C23H27NO9	2.16	461.46	2.79±0.70	8.09±0.40	-1.82	-1.86	-2.15	0.685±0.750	zwitterionic

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{ow}$ pH = 6	$\log D_{ow}$ pH = 7	$\log D_{ow}$ pH = 8	$\log K_{ow}$	Charge pH = 7
Analgesics/anti-inflammatories	Naproxen	22204-53-1	M01AE02	C14H14O3	1.82	230.26	4.84±0.30	-	1.69	1.69	-0.18	2.876±0.239	anion
Analgesics/anti-inflammatories	<i>Norfentanyl</i>	1609-66-1	-	C14H20N2O	73	232.32	-	9.81±0.10	-1.3	-0.78	0.12	1.667±0.361	cationic
Analgesics/anti-inflammatories	<i>Norpethidine</i>	77-17-8	-	C14H19NO2	29.2	233.31	-	9.58±0.10	-1.34	-0.82	0.06	1.639±0.568	cationic
Analgesics/anti-inflammatories	<i>Norpropoxyphene</i>	3376-94-1	-	C21H27NO2	4.35	325.45	-	10.08±0.20	0.68	0.95	1.69	3.737±0.525	cationic
Analgesics/anti-inflammatories	<i>O-Desmethyltramadol</i>	73986-53-5	-	C15H23NO2	10.1	249.35	10.00±0.10	9.61±0.28	-1.16	-0.59	0.31	1.779±0.266	cationic
Analgesics/anti-inflammatories	Oxycodone	76-42-6	N02AA05	C18H21NO4	8.04	315.36	13.13±0.20	7.57±0.40	-0.08	0.83	1.42	1.588±0.572	cationic
Analgesics/anti-inflammatories	Oxymorphone	76-41-5	N02AA11	C17H19NO4	4.58	301.34	9.17±0.40	7.58±0.40	-0.41	0.48	0.96	1.148±0.555	cationic
Analgesics/anti-inflammatories	Pentazocine	359-83-1	N02AD01	C19H27NO	0.51	285.42	10.10±0.60	8.94±0.60	1.44	2.23	3.16	4.147±0.388	cationic
Analgesics/anti-inflammatories	Pethidine	57-42-1	N02AB02	C15H21NO2	19.7	247.33	-	7.84±0.10	0.37	1.29	1.96	2.185±0.360	cationic
Analgesics/anti-inflammatories	Phenylbutazone	50-33-9	M01AA01	C19H20N2O2	1.09	308.38	4.64±0.10	-0.29±0.40	2.03	1.25	0.93	3.376±0.263	anion
Analgesics/anti-inflammatories	Procaine	59-46-1	N01BA02	C13H20N2O2	3.87	236.31	-	9.24±0.25	-0.61	0.05	0.98	2.256±0.523	cationic
Analgesics/anti-inflammatories	Tolfenamic acid	13710-19-5	M01AG02	C14H12ClNO2	0.19	261.7	3.66±0.36	-2.48±0.50	3.19	2.53	2.34	5.468±0.431	anion
Analgesics/anti-inflammatories	Tramadol	27203-92-5	N02AX02	C16H25NO2	8.65	263.38	14.47±0.40	9.61±0.28	-0.63	-0.06	0.85	2.316±0.273	cationic
Antiarrhythmic agents	Amiodarone	1951-25-3	C01BD01	C25H29I2NO3	0.0011	645.31	-	9.37±0.25	4.9	5.51	6.43	7.815±0.731	cationic
Antiarrhythmic agents	Digitoxin	71-63-6	C01AA04	C41H64O13	0.88	764.94	13.50±0.70	-	2.74	2.74	2.74	2.740±0.779	neutral

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{\text{ow}}$ pH = 6	$\log D_{\text{ow}}$ pH = 7	$\log D_{\text{ow}}$ pH = 8	$\log K_{\text{ow}}$	Charge pH = 7
Antiarrhythmic agents	Propafenone	54063-53-5	C01BC03	C21H27NO3	0.85	341.44	13.82±0.20	9.31±0.10	0.42	1.02	1.93	3.351±0.300	cationic
Antiarrhythmic agents	Strophanthidin	66-28-4	--	C23H32O6	57.7	404.5	13.92±0.70		0.66	0.66	0.66	0.663±0.570	neutral
Antiarrhythmic agents	Strophanthin	11005-63-3	--	C36H54O14	14.3	--	--	--	--	--	--	0.55	-
Antibiotics	2-NP-AOZ	19687-73-1	--	C10H9N3O4	3.2	235.2	-	-1.38±0.20	0.26	0.26	0.26	0.263±0.317	neutral
Antibiotics	Amoxicillin	61336-70-7	J01CA04	C16H19N3O5S	0.078	365.41	2.44±0.50	7.14±0.10	-1.69	-2.08	-2.64	0.883±0.301	zwitterionic
Antibiotics	Azithromycin	83905-01-5	J01FA10	C38H72N2O12	0.019	748.99	13.28±0.70	8.59±0.70	-1.37	-0.06	1.59	2.582±0.853	cationic
Antibiotics	Cinoxacin	28657-80-9	J01MB06	C12H10N2O5	3.69	262.22	4.33±0.20	-	-3.12	-3.12	-3.26	0.489±0.742	anion
Antibiotics	Ciprofloxacin	85721-33-1	J01MA02	C17H18FN3O3	0.089	331.34	6.43±0.41	8.68±0.10	-0.75	-0.33	-0.35	1.625±0.831	zwitterionic
Antibiotics	Clarithromycin	81103-11-9	J01FA09	C38H69NO13	0.12	747.95	13.08±0.70	8.16±0.70	0.78	1.71	2.47	2.805±0.845	cationic
Antibiotics	Doxycycline	24390-14-5	J01AA02	C22H24N2O8	0.46	444.44	4.50±1.00	10.84±0.70	-0.75	-0.92	-1.47	1.777±0.760	zwitterionic
Antibiotics	Enoxacin	74011-58-8	J01MA04	C15H17FN4O3	2.51	320.32	6.04±0.70	8.19±0.10	-0.71	-0.6	-0.76	1.589±0.955	zwitterionic
Antibiotics	Erythromycin	114-07-8	J01FA01	C37H67NO13	0.2	733.93	13.09±0.70	8.16±0.70	-0.12	0.81	1.58	1.909±0.841	cationic
Antibiotics	Flumequine	42835-25-6	J01MB07	C14H12FN3O3	1.5	261.25	5.70±0.40	-1.98±0.60	-0.05	-1	-1.94	0.882±0.669	anion
Antibiotics	Furazolidon	67-45-8	G01AX06	C8H7N3O5	2.5	225.16	-	-1.98±0.20	-0.05	-0.05	-0.05	-0.050±0.342	neutral
Antibiotics	Lomefloxacin	98079-51-7	J01MA07	C17H19FN3O3	0.83	351.35	-0.25±0.20	8.57±0.40	0	0.06	-0.07	2.459±0.934	zwitterionic
Antibiotics	Metronidazole	443-48-1	J01XD01	C6H9N3O3	33.1	171.15	14.44±0.10	2.58±0.34	-0.14	-0.14	-0.14	-0.135±0.301	neutral
Antibiotics	Minocycline	13614-98-7	J01AA08	C23H27N3O7	0.041	457.48	4.50±1.00	11.06±0.70	-0.44	-0.51	-0.99	2.124±0.757	zwitterionic
Antibiotics	Nalidixic acid	389-08-2	J01MB02	C12H12N2O3	4.66	232.24	3.45±0.20	6.12±0.70	-0.66	-1.2	-2.1	0.025±0.768	anion
Antibiotics	Norfloxacin	70458-96-7	J01MA06	C16H18FN3O3	0.78	319.33	0.16±0.20	8.68±0.10	-0.74	-0.65	-0.75	1.744±0.831	zwitterionic
Antibiotics	Ofloxacin	82419-36-1	J01MA01	C18H20FN3O4	0.14	361.37	5.19±0.40	7.37±0.42	-0.07	-0.2	-0.82	1.855±0.875	zwitterionic
Antibiotics	Oleandomycin	3922-90-5	J01FA05	C35H61NO12	0.87	687.86	13.49±0.70	8.16±0.70	0.28	1.21	1.98	2.308±0.846	cationic
Antibiotics	Oxolinic acid	14698-29-4	J01MB05	C13H11NO5	15.0	261.23	5.94±0.20	-2.04±0.40	-0.72	-1.48	-2.44	-0.382±1.271	anion
Antibiotics	Oxytetracycline	2058-46-0	D06AA03	C22H24N2O9	0.32	460.43	4.50±1.00	10.80±0.70	-2.06	-2.25	-2.82	0.479±0.784	zwitterionic

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge pH = 7
Antibiotics	Penicillin G	113-98-4	J01CE01	C16H18N2O4S	-	334.39	2.45±0.50	-1.32±0.60	-1.42	-1.77	-1.83	1.918±0.197	anion
Antibiotics	Pipemidic acid	51940-44-4	J01MB04	C14H17N5O3	0.95	303.32	4.14±0.20	8.51±0.10	-2.69	-2.7	-2.81	-0.194±0.775	zwitterionic
Antibiotics	Roxithromycin	80214-83-1	J01FA06	C41H76N2O15	0.083	837.05	13.00±0.70	8.16±0.70	0.81	1.75	2.51	2.842±0.869	cationic
Antibiotics	Silvadene	68-35-9	D06BA01	C10H10N4O2S	4.6	250.28	6.81±0.10	1.64±0.10	-0.19	-0.68	-1.46	-0.074±0.255	anion
Antibiotics	Spiramycin	8025-81-8	J01FA02	C43H74N2O14	0.12	-	-	-	-	-	-	<u>2.50</u>	-
Antibiotics	Sulfabenzamide	127-71-9	-	C13H12N2O3S	3.05	276.31	4.85±0.10	1.11±0.10	0.75	0.04	-0.22	1.737±0.426	anion
Antibiotics	Sulfadimethoxine	122-11-2	J01ED02	C12H14N4O4S	1.21	310.33	6.21±0.50	3.00±0.10	-0.69	-1.16	-1.26	0.729±0.386	anion
Antibiotics	Sulfadimidine	57-68-1	J01EB03	C12H14N4O2S	1.12	278.33	7.89±0.10	1.69±0.10	0.28	0.15	-0.37	0.296±0.278	neutral
Antibiotics	Sulfafurazole	127-69-5	J01EB05	C11H13N3O3S	4.63	267.31	4.83±0.50	1.52±0.10	0.51	-0.27	-0.83	1.010±0.450	anion
Antibiotics	Sulfaguandine	57-67-0	A07AB03	C7H10N4O2S	10.6	214.25	11.22±0.70	2.22±0.70	-1.22	-1.22	-1.22	-1.220±0.310	neutral
Antibiotics	Sulfamerazine	127-79-7	D06BA06	C11H12N4O2S	1.12	264.31	7.35±0.10	1.64±0.10	0.07	-0.18	-0.88	0.107±0.267	neutral
Antibiotics	Sulfamethizole	144-82-1	D06BA04	C9H10N4O2S2	1.5	270.33	5.51±0.50	2.07±0.10	-0.13	-0.92	-1.37	0.520±0.255	anion
Antibiotics	Sulfamethoxazole	723-46-6	J01EC01	C10H11N3O3S	0.6	253.28	5.81±0.50	1.39±0.10	0.43	-0.22	-0.96	0.659±0.409	anion
Antibiotics	Sulfamethoxydiazine	651-06-9	J01ED04	C11H12N4O3S	1.03	280.3	6.58±0.10	1.54±0.10	0.31	-0.15	-0.94	0.410±0.270	anion
Antibiotics	Sulfamethoxyipyridazine	80-35-3	J01ED05	C11H12N4O3S	1.38	280.3	7.19±0.30	2.04±0.10	-0.05	-0.75	-1.42	0.320±0.527	neutral
Antibiotics	Sulfanilamide	63-74-1	J01EB06	C6H8N2O2S	17.5	172.21	10.10±0.10	1.85±0.10	-0.67	-0.67	-0.67	-0.667±0.221	neutral
Antibiotics	Sulfaphenazole	526-08-9	J01ED08	C15H14N4O2S	0.12	314.36	6.47±0.50	1.79±0.10	1.34	1.08	0.38	1.386±0.588	anion
Antibiotics	Sulfapyridine	144-83-2	J01EB04	C11H11N3O2S	1.83	249.29	8.54±0.30	2.13±0.10	0.44	0.43	0.37	0.469±0.315	neutral
Antibiotics	Sulfathiazole	72-14-0	D06BA02	C9H9N3O2S2	1.92	255.32	7.24±0.10	2.19±0.10	0.03	-0.15	-0.76	0.050±0.310	neutral
Antibiotics	Tinidazole	19387-91-8	J01XD02	C8H13N3O4S	14.6	247.27	-	2.30±0.34	-0.29	-0.29	-0.29	-0.293±0.358	neutral
Antibiotics	Trimethoprim	738-70-5	J01EA01	C14H18N4O3	100	290.32	-	7.04±0.10	-0.48	0.27	0.55	0.594±0.385	cationic
Antifungals	Sulfacetamide	144-80-9	D10AF06	C8H10N2O3S	14.3	214.24	5.43±0.10	0.93±0.10	-1.46	-2.24	-2.8	-0.960±0.397	anion
Antifungals	Terbinafine	91161-71-6	D01AE15	C21H25N	0.011	291.43	-	6.92±0.50	4.62	5.32	5.55	5.584±0.278	neutral
Antifungals	Tiabendazole	148-79-8	D01AC06	C10H7N3S	3.3	201.25	10.53±0.10	3.40±0.10	2.47	2.47	2.47	2.470±0.570	neutral
Antihistamines	Diphenhydramine	58-73-1	D04AA32	C17H21NO	0.99	255.36	-	8.76±0.28	0.4	1.25	2.17	2.997±0.366	cationic

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge pH = 7
Antihistamines	Promethazine	60-87-7	D04AA10	C17H20N2S	0.13	284.42	-	8.98±0.50	2.21	3.03	3.96	4.887±0.317	cationic
Antihypertensive	Clonidine	4205-90-7	C02AC01	C9H9Cl2N3	2.83	230.09	-	8.10±0.50	0.61	1.28	2.01	2.362±0.603	cationic
Antiparasitics	Albendazole	54965-21-8	P02CA03	C12H15N3O2S	0.26	265.33	10.72±0.10	5.37±0.10	2.91	2.99	2.99	3.001±0.805	neutral
Antiparasitics	Flubendazole	31430-15-6	P02CA05	C16H12FN3O3	0.24	313.28	10.66±0.10	4.45±0.10	3.07	3.08	3.07	3.084±0.586	neutral
Antiparasitics	Levamisole	14769-73-4	P02CE01	C11H12N2S	1.81	204.29	-	10.00±0.40	-0.16	-0.12	0.14	1.840±0.572	cationic
Antiparasitics	Mebendazole	31431-39-7	P02CA01	C16H13N3O3	0.16	295.29	10.81±0.10	4.70±0.10	2.8	2.83	2.82	2.830±0.560	neutral
Antiparasitics	Praziquantel	55268-74-1	P02BA01	C19H24N2O2	2.22	312.41	-	-0.98±0.20	2.66	2.66	2.66	2.661±0.714	neutral
Antiparasitics	Triclabendazole	68786-66-3	P02BX04	C14H9Cl3N2OS	0.0071	359.66	7.91±0.10	3.65±0.10	5.38	5.34	5.04	5.390±0.418	neutral
Antiseptic	Nitrofurantoin	59-87-0	D08AF02	C6H6N4O4	5.29	198.14	10.98±0.46	-0.45±0.70	0.47	0.47	0.47	0.470±0.304	neutral
Beta-blockers	Atenolol	29122-68-7	C07AB03	C14H22N2O3	150	266.34	13.88±0.20	9.43±0.10	-2.63	-2.09	-1.2	0.335±0.279	cationic
Beta-blockers	Bisoprolol	66722-44-9	C07AB07	C18H31NO4	3.18	325.44	13.86±0.20	9.42±0.10	-1.07	-0.54	0.36	1.888±0.384	cationic
Beta-blockers	Metoprolol	37350-58-6	C07AB02	C15H25NO3	8.6	267.36	13.89±0.20	9.43±0.10	-1.33	-0.81	0.09	1.632±0.263	cationic
Calcium channel blocker	Verapamil	52-53-9	C08DA01	C27H38N2O4	2.53	454.6	-	8.97±0.50	1.29	2.08	3.01	4.024±0.380	cationic
Diuretic	Torsemide	56211-40-6	C03CA04	C16H20N4O3S	0.49	348.42	3.37±0.10	5.33±0.38	0.26	0.01	-0.03	1.964±0.828	anion
Hormones	Fludrocortisone acetate	514-36-3	-	C23H31FO6	21.4	422.49	12.06±0.70	-	2.72	2.72	2.72	2.716±0.573	neutral
Hormones	Flumethasone	2135-17-3	D07AB03	C22H28F2O5	19.4	410.45	11.98±0.70	-	1.84	1.84	1.84	1.838±0.631	neutral
Hormones	Hydrocortisone	50-23-7	-	C21H30O5	28.8	362.46	12.47±0.70	-	1.76	1.76	1.76	1.762±0.471	neutral
Hormones	Methylprednisolone	83-43-2	D07AA01	C22H30O5	17.4	374.47	12.46±0.70	-	2.17	2.17	2.17	2.170±0.528	neutral
Hormones	Mometasone furoate	83919-23-7	D07AC13	C27H30Cl2O6	1.26	521.43	13.02±0.70	-	3.59	3.59	3.59	3.594±0.563	neutral
Hormones	Prednicarbate	73771-04-7	D07AC18	C27H36O8	4.59	488.57	14.05±0.70	-	2.83	2.83	2.83	2.832±0.615	neutral
Hormones	Prednisolone	50-24-8	A07EA01; C05AA04; D07AA03	C21H28O5	24.4	360.44	12.46±0.70	-	1.63	1.63	1.63	1.635±0.526	neutral
Hormones	Triamcinolone	124-94-7	D07AB09	C21H27FO6	25.2	394.43	11.57±0.70	-	0.53	0.53	0.53	0.529±0.607	neutral
Hormones	Triamcinolone acetonide	76-25-5	D07AB09	C24H31FO6	14.9	434.5	12.87±0.10	-	2.43	2.43	2.43	2.428±0.666	neutral

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge pH = 7
Illicit drugs	Amphetamine	300-62-9	N06BA01	C9H13N	24.8	135.21	-	9.94±0.10	-1.25	-0.92	-0.13	1.789±0.197	cationic
Illicit drugs	<i>Benzoylcegonine</i>	519-09-5	-	C16H19NO4	-	289.33	3.35±0.40	10.83±0.40	-0.24	-0.24	-0.24	2.263±0.397	zwitterionic
Illicit drugs	Cannabinol	521-35-7	-	C21H26O2	0.08	310.43	9.40±0.40	-	6.93	6.93	6.91	6.929±0.364	neutral
Illicit drugs	<i>Cocaethylene</i>	529-38-4	-	C23H32O5	1.55	317.38	-	9.04±0.60	0.01	0.77	1.71	2.785±0.404	cationic
Illicit drugs	Cocaine	50-36-2	N01BC01	C29H47NO6	2.46	303.35	8.97±0.60	-	-0.45	0.33	1.27	2.275±0.404	neutral
Illicit drugs	<i>Ecgonine methyl ester</i>	7143-09-1	-	C10H17NO3	88.8	199.25	14.12±0.40	9.57±0.60	-3.15	-2.68	-1.81	-0.157±0.435	cationic
Illicit drugs	Ketamine	6740-88-1	N01AX03	C13H16ClNO	5.71	237.73	-	6.46±0.20	2.43	2.43	3	3.012±0.406	neutral
Illicit drugs	MDA	4764-17-4	-	C10H13NO2	50.3	179.22	-	9.94±0.10	-1.4	-1.08	-0.28	1.637±0.311	cationic
Illicit drugs	MDEA	82801-81-8	-	C12H17NO2	26	207.27	-	10.34±0.19	-0.52	-0.34	0.29	2.560±0.321	cationic
Illicit drugs	MDMA	42542-10-9	-	C11H15NO2	47.6	193.24	-	10.32±0.10	-1.02	-0.85	-0.21	2.050±0.321	cationic
Illicit drugs	Methamphetamine	537-46-2	N06BA03	C10H15N	9.74	149.23	-	10.38±0.10	-0.88	-0.72	-0.11	2.202±0.211	cationic
Illicit drugs	Phencyclidine	77-10-1	-	C17H25N	0.17	243.39	-	8.21±0.20	2.09	3.02	3.83	4.251±0.270	cationic
Illicit drugs	THC	1972-08-3	A04AD10	C13H19NO2S	0.072	314.46	9.81±0.60	-	6.84	6.84	6.84	6.838±0.348	neutral
Plastic additives	Benzotriazole	95-14-7	-	C6H5N3	7.77	119.12	8.38±0.10	1.17±0.30	1.44	1.42	1.29	1.440±0.251	neutral
Plastic additives	p-Toluenesulfonamide	70-55-3	-	C7H9NO2S	150	171.22	10.20±0.10	-6.46±0.70	0.97	0.97	0.97	0.971±0.207	neutral
Psychiatric drugs	<i>10-Hydroxycarbazepine</i>	29331-92-8	-	C15H14N2O2	4.03	254.28	13.75±0.20	-0.53±0.40	0.65	0.65	0.65	0.647±0.599	neutral
Psychiatric drugs	<i>7-Aminoclonazepam</i>	4959-17-5	-	C15H12ClN3O	0.38	285.73	12.15±0.70	3.80±0.20	1.28	1.29	1.29	1.288±1.120	neutral
Psychiatric drugs	<i>7-Aminoflunitrazepam</i>	34084-50-9	-	C16H14FN3O	0.98	283.3	-	4.06±0.20	1.44	1.44	1.44	1.441±1.222	neutral
Psychiatric drugs	Alprazolam	28981-97-7	N05BA12	C17H13ClN4	0.077	308.77	-	2.37±0.40	1.92	1.92	1.92	1.916±1.071	neutral
Psychiatric drugs	Amisulpride	71675-85-9	N05AL05	C17H27N3O4S	1.43	369.48	13.73±0.46	8.97±0.50	-1.37	-0.7	0.23	1.495±0.582	cationic
Psychiatric drugs	Amitriptyline	50-48-6	N06AA09	C20H23N	0.14	277.4	-	9.18±0.28	1.57	2.28	3.21	4.410±0.266	cationic
Psychiatric drugs	Amoxapine	14028-44-5	N06AA17	C17H16ClN3O	0.42	313.78	-	8.62±0.10	0.51	1.41	2.3	2.930±1.068	cationic
Psychiatric drugs	Bromazepam	1812-30-2	N05BA08	C14H10BrN3O	0.59	316.15	11.39±0.70	2.00±0.19	2.28	2.28	2.28	2.277±0.839	neutral
Psychiatric drugs	Carbamazepine	298-46-4	N03AF01	C15H12N2O	0.05	236.27	13.94±0.20	-0.49±0.20	1.89	1.89	1.89	1.895±0.597	neutral
Psychiatric drugs	Chlordiazepoxide	58-25-3	N05BA02	C16H14ClN3O	0.57	299.76	-	2.38±0.20	2.49	2.49	2.49	2.492±0.643	neutral

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{\text{ow}}$ pH = 6	$\log D_{\text{ow}}$ pH = 7	$\log D_{\text{ow}}$ pH = 8	$\log K_{\text{ow}}$	Charge pH = 7
Psychiatric drugs	Chlorprothixene	113-59-7	N05AF03	C18H18ClNS	0.075	315.86	-	9.05±0.28	2.44	3.2	4.13	5.211±0.341	cationic
Psychiatric drugs	Citalopram	59729-33-8	N06AB04	C20H21FN2O	16.0	324.39	-	9.57±0.28	0.5	1.02	1.91	3.475±0.600	cationic
Psychiatric drugs	Clobazam	22316-47-8	N05BA09	C16H13ClN2O2	1.17	300.74	8.59±0.20	-0.13±0.20	1.25	1.24	1.15	1.252±0.900	neutral
Psychiatric drugs	Clomipramine	303-49-1	N06AA04	C19H23ClN2	0.11	314.85	9.46±0.28	-	2.01	2.6	3.51	4.940±0.321	neutral
Psychiatric drugs	Clonazepam	1622-61-3	N03AE01	C15H10ClN3O3	0.3	315.71	11.21±0.70	1.55±0.10	2.52	2.52	2.52	2.521±0.879	neutral
Psychiatric drugs	Clorazepate	23887-31-2	N05BA05	C16H13ClN2O4	0.11	314.72	0.80±0.40	3.43±0.50	-0.65	-1.11	-1.2	2.536±0.836	anion
Psychiatric drugs	Clozapine	5786-21-0	N05AH02	C18H19ClN4	0.18	326.82	-	7.33±0.20	2.17	3.23	3.8	3.939±1.082	cationic
Psychiatric drugs	<i>Desalkylflurazepam</i>	2886-65-9	-	C15H10ClFN2O	0.78	288.7	11.55±0.70	2.36±0.10	2.6	2.6	2.6	2.597±0.849	neutral
Psychiatric drugs	Desipramine	50-47-5	N06AA01	C18H22N2	0.29	266.38	-	10.40±0.10	0.9	1.07	1.71	3.972±0.285	cationic
Psychiatric drugs	Desvenlafaxine	93413-62-8	N06AX23	C16H25NO2	7.11	263.38	10.04±0.26	9.33±0.28	-1.08	-0.37	0.56	1.741±0.261	cationic
Psychiatric drugs	Dexametasone	382-67-2	N06AA01	C22H29FO4	24.6	376.46	12.98±0.10	-	2.22	2.22	2.22	2.224±0.515	neutral
Psychiatric drugs	Diazepam	439-14-5	N05BA01	C16H13ClN2O	0.29	284.74	-	3.40±0.10	2.8	2.8	2.8	2.801±0.694	neutral
Psychiatric drugs	Dothiepin	113-53-1	N06AA16	C19H21NS	0.12	295.44	-	9.35±0.28	1.36	1.98	2.9	4.268±0.410	cationic
Psychiatric drugs	Doxepin	1668-19-5	D04AX01 N06AA12	C19H21NO	0.36	279.38	-	9.40±0.28	0.91	1.51	2.43	3.836±0.352	cationic
Psychiatric drugs	<i>EDDP</i>	30223-73-5	-	C11H17O3PS	0.14	277.4	-	7.71±0.60	3.83	4.6	5.19	5.363±0.335	cationic
Psychiatric drugs	Felbamate	25451-15-4	N03AX10	C11H14N2O4	11.1	238.24	12.99±0.50	-1.12±0.70	0.73	0.73	0.73	0.732±0.499	neutral
Psychiatric drugs	Fluoxetine	54910-89-3	N06AB03	C17H18F3NO	0.1	309.33	-	10.05±0.10	0.88	1.15	1.91	3.930±0.434	cationic
Psychiatric drugs	Flupentixol	2709-56-0	N05AF01	C23H25F3N2OS	0.082	434.52	14.96±0.10	7.26±0.10	2.26	3.13	3.57	3.667±0.606	cationic
Psychiatric drugs	Flurazepam	17617-23-1	N05CD01	C21H23ClFN3O	0.092	387.88	-	9.79±0.25	1.81	2.19	3.02	4.842±0.800	cationic
Psychiatric drugs	Fluvoxamine	54739-18-3	N06AB08	C15H21F3N2O2	2.49	318.34	-	9.39±0.10	0.79	1.4	2.32	3.713±0.504	cationic
Psychiatric drugs	Gabapentin	60142-96-3	N03AX12	C9H17NO2	10.0	171.24	4.72±0.10	10.27±0.29	-1.43	-1.42	-1.42	1.083±0.235	zwitterionic
Psychiatric drugs	Haloperidol	52-86-8	N05AD01	C21H23ClFNO2	0.76	375.86	13.86±0.20	8.04±0.20	1.64	2.58	3.37	3.757±0.474	cationic
Psychiatric drugs	Imipramine	50-49-7	N06AA02	C19H24N2	0.19	280.41	-	9.49±0.28	1.42	2	2.91	4.355±0.302	cationic
Psychiatric drugs	Lamotrigine	84057-84-1	N03AX09	C9H7Cl2N5	10.0	256.09	-	5.39±0.63	1.15	1.23	1.24	1.244±0.634	neutral

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge pH = 7
Psychiatric drugs	Lorazepam	846-49-1	N05BA06	C15H10Cl2N2O2	0.096	321.16	10.80±0.70	0.17±0.50	2.38	2.38	2.38	2.382±0.915	neutral
Psychiatric drugs	Maprotiline	10262-69-8	N06AA21	C20H23N	0.3	277.4	10.62±0.10	-	1.28	1.38	1.87	4.364±0.340	neutral
Psychiatric drugs	Medazepam	2898-12-6	N05BA03	C16H15ClN2	0.21	270.76	-	6.18±0.10	3.66	3.86	3.89	3.890±0.474	neutral
Psychiatric drugs	Memantine	19982-08-2	N06DX01	C12H21N	1.84	179.3	-	10.79±0.60	-0.09	-0.02	0.38	3.004±0.270	cationic
Psychiatric drugs	Methadone	76-99-3	N07BC02	C11H15NO2	0.84	309.45	-	9.05±0.50	1.16	1.92	2.85	3.930±0.350	cationic
Psychiatric drugs	Methylphenidate	113-45-1	N06BA04	C14H19NO2	11.6	233.31	-	9.51±0.10	-0.65	-0.11	0.79	2.310±0.280	cationic
Psychiatric drugs	Mianserin	24219-97-4	N06AX03	C18H20N2	0.32	264.37	-	8.26±0.20	-0.4	0.49	1.01	1.143±0.752	cationic
Psychiatric drugs	Mirtazapine	61337-67-5	N06AX11	C17H19N3	1.0	265.35	-	8.10±0.20	-0.98	-0.05	0.64	0.888±0.854	cationic
Psychiatric drugs	Naltrexone	16590-41-3	N07BB04	C20H23NO4	1.92	341.4	9.16±0.40	7.50±0.40	0.42	1.32	1.86	2.048±0.557	cationic
Psychiatric drugs	<i>N-Desmethylozapine</i>	6104-71-8	-	C17H17ClN4	0.054	312.8	-	8.49±0.10	1.38	2.8	3.84	4.462±1.027	cationic
Psychiatric drugs	Nitrazepam	146-22-5	N05CD02	C15H11N3O3	0.49	281.27	11.35±0.70	2.55±0.10	2.35	2.35	2.35	2.355±0.799	neutral
Psychiatric drugs	<i>Norbuprenorphine</i>	78715-23-8	-	C25H35NO4	1.06	413.55	9.14±0.60	9.77±0.60	-1.76	-1.23	-0.36	1.201±0.607	cationic
Psychiatric drugs	Nordiazepam	1088-11-5	N05BA16	C15H11ClN2O	0.43	270.71	11.72±0.70	3.22±0.10	2.77	2.78	2.78	2.776±0.802	neutral
Psychiatric drugs	Nortriptyline	72-69-5	N06AA10	C19H21N	0.19	263.38	-	10.00±0.10	0.92	1.22	2	3.972±0.238	cationic
Psychiatric drugs	Olanzapine	132539-06-1	N05AH03	C17H20N4S	0.054	312.43	-	7.78±0.20	0.95	1.99	2.76	3.076±1.424	cationic
Psychiatric drugs	Opipramol	315-72-0	N06AA05	C23H29N3O	0.5	363.5	14.96±0.10	7.45±0.10	1.74	2.63	3.14	3.268±0.453	cationic
Psychiatric drugs	Oxazepam	604-75-1	N05BA04	C15H11ClN2O2	0.37	286.71	10.94±0.70	1.17±0.50	2.22	2.22	2.22	2.216±0.838	neutral
Psychiatric drugs	Oxcarbazepine	28721-07-5	N03AF02	C15H12N2O2	2.95	252.27	13.73±0.20	-0.53±0.20	1.66	1.66	1.66	1.656±0.602	neutral
Psychiatric drugs	Paliperidone	144598-75-4	N05AX13	C23H27FN4O3	0.61	426.48	13.00±0.60	8.07±0.10	-0.68	0.26	1.04	1.410±0.415	cationic
Psychiatric drugs	Paroxetine	61869-08-7	N06AB05	C19H20FNO3	1.41	329.37	-	9.68±0.10	0.7	1.16	2.03	3.701±0.436	cationic
Psychiatric drugs	Phenazepam	51753-57-2	N05BX	C15H10BrClN2O	0.32	349.61	11.58±0.70	2.18±0.10	3.37	3.37	3.37	3.371±0.913	neutral
Psychiatric drugs	Phenytoin	57-41-0	N03AB02	C15H12N2O2	0.87	252.27	8.28±0.10	-2.81±0.40	1.42	1.41	1.29	1.421±0.369	neutral
Psychiatric drugs	Pipamperone	1893-33-0	N05AD05	C21H30FN3O2	1.66	375.48	16.20±0.20	8.08±0.10	0.31	1.26	2.07	2.465±0.592	cationic
Psychiatric drugs	Prazepam	2955-38-6	N05BA11	C19H17ClN2O	0.21	324.8	-	3.44±0.20	3.7	3.7	3.7	3.701±0.695	neutral
Psychiatric drugs	Promazine	58-40-2	N05AA03	C17H20N2S	0.12	284.42	-	9.43±0.28	1.77	2.37	3.29	4.689±0.251	cationic

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{\text{ow}}$ pH = 6	$\log D_{\text{ow}}$ pH = 7	$\log D_{\text{ow}}$ pH = 8	$\log K_{\text{ow}}$	Charge pH = 7
Psychiatric drugs	Protriptyline	438-60-8	N06AA11	C19H21N	0.37	263.38	-	10.61±0.10	1.27	1.38	1.87	4.360±0.243	cationic
Psychiatric drugs	Quetiapine	111974-69-7	N05AH04	C21H25N3O2S	0.14	383.51	14.41±0.10	6.74±0.10	1.76	2.4	2.58	2.600±0.788	neutral
Psychiatric drugs	Risperidone	106266-06-2	N05AX08	C23H27FN4O2	0.38	410.49	-	8.07±0.10	0.6	1.53	2.31	2.678±0.406	cationic
Psychiatric drugs	<i>Ritalinic acid</i>	19395-41-6	-	C13H17NO2	14.2	219.28	3.50±0.10	10.54±0.10	-0.62	-0.62	-0.62	1.884±0.283	zwitterionic
Psychiatric drugs	Secobarbital	76-73-3	N05CA06	C12H18N2O3	4.24	238.28	7.81±0.10	-	2.29	2.24	1.9	2.300±0.259	neutral
Psychiatric drugs	Sertraline	79617-96-2	N06AB06	C17H17Cl2N	0.091	306.23	-	9.47±0.40	2.13	2.7	3.6	5.079±0.348	cationic
Psychiatric drugs	Temazepam	846-50-4	N05CD07	C16H13ClN2O2	0.071	300.74	11.66±0.40	1.58±0.50	2.19	2.19	2.19	2.188±0.720	neutral
Psychiatric drugs	Topiramate	97240-79-4	N03AX11	C12H21NO8S	15.3	339.36	9.22±0.70	-8.22±0.70	2.16	2.15	2.13	2.157±0.671	neutral
Psychiatric drugs	Trazodone	19794-93-5	N06AX05	C19H22ClN5O	0.016	371.86	-	7.52±0.10	1.63	2.41	2.71	2.756±0.655	cationic
Psychiatric drugs	Triazolam	28911-01-5	N05CD05	C17H12Cl2N4	0.029	343.21	2.29±0.40	-	2.08	2.08	2.08	2.082±1.132	anion
Psychiatric drugs	Trimipramine	739-71-9	N06AA10	C20H26N2	0.17	294.43	-	9.38±0.28	1.8	2.41	3.33	4.708±0.308	cationic
Psychiatric drugs	Venlafaxine	93413-69-5	N06AX16	C17H27NO2	0.038	277.4	14.84±0.20	9.26±0.28	-0.34	0.39	1.32	2.475±0.268	cationic
Psychiatric drugs	Zolpidem	82626-48-0	N05CF02	C19H21N3O	0.18	307.39	-	6.77±0.50	2.42	2.95	3.07	3.089±0.594	neutral
Psychiatric drugs	Zopiclone	43200-80-2	N05CF01	C17H17ClN6O3	0.077	388.81	-	6.70±0.10	1.93	2.53	2.69	2.713±0.847	neutral
Psychiatric drugs	α -Hydroxyalprazolam	37115-43-8	-	C17H13ClN4O	0.31	324.76	12.90±0.10	1.47±0.40	0.62	0.62	0.62	0.616±1.079	neutral
Psychiatric drugs	α -Hydroxymidazolam	59468-90-5	-	C18H13ClFN3O	0.15	341.77	13.59±0.10	3.63±0.40	2.49	2.5	2.5	2.498±0.906	neutral
Psychiatric drugs	α -Hydroxytriazolam	37115-45-0	-	C17H12Cl2N4O	0.087	359.21	12.90±0.10	1.39±0.40	0.78	0.78	0.78	0.783±1.140	neutral
Receptor antagonists	Atropine	51-55-8	A03BA01; S01FA01	C17H23NO3	11.5	289.37	14.12±0.10	9.98±0.40	-1.67	-1.36	-0.58	1.380±0.365	cationic
Receptor antagonists	Flumazenil	78755-81-4	V03AB25	C15H14FN3O3	1.69	303.29	-	0.86±0.20	2.15	2.15	2.15	2.151±0.610	neutral
Stimulants	Caffeine	58-08-2	N06BC01	C8H10N4O2	1.2	194.19	-	0.52±0.70	-0.63	-0.63	-0.63	-0.628±0.753	neutral
Stimulants	Cotinine	486-56-6	-	C14H12O2	10	176.22	-	4.72±0.12	0.05	0.07	0.07	0.075±0.379	neutral
Stimulants	Phentermine	122-09-8	A08AA01	C10H15N	16.5	149.23	-	9.94±0.25	-0.84	-0.51	0.28	2.200±0.212	cationic
UV filter	Octinoxate	5466-77-3	D02BA02	C18H26O3	0.026	290.4	-	-	5.92	5.92	5.92	5.921±0.246	anion
Veterinary drugs	Carprofen	53716-49-7	QM01AE91	C15H12ClNO2	0.19	273.71	4.84±0.30	-5.73±0.50	2.71	1.75	0.83	3.843±0.727	anion

Table S1. (continued)

Class	Compound	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{\text{ow}}$ pH = 6	$\log D_{\text{ow}}$ pH = 7	$\log D_{\text{ow}}$ pH = 8	$\log K_{\text{ow}}$	Charge pH = 7
Veterinary drugs	Diaveridine	5355-16-8	QP51AX18	C13H16N4O2	0.36	260.29	-	7.11±0.10	-0.18	0.59	0.9	0.951±0.375	cationic
Veterinary drugs	Difloxacin	98106-17-3	QJ01MA94	C21H19F2N3O3	1.55	399.39	6.17±0.41	7.41±0.42	-0.45	-0.28	-0.89	0.843±0.832	zwitterionic
Veterinary drugs	Dimetridazole	551-92-8	QP51AA07	C5H7N3O2	29.5	141.13	-	2.81±0.25	0.09	0.09	0.09	0.095±0.235	neutral
Veterinary drugs	Enrofloxacin	93106-60-6	QJ01MA90	C19H22FN3O3	1.61	359.4	6.43±0.41	7.76±0.10	0.84	1.18	0.72	2.306±0.819	zwitterionic
Veterinary drugs	Flunixin	38677-85-9	QM01AG90	C14H11F3N2O2	0.16	296.25	1.70±0.36	4.80±0.29	2.06	1.66	1.59	4.728±0.548	anion
Veterinary drugs	Furaltadone	139-91-3	QJ01XX93	C13H16N4O6	19.2	324.29	-	6.19±0.10	-0.83	-0.48	-0.43	-0.423±0.453	neutral
Veterinary drugs	Iprnidazole	14885-29-1	QP51AA10	C7H11N3O2	6.6	169.18	-	2.55±0.25	0.96	0.96	0.96	0.958±0.239	neutral
Veterinary drugs	Marbofloxacin	115550-35-1	QJ01MA93	C17H19FN4O4	7.78	362.36	6.02±0.20	7.34±0.42	-2.27	-2.35	-3.07	-0.641±0.921	zwitterionic
Veterinary drugs	Monensin	17090-79-8	QA16QA06	C36H62O11	1.36	670.87	4.26±0.27	-	2.26	1.3	0.56	4.011±0.729	anion
Veterinary drugs	Orbifloxacin	113617-63-3	QJ01MA95	C19H20F3N3O3	0.024	395.38	6.36±0.50	8.48±0.60	0.72	1.14	1.07	2.968±0.948	zwitterionic
Veterinary drugs	Oxibendazole	20559-55-1	QP52AC07	C12H15N3O3	1.3	249.27	10.60±0.10	5.84±0.10	2.32	2.5	2.52	2.532±0.812	neutral
Veterinary drugs	Ronidazole	7681-76-7	QP51AA08	C6H8N4O4	16.7	200.15	12.99±0.50	1.32±0.25	-0.11	-0.11	-0.11	-0.109±0.433	neutral
Veterinary drugs	Salinomycin	53003-10-4	QP51AH01	C42H70O11	0.16	751	4.36±0.10	-	3.95	2.99	2.21	5.596±0.735	anion
Veterinary drugs	Sarafloxacin	98105-99-8	QJ01MA98	C20H17F2N3O3	1.87	385.36	6.17±0.41	8.68±0.10	-1.71	-1.39	-1.44	0.671±0.844	zwitterionic
Veterinary drugs	Sulfachlorpyridazine	80-32-0	-	C10H9CIN4O2S	0.73	284.72	5.90±0.30	1.88±0.10	-0.49	-1.12	-1.3	0.677±0.477	anion
Veterinary drugs	Sulfaclozine	102-65-8	QP51AG04	C10H9CIN4O2S	1.09	284.72	4.83±0.10	1.12±0.10	-0.14	-0.84	-1.08	0.877±0.407	anion
Veterinary drugs	Sulfadoxine	2447-57-6	QJ01EQ13	C12H14N4O4S	1.47	310.33	6.16±0.50	2.18±0.10	-0.49	-1.21	-1.49	0.460±0.419	anion
Veterinary drugs	Sulfamonomethoxine	1220-83-3	QJ01EQ18	C11H12N4O3S	1.87	280.3	6.67±0.30	2.81±0.10	0	-0.69	-0.93	1.032±0.398	anion
Veterinary drugs	Sulfanitran	122-16-7	-	C14H13N3O5S	0.89	335.34	7.42±0.10	-3.57±0.50	2.41	2.24	1.64	2.436±0.359	neutral
Veterinary drugs	Sulfaquinoxaline	59-40-5	QP51AG03	C14H12N4O2S	0.14	300.34	5.65±0.10	1.99±0.30	1.36	1.01	0.25	1.429±0.371	anion
Veterinary drugs	Tilmicosin	108050-54-0	QJ01FA91	C46H80N2O13	0.069	869.13	13.16±0.70	9.58±0.10	-0.2	0.74	2.07	3.736±0.859	cationic
X-ray contrast medium	Iopromide	73334-07-3	V08AB05	C18H24I3N3O8	0.14	791.11	10.62±0.70	-2.60±0.70	-2.66	-2.66	-2.66	-2.658±0.952	neutral

Table S2. Main physicochemical properties and Predicted No-Effect Concentration (PNEC) in freshwater of the non-target OMPs analyzed. The compound classes were attributed according to the Anatomic Therapeutic Chemical (ATC) classification. The transformation products are written in *italics*. Data on (predicted) physicochemical properties were obtained from CAS Scifinder (<https://scifinder.cas.org>) and the PNEC values from the NORMAN database (<https://www.norman-network.com/nds/ecotox/>). The charge was obtained from pKa values by calculating the molecular/ionic species at pH 7 (see **Text S1**).

Class	Name	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge at pH 7
Analgesics/anti-inflammatories	<i>2,6-Xylidine / Lidocaine-M / Dimethylaniline</i>	87-62-7	-	C8H11N	12.7	121.18	-	4.31±0.10	1.62	1.63	1.63	1.631±0.223	neutral
Analgesics/anti-inflammatories	Azelastine	58581-89-8	R01AC03	C22H24ClN3O	-	381.9	-	9.16±0.40	0.57	1.21	2.13	3.468±0.753	cationic
Analgesics/anti-inflammatories	Benzocaine	94-09-7	N01BA05	C9H11NO2	-	165.19	-	2.51±0.10	1.84	1.84	1.84	1.835±0.251	neutral
Analgesics/anti-inflammatories	<i>Depropionylbezitramide</i>	83898-28-6	-	C28H28N4O	0.0037	436.55	12.04±0.30	8.21±0.10	2.09	3.01	3.63	3.818±0.445	cationic
Analgesics/anti-inflammatories	<i>Dimethylaminophenazone</i>	58-15-1	-	C13H17N3O	17.6	231.29	-	4.50±0.65	0.84	0.85	0.85	0.854±0.283	neutral
Analgesics/anti-inflammatories	Fenoprofen	31879-05-7	M01AE04	C15H14O3	2.6	242.27	4.20±0.10	-	1.92	0.97	0.25	3.723±0.342	anion
Analgesics/anti-inflammatories	Metaxalone	1665-48-1	-	C12H15NO3	15.3	221.25	12.26±0.40	-1.42±0.40	1.18	1.18	1.18	1.181±0.710	neutral
Analgesics/anti-inflammatories	Niflumic acid	4394-00-7	M02AA17; M01AX02	C13H9F3N2O2	0.15	282.22	1.70±0.36	4.71±0.29	1.79	1.39	1.32	4.460±0.545	anion
Analgesics/anti-inflammatories	Parsamide	30653-83-9	-	C14H18N2O2	2.25	246.31	14.83±0.46	3.94±0.10	1.04	1.04	1.04	1.044±0.390	neutral
Analgesics/anti-inflammatories	Propacetamol	66532-85-2	N02BE05	C14H20N2O3	3.86	264.32	14.20±0.70	8.08±0.25	-0.55	0.38	1.17	1.536±0.291	cationic
Analgesics/anti-inflammatories	Tapentadol	175591-23-8	N02AX06	C14H23NO	-	221.34	9.97±0.10	9.45±0.28	0.08	0.66	1.56	3.017±0.243	cationic
Analgesics/anti-inflammatories	<i>Tramadol-N-oxide</i>	147441-56-3	-	C16H25NO3	59.4	279.38	14.08±0.40	4.74±0.40	-0.27	-0.25	-0.25	-0.247±0.628	neutral
Antiacid	Lansoprazole	103577-45-3	A02BC03	C16H14F3N3O2S	0.47	369.36	9.56±0.10	3.64±0.30	2.58	2.58	2.58	2.581±0.810	neutral
Antiacid	Omeprazole	73590-58-6	A02BC01	C17H19N3O3S	-	345.42	8.78±0.10	4.72±0.40	2.34	2.35	2.33	2.359±0.736	neutral
Antiacid	Troxipide	30751-05-4	A02BX11	C15H22N2O4	-	294.35	13.66±0.20	9.32±0.10	-1.16	-0.5	0.43	1.710±0.706	cationic
Antiarrhythmic agents	Flecainide	54143-55-4	C01BC04	C17H20F6N2O3	0.64	414.34	14.15±0.46	9.69±0.10	0.21	0.72	1.61	3.188±0.811	cationic
Antibiotics	<i>2-Hydroxyquinoline</i>	59-31-4	-	C9H7NO	7.46	145.16	11.80±0.50	-0.41±0.10	1.17	1.17	1.17	1.174±0.490	neutral
Antibiotics	<i>Azithromycin 3'-N-oxide</i>	90503-06-3	-	C38H72N2O13	-	764.99	12.51±0.60	8.59±0.70	-3.07	-2.18	-1.28	-0.622±0.925	cationic
Antibiotics	<i>Azithromycin N'-(Desmethyl)</i>	172617-84-4	-	C37H70N2O12	-	734.96	13.28±0.70	9.07±0.70	-2.48	-1.84	-0.11	1.591±0.831	cationic
Antibiotics	Cefalexin	15686-71-2	J01DB01	C16H17N3O4S	4.03	347.39	3.12±0.50	6.84±0.10	-2.22	-2.68	-3.22	0.350±0.254	anion
Antibiotics	Cefoxitin	35607-66-0	J01DC01	C16H17N3O7S2	1.3	427.45	2.63±0.50	-1.41±0.70	-3.23	-3.66	-3.74	2 x 10 ⁻³ ±0.879	anion
Antibiotics	<i>Clarithromycin-N-oxide</i>	118074-07-0	-	C38H69NO14	1.67	763.95	12.50±0.60	4.11±0.70	-0.4	-0.4	-0.4	-0.399±0.919	neutral
Antibiotics	<i>Erythromycin A enol ether</i>	33396-29-1	-	C37H65NO12	-	715.91	13.45±0.70	8.13±0.70	1.32	2.25	3.01	3.325±0.864	cationic
Antibiotics	Gatifloxacin	112811-59-3	J01MA16	C19H22FN3O4	0.27	375.39	6.43±0.50	8.72±0.40	-0.46	-0.16	-0.21	2.104±0.936	zwitterionic

Table S2. (continued)

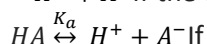
Class	Name	CAS#	ATC code	Formula	PNEC freshwater ($\mu\text{g/L}$)	Molecular weight	Strongest acidic pK_a at 25°C	Strongest basic pK_a at 25°C	$\log D_{ow}$ pH = 6	$\log D_{ow}$ pH = 7	$\log D_{ow}$ pH = 8	$\log K_{ow}$	Charge at pH 7
Antibiotics	Moxifloxacin	354812-41-2	J01MA14	C ₂₁ H ₂₄ FN ₃ O ₄	0.077	401.43	6.43±0.50	10.63±0.20	0.04	0.28	0.33	2.825±0.931	zwitterionic
Antibiotics	N4-Acetylsulfamethoxazole	21312-10-7	-	C ₁₂ H ₁₃ N ₃ O ₄ S	2.38	295.32	5.60±0.50	-3.38±0.50	0.65	-0.06	-0.76	0.955±0.416	anion
Antibiotics	Pazufloxacin	127045-41-4	J01MA18	C ₁₆ H ₁₅ FN ₂ O	1.03	318.3	5.05±0.40	7.08±0.20	-2.11	-2.26	-2.84	0.116±0.739	zwitterionic
Antibiotics	Rifaximin	80621-81-4	A07AA11	C ₄₃ H ₅₁ N ₃ O ₁₁	0.0025	785.88	2.83±0.70	5.60±0.70	1.19	0.49	0.15	3.353±1.798	anion
Anti-cancer drugs	Cyclophosphamide	50-18-0	L01AA01	C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	6.96	261.09	-	2.84±0.20	0.73	0.73	0.73	0.727±0.355	neutral
Anti-cancer drugs	Cytarabine	147-94-4	L01BC01	C ₉ H ₁₃ N ₃ O ₅	22.6	243.22	13.48±0.70	4.26±0.10	-1.81	-1.81	-1.81	-1.808±0.269	neutral
Anti-cancer drugs	Flutamide	13311-84-7	L02BB01	C ₁₁ H ₁₁ F ₃ N ₂ O ₃	1.15	276.21	13.12±0.70	-4.58±0.50	3.52	3.52	3.52	3.522±0.332	neutral
Anti-cancer drugs	Lapatinib	231277-92-2	L01XE07	C ₂₉ H ₂₆ Cl ₂ FN ₄ O ₄ S	-	581.06	-	6.34±0.19	5.7	6.21	6.29	6.302±1.084	neutral
Antidiabetic drugs	Metformin	657-24-9	A10BA02	C ₄ H ₁₁ N ₅	-	129.16	-	12.27±0.10	-3.25	-3.25	-3.2	-1.254±0.377	cationic
Antidiabetic drugs	Sitagliptin	486460-32-6	A10BH01	C ₁₆ H ₁₅ F ₆ N ₅ O	-	407.31	-	7.20±0.10	1.1	1.8	2.02	2.055±0.673	cationic
Antiemetic	Metoclopramide	364-62-5	A03FA01	C ₁₄ H ₂₂ Cl ₂ N ₃ O ₂	1.34	299.8	13.84±0.46	9.08±0.10	-0.72	-0.06	0.86	2.161±0.419	cationic
Antigout preparation	Allopurinol	315-30-0	M04AA01	C ₅ H ₄ N ₄ O	20.6	136.11	9.20±0.50	1.37±0.20	-0.55	-0.55	-0.56	-0.550±0.424	neutral
Antihistamine	Fexofenadine	83799-24-0	R06AX26	C ₃₂ H ₃₉ N ₃ O ₄	-	501.66	4.43±0.10	9.42±0.10	1.22	1.23	1.22	3.732±0.431	zwitterionic
Antihypertensives	Candesartan	139481-59-7	C09DB07	C ₂₄ H ₂₀ N ₆ O ₃	-	440.45	2.06±0.10	5.60±0.10	1.02	0.59	0.51	4.652±0.838	anion
Antihypertensives	Irbesartan	138402-11-6	C09DA04	C ₂₅ H ₂₈ N ₆ O	-	428.53	4.16±0.10	2.60±0.20	3.67	3.31	3.25	5.246±0.633	anion
Antihypertensives	Losartan	114798-26-4	C09CA01	C ₂₂ H ₂₃ Cl ₂ N ₆ O	-	422.91	4.15±0.10	4.39±0.60	1.83	1.51	1.46	3.455±0.507	anion
Antihypertensives	Nitrendipin	39562-70-4	C08CA08	C ₁₈ H ₂₀ N ₂ O ₆	0.0092	360.36	-	2.79±0.70	3.81	3.81	3.81	3.807±0.587	neutral
Antihypertensives	Olmesartan	144689-63-4	C09CA08	C ₂₄ H ₂₆ N ₆ O ₃	0.0024	558.59	4.15±0.10	4.54±0.70	1.17	0.86	0.8	2.798±0.633	anion
Antihypertensives	Sotalol	3930-20-9	C07AA07	C ₁₂ H ₂₀ N ₂ O ₃ S	6.52	272.37	8.28±0.10	9.31±0.10	-2.65	-2.01	-1.23	0.240±0.369	cationic
Antihypertensives	Telmisartan	144701-48-4	C09CA07	C ₃₃ H ₃₀ N ₄ O ₂	-	514.62	3.86±0.36	5.01±0.10	4.34	3.65	3.65	6.477±1.193	anion
Antihypertensives	Valsartan	137862-53-4	C09CA03	C ₂₄ H ₂₉ N ₅ O ₃	-	435.52	3.56±0.10	0.60±0.10	-0.21	-0.68	-0.72	4.022±0.606	anion
Antiparasitic	Hydroxychloroquine	118-42-3	P01BA02	C ₁₈ H ₂₆ Cl ₂ N ₃ O	0.071	335.87	14.76±0.10	8.87±0.50	0.38	1.57	2.58	3.534±0.764	cationic
Antiseptics	4-Chloroaniline	106-47-8	--	C ₆ H ₆ ClN	-	127.57	-	3.97±0.10	1.95	1.95	1.95	1.952±0.218	neutral
Antiseptics	Chlorhexidine	55-56-1	--	C ₂₂ H ₃₀ Cl ₂ N ₁₀	0.0068	505.45	-	11.51±0.10	1.57	1.58	1.58	4.575±0.330	cationic
Antithrombotics	Clopidogrel	113665-84-2	B01AC04	C ₁₆ H ₁₆ Cl ₂ N ₂ O ₂ S	-	321.82	-	4.56±0.20	2.57	2.58	2.58	2.583±0.441	neutral
Antithrombotics	Dabigatran	211914-51-1	B01AE07	C ₂₅ H ₂₅ N ₇ O ₃	0.049	471.51	4.17±0.10	12.92±0.50	-1.47	-1.48	-1.48	1.024±0.631	zwitterionic
Beta-blockers	Desacetylmepitranolol	57193-14-3	--	C ₁₅ H ₂₅ N ₃ O ₃	-	267.36	11.10±0.30	9.67±0.10	-1.26	-0.85	-0.01	1.762±0.340	cationic
Beta-blockers	Metoprolol acid	56392-14-4	--	C ₁₄ H ₂₁ N ₃ O ₄	47.7	267.32	4.41±0.10	9.45±0.10	-1.66	-1.65	-1.66	0.850±0.265	zwitterionic
Bronchodilators	Terbutaline	23031-25-6	R03AC03	C ₁₂ H ₁₉ N ₃ O ₃	-	225.28	9.11±0.10	9.65±0.10	-2.28	-1.77	-0.9	0.696±0.360	cationic
Bronchodilators	Theophylline	58-55-9	R03DA04	C ₇ H ₈ N ₄ O ₂	14.8	180.16	8.60±0.50	1.64±0.70	-0.28	-0.28	-0.37	-0.276±0.296	neutral
Food additives	Methylsalicylate	119-36-8	--	C ₈ H ₈ O ₃	18.6	152.15	9.76±0.10	-	2.52	2.52	2.52	2.523±0.240	neutral
Food additives	Triethyl citrate	77-93-0	--	C ₁₂ H ₂₀ O ₇	73.9	276.28	11.57±0.29	-	1.27	1.27	1.27	1.267±0.411	neutral
Hormones	Boldione	897-06-3	--	C ₁₉ H ₂₄ O ₂	2.23	284.39	-	-	2.62	2.62	2.62	2.623±0.412	neutral
Hormones	Paramethasone acetate	1597-82-6	--	C ₂₄ H ₃₁ F ₆ O ₆	6.48	434.5	12.29±0.70	-	2.26	2.26	2.26	2.262±0.616	neutral
Illicit drug	Norcocaine	129944-99-6	--	C ₁₆ H ₁₉ N ₃ O ₅	7.07	305.33	3.25±0.40	10.64±0.40	-0.7	-0.7	-0.73	1.805±0.405	zwitterionic
Lipid regulators	Atorvastatin	134523-00-5	C10AA05	C ₃₃ H ₃₅ FN ₂ O ₅	-	558.64	4.29±0.10	0.38±0.50	2.03	1.08	0.37	3.846±0.731	anion
Lipid regulators	Bezafibrate	41859-67-0	C10AB02	C ₁₉ H ₂₀ Cl ₂ N ₄ O ₄	-	361.82	3.29±0.10	-2.06±0.70	-0.17	-0.93	-1.2	2.504±0.419	anion
Other	1,2-Benzisothiazolinone	2634-33-5	-	C ₇ H ₅ N ₂ O ₂ S	7.11	151.19	10.19±0.20	-1.97±0.20	1.95	1.95	1.95	1.953±0.401	neutral
Other	1-Methylimidazole	616-47-7	-	C ₄ H ₆ N ₂	14.5	82.1	-	82.1	-1.13	-0.4	-0.14	-0.094±0.227	cationic
Other	1-Naphthylamine	134-32-7	-	C ₁₀ H ₉ N	0.93	143.19	-	4.21±0.10	2.31	2.32	2.32	2.320±0.192	neutral

Table S2. (continued)

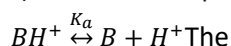
Class	Name	CAS#	ATC code	Formula	PNEC freshwater (µg/L)	Molecular weight	Strongest acidic pK _a at 25°C	Strongest basic pK _a at 25°C	logD _{ow} pH = 6	logD _{ow} pH = 7	logD _{ow} pH = 8	logK _{ow}	Charge at pH 7
Other	2,2'-Oxamido bis-[ethyl-3-(3,5-di-t-butyl-4-hydroxyphenyl) propionate	70331-94-1	-	C40H60N2O8	2.58	696.91	11.48±0.46	-1.26±0.70	8.46	8.46	8.46	8.455±0.809	neutral
Other	Indole	120-72-9	-	C8H7N	2.08	117.15	17.00±0.30	-2.40±0.50	2.59	2.59	2.59	2.588±0.172	neutral
Other	MIT / Methylisothiazolinone	2682-20-4	-	C4H5NOS	-	115.15	-	-2.03±0.20	0.12	0.12	0.12	0.119±0.406	neutral
Other	NDEA / Nitrosodiethylamine	55-18-5	-	C4H10N2O	27	102.14	-	-3.14±0.70	0.52	0.52	0.52	0.523±0.228	neutral
Other	Nicopholine	492-85-3	-	C10H12N2O2	36.8	192.21	-	4.11±0.10	-0.2	-0.2	-0.2	-0.196±0.411	neutral
Other	Picaridin / Bayrepel / Icaridin	119515-38-7	-	C12H23NO3	-	229.32	15.15±0.10	-1.71±0.40	1.82	1.82	1.82	1.819±0.565	neutral
Pesticide	DEET / Diethyltoluamide	134-62-3	-	C12H17NO	-	191.27	-	-1.37±0.70	2.42	2.42	2.42	2.419±0.233	neutral
Plastic additive	5-Methyl-1H-benzotriazole	136-85-6	-	C7H7N3	-	133.15	8.74±0.40	1.65±0.30	1.98	1.98	1.91	1.983±0.734	neutral
Psychiatric drugs	10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	-	C15H14N2O2	-	254.28	13.75±0.20	-0.53±0.40	0.65	0.65	0.65	0.647±0.599	neutral
Psychiatric drugs	Acridine / Carbamazepine-M	260-94-6	-	C13H9N	0.27	179.22	-	5.56±0.10	3.32	3.43	3.45	3.450±0.252	neutral
Psychiatric drugs	Carbamazepine 10,11-epoxide	36507-30-9	-	C15H12N2O2	2.57	252.27	13.91±0.20	-0.50±0.20	0.16	0.16	0.16	0.155±0.718	neutral
Psychiatric drugs	Levetiracetam	102767-28-2	N03AX14	C8H14N2O2	38	170.21	-	-	-	-	-	-	-
Psychiatric drugs	Norcitalopram / Desmethylcitalopram	62498-67-3	-	C19H19FN2O	0.5	310.37	-	10.50±0.10	-0.27	-0.14	0.41	2.814±0.578	cationic
Psychiatric drugs	Pregabalin	148553-50-8	N03AX16	C8H17NO2	-	159.23	4.23±0.10	11.31±0.10	-1.41	-1.41	-1.41	1.089±0.221	zwitterionic
Psychiatric drugs	Propyperone	3781-28-0	-	C23H33FN2O2	-	388.52	-	7.91±0.10	1.52	2.47	3.25	3.603±0.543	cationic
Psychiatric drugs	Sulpiride	15676-16-1	N05AL01	C15H23N3O4S	4.09	341.43	9.98±0.60	8.97±0.50	-2.1	-1.44	-0.51	0.776±0.414	cationic
Stimulants	3-Hydroxycotinine	34834-67-8	-	C10H12N2O2	9.71	192.21	13.02±0.40	4.72±0.12	-1.14	-1.12	-1.12	-1.121±0.455	neutral
Stimulants	Nicotine	54-11-5	N07BA01	C10H14N2	-	162.23	-	8.00±0.50	-1.89	-0.99	-0.1	0.570±0.357	cationic
Stimulants	Paraxanthine	611-59-6	-	C7H8N4O2	21.4	180.16	8.50±0.50	0.21±0.70	-0.94	-0.95	-1.06	-0.941±0.916	neutral
Stimulants	Theobromine	83-67-0	C03BD01; R03DA07	C7H8N4O2	-	180.16	9.90±0.50	0.41±0.70	-1.06	-1.06	-1.06	-1.058±0.782	neutral
Synthetic musks	AHDI / Phantolide	15323-35-0	-	C17H24O	0.048	244.37	-	-	4.54	4.54	4.54	4.536±0.415	-
Synthetic musks	Celestolide	13171-00-1	-	C17H24O	0.043	244.37	-	-	3.76	3.76	3.76	3.761±0.420	-
UV filters	Dioxybenzone / Benzophenone-8	131-53-3	-	C14H12O4	0.86	244.24	7.11±0.35	-	4.27	3.98	2.97	4.311±0.409	neutral
X-ray contrast media	Diatrizoate / Amidotrizoic acid	117-96-4	-	C11H9I3N2O4	0.073	613.91	0.92±0.10	-2.76±0.50	-2.65	-2.66	-2.66	0.492±0.943	anion
X-ray contrast media	Iohexol	66108-95-0	V08AB02	C19H26I3N3O9	0.14	821.14	11.35±0.46	-2.72±0.70	-2.92	-2.92	-2.92	-2.921±0.946	neutral
X-ray contrast media	Iopamidol	60166-93-0	V08AB04	C17H22I3N3O8	0.03	777.09	10.87±0.46	-2.85±0.70	-2.54	-2.54	-2.54	-2.545±1.056	neutral

Text S3. Calculation of the OMP charge (ionic form).

The charge of the OMPs can be estimated by calculating the proportion of ionic species as a function of the acid dissociation constant (K_a) of the compound and the pH value of the wastewater (Sukul et al., 2008). The (predicted) pK_a values of the most acidic and/or basic groups of the molecule (strongest acidic/basic pK_a at 25 °C in **Table S1** and **S2**) were obtained from CAS Scifinderⁿ, which allowed the calculation of the speciation of the analyzed OMPs at pH values ranging from 1 to 14 (in this study, the pH was set as pH = 7) (Kovalova et al., 2013; Schwarzenbach et al., 2003). Depending on whether the compound has one or two pK_a values, the speciation goes as follows: One pK_a value If the compound has only the strongest acidic pK_a , it is defined as the pK_a of an acidic pharmaceutical (HA), $HA \xrightleftharpoons{K_a} H^+ + A^-$ If the compound has only the strongest basic pK_a , it



is defined as the pK_a of the conjugate acid (BH^+) of a basic compound (Schwarzenbach et al., 2003), $BH^+ \xrightleftharpoons{K_a} B +$



$$x_0 = \frac{[HA]}{[HA] + [A^-]} = \frac{[BH^+]}{[BH^+] + [B]} = \frac{[H^+]}{[H^+] + K_a} \quad x_1 = \frac{[A^-]}{[HA] + [A^-]} = \frac{[B]}{[BH^+] + [B]} = \frac{K_a}{[H^+] + K_a} \quad \text{where, } x_0 + x_1$$

$$x_1 = \frac{[A^-]}{[HA] + [A^-]} = \frac{[B]}{[BH^+] + [B]} = \frac{K_a}{[H^+] + K_a} \quad \text{where, } x_0 + x_1 = 1 \text{ being}$$

$$= 1 \text{ being}$$

$$x_0 + x_1 = 1 \text{ being}$$

$$x_0 = \frac{[H^+]^2}{[H^+]^2 + K_1 \cdot [H^+] + K_1 \cdot K_2} \quad x_1 = \frac{K_1 \cdot [H^+]}{[H^+]^2 + K_1 \cdot [H^+] + K_1 \cdot K_2} \quad x_2$$

$$x_1 = \frac{K_1 \cdot [H^+]}{[H^+]^2 + K_1 \cdot [H^+] + K_1 \cdot K_2} \quad x_2 = \frac{K_1 \cdot K_2}{[H^+]^2 + K_1 \cdot [H^+] + K_1 \cdot K_2} \quad \text{where, } x_0 + x_1 + x_2 = 1 \text{ Being}$$

$$x_2 = \frac{K_1 \cdot K_2}{[H^+]^2 + K_1 \cdot [H^+] + K_1 \cdot K_2} \quad \text{where, } x_0 + x_1 + x_2 = 1 \text{ Being}$$

$$= \frac{K_1 \cdot K_2}{[H^+]^2 + K_1 \cdot [H^+] + K_1 \cdot K_2} \quad \text{where, } x_0 + x_1 + x_2 = 1 \text{ Being}$$

$$x_0 + x_1 + x_2 = 1 \text{ Being}$$

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Analgesics/anti-inflammatories	4-Acetylaminoantipyrine		100	
Analgesics/anti-inflammatories	4-FormylAminoAntipyrine		100	
Analgesics/anti-inflammatories	6-Acetylmorphine	91.43	8.53	0.03
Analgesics/anti-inflammatories	Acetaminophen		99.86	0.14
Analgesics/anti-inflammatories	Acetylcodeine	91.28	8.72	
Analgesics/anti-inflammatories	Acetylsalicylic acid		0.03	99.97
Analgesics/anti-inflammatories	Alfentanil	86.85	13.15	
Analgesics/anti-inflammatories	Aminopyrine	0.32	99.68	
Analgesics/anti-inflammatories	Betamethasone 17,21-dipropionate		100	
Analgesics/anti-inflammatories	Buprenorphine	95.32	4.67	0.02
Analgesics/anti-inflammatories	Buprenorphine glucuronide	0.01	95.12	4.88
Analgesics/anti-inflammatories	Carisoprodol		100	
Analgesics/anti-inflammatories	Codeine	94.44	5.56	
Analgesics/anti-inflammatories	Dextromethorphan	99.26	0.74	
Analgesics/anti-inflammatories	Dextropropoxyphene	99.36	0.64	
Analgesics/anti-inflammatories	Diclofenac		0.15	99.85
Analgesics/anti-inflammatories	Etodolac		0.20	99.80
Analgesics/anti-inflammatories	Fentanyl	98.81	1.19	
Analgesics/anti-inflammatories	Hydrocodone	97.07	2.93	
Analgesics/anti-inflammatories	Hydromorphone	97.12	2.87	0.01
Analgesics/anti-inflammatories	Ibuprofen		0.26	99.74
Analgesics/anti-inflammatories	Ketoprofen		0.17	99.83
Analgesics/anti-inflammatories	Lidocaine	90.12	9.88	
Analgesics/anti-inflammatories	Meloxicam		0.32	99.68
Analgesics/anti-inflammatories	Morphine	94.66	5.32	0.02
Analgesics/anti-inflammatories	Morphine-6-β-D-glucuronide	0.01	92.48	7.52
Analgesics/anti-inflammatories	Naproxen		0.69	99.31
Analgesics/anti-inflammatories	Norfentanyl	99.85	0.15	
Analgesics/anti-inflammatories	Norpethidine	99.74	0.26	
Analgesics/anti-inflammatories	Norpropoxyphene	99.92	0.08	
Analgesics/anti-inflammatories	O-Desmethyltramadol	99.75	0.24	
Analgesics/anti-inflammatories	Oxycodone	78.79	21.21	
Analgesics/anti-inflammatories	Oxymorphone	79.06	20.80	0.14
Analgesics/anti-inflammatories	Pentazocine	98.86	1.14	
Analgesics/anti-inflammatories	Pethidine	87.37	12.63	
Analgesics/anti-inflammatories	Phenylbutazone		0.43	99.57
Analgesics/anti-inflammatories	Procaine	99.43	0.57	
Analgesics/anti-inflammatories	Tolfenamic acid		0.05	99.95
Analgesics/anti-inflammatories	Tramadol	99.76	0.24	
Antiarrhythmic agents	Amiodarone	99.58	0.42	
Antiarrhythmic agents	Digitoxin		100	

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Antiarrhythmic agents	Propafenone	99.51	0.49	
Antiarrhythmic agents	Strophanthidin		100	
Antiarrhythmic agents	Strophanthin	n.a.	n.a.	n.a.
Antibiotics	2-NP-AOZ		100	
Antibiotics	Amoxicillin	0.00	57.99	42.01
Antibiotics	Azithromycin	97.49	2.51	
Antibiotics	Cinoxacin		0.21	99.79
Antibiotics	Ciprofloxacin	20.86	77.52	1.62
Antibiotics	Clarithromycin	93.53	6.47	
Antibiotics	Doxycycline	0.32	99.67	0.01
Antibiotics	Enoxacin	9.34	85.16	5.50
Antibiotics	Erythromycin	93.53	6.47	
Antibiotics	Flumequine		4.77	95.23
Antibiotics	Furazolidon		100	
Antibiotics	Lomefloxacin		97.38	2.62
Antibiotics	Metronidazole		100	
Antibiotics	Minocycline	0.32	99.68	0.01
Antibiotics	Nalidixic acid		11.65	88.35
Antibiotics	Norfloxacin		97.95	2.05
Antibiotics	Ofloxacin	1.07	69.34	29.58
Antibiotics	Oleandomycin	93.53	6.47	
Antibiotics	Oxolinic acid		8.01	91.99
Antibiotics	Oxytetracycline	0.32	99.67	0.02
Antibiotics	Penicillin G			100
Antibiotics	Pipemidic acid	0.13	96.87	2.99
Antibiotics	Roxithromycin	93.53	6.47	
Antibiotics	Silvadene		39.23	60.77
Antibiotics	Spiramycin	n.a.	n.a.	n.a.
Antibiotics	Sulfabenzamide		0.70	99.30
Antibiotics	Sulfadimethoxine		13.95	86.05
Antibiotics	Sulfadimidine		88.59	11.41
Antibiotics	Sulfafurazole		0.67	99.33
Antibiotics	Sulfaguanidine		99.99	0.01
Antibiotics	Sulfamerazine		69.12	30.88
Antibiotics	Sulfamethizole		3.13	96.87
Antibiotics	Sulfamethoxazole		6.06	93.94
Antibiotics	Sulfamethoxydiazine		27.55	72.45
Antibiotics	Sulfamethoxypyridazine		60.77	39.23
Antibiotics	Sulfanilamide		99.92	0.08
Antibiotics	Sulfaphenazole		22.79	77.21
Antibiotics	Sulfapyridine	0.00	97.20	2.80
Antibiotics	Sulfathiazole		63.47	36.53

Table S3. (continued)

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Antibiotics	Tinidazole		100	
Antibiotics	Trimethoprim	52.30	47.70	
Antifungals	Sulfacetamide		2.62	97.38
Antifungals	Terbinafine	45.41	54.59	
Antifungals	Tiabendazole	0.03	99.95	0.03
Antihistamines	Diphenhydramine	98.29	1.71	
Antihistamines	Promethazine	98.96	1.04	
Antihypertensive	Clonidine	92.64	7.36	
Antiparasitics	Albendazole	2.29	97.69	0.02
Antiparasitics	Flubendazole	0.28	99.70	0.02
Antiparasitics	Levamisole	99.90	0.10	
Antiparasitics	Mebendazole	0.50	99.49	0.01
Antiparasitics	Praziquantel		100	
Antiparasitics	Triclabendazole	0.04	89.01	10.95
Antiseptic	Nitrofurantoin		99.99	0.01
Beta-blockers	Atenolol	99.63	0.37	
Beta-blockers	Bisoprolol	99.62	0.38	
Beta-blockers	Metoprolol	99.63	0.37	
Calcium channel blocker	Verapamil	98.94	1.06	
Diuretic	Torsemide		2.09	97.91
Hormones	Fludrocortisone acetate		100	
Hormones	Flumethasone		100	
Hormones	Hydrocortisone		100	
Hormones	Methylprednisolone		100	
Hormones	Mometasone furoate		100	
Hormones	Prednicarbate		100	
Hormones	Prednisolone		100	
Hormones	Triamcinolone		100	
Hormones	Triamcinolone acetonide		100	
Illicit drugs	Amphetamine	99.89	0.11	
Illicit drugs	Benzoyllecgonine	0.02	99.96	0.01
Illicit drugs	Cannabinol		99.60	0.40
Illicit drugs	Cocaine	99.10	0.90	
Illicit drugs	Cocaine		98.94	1.06
Illicit drugs	Ecgonine methyl ester	99.73	0.27	
Illicit drugs	Ketamine	22.38	77.62	
Illicit drugs	MDA	99.89	0.11	
Illicit drugs	MDEA	99.95	0.05	
Illicit drugs	MDMA	99.95	0.05	
Illicit drugs	Methamphetamine	99.96	0.04	
Illicit drugs	Phencyclidine	94.19	5.81	
Illicit drugs	THC		99.85	0.15

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Plastic additives	Benzotriazole		96.00	4.00
Plastic additives	p-Toluenesulfonamide		99.94	0.06
Psychiatric drugs	10-Hydroxycarbazepine		100	
Psychiatric drugs	7-Aminoclonazepam	0.06	99.94	
Psychiatric drugs	7-Aminoflunitrazepam	0.11	99.89	
Psychiatric drugs	Alprazolam	0.00	100	
Psychiatric drugs	Amisulpride	98.94	1.06	
Psychiatric drugs	Amitriptyline	99.34	0.66	
Psychiatric drugs	Amoxapine	97.66	2.34	
Psychiatric drugs	Bromazepam		100	
Psychiatric drugs	Carbamazepine		100	
Psychiatric drugs	Chlordiazepoxide		100	
Psychiatric drugs	Chlorprothixene	99.12	0.88	
Psychiatric drugs	Citalopram	99.73	0.27	
Psychiatric drugs	Clobazam		97.49	2.51
Psychiatric drugs	Clomipramine		99.65	0.35
Psychiatric drugs	Clonazepam		99.99	0.01
Psychiatric drugs	Clorazepate		0.03	99.97
Psychiatric drugs	Clozapine	68.13	31.87	
Psychiatric drugs	Desalkylflurazepam		100	
Psychiatric drugs	Desipramine	99.96	0.04	
Psychiatric drugs	Desvenlafaxine	99.53	0.47	
Psychiatric drugs	Dexametasone		100	
Psychiatric drugs	Diazepam	0.03	99.97	
Psychiatric drugs	Dothiepin	99.56	0.44	
Psychiatric drugs	Doxepin	99.60	0.40	
Psychiatric drugs	EDDP	83.68	16.32	
Psychiatric drugs	Felbamate		100	
Psychiatric drugs	Fluoxetine	99.91	0.09	
Psychiatric drugs	Flupentixol	64.54	35.46	
Psychiatric drugs	Flurazepam	99.84	0.16	
Psychiatric drugs	Fluvoxamine	99.59	0.41	
Psychiatric drugs	Gabapentin	0.52	99.42	0.05
Psychiatric drugs	Haloperidol	91.64	8.36	
Psychiatric drugs	Imipramine	99.68	0.32	
Psychiatric drugs	Lamotrigine	2.40	97.60	
Psychiatric drugs	Lorazepam		99.98	0.02
Psychiatric drugs	Maprotiline		99.98	0.02
Psychiatric drugs	Medazepam	13.15	86.85	
Psychiatric drugs	Memantine	99.98	0.02	
Psychiatric drugs	Methadone	99.12	0.88	
Psychiatric drugs	Methylphenidate	99.69	0.31	

Table S3. (continued)

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Psychiatric drugs	Mianserin	94.79	5.21	
Psychiatric drugs	Mirtazapine	92.64	7.36	
Psychiatric drugs	Naltrexone	75.85	23.99	0.17
Psychiatric drugs	<i>N-Desmethylclozapine</i>	96.87	3.13	
Psychiatric drugs	Nitrazepam		100	
Psychiatric drugs	<i>Norbuprenorphine</i>	99.28	0.72	
Psychiatric drugs	Nordiazepam	0.02	99.98	
Psychiatric drugs	Nortriptyline	99.90	0.10	
Psychiatric drugs	Olanzapine	85.77	14.23	
Psychiatric drugs	Opipramol	73.81	26.19	
Psychiatric drugs	Oxazepam		99.99	0.01
Psychiatric drugs	Oxcarbazepine		100	
Psychiatric drugs	Paliperidone	92.16	7.84	
Psychiatric drugs	Paroxetine	99.79	0.21	
Psychiatric drugs	Phenazepam		100.00	
Psychiatric drugs	Phenytol		95.01	4.99
Psychiatric drugs	Pipamperone	92.32	7.68	
Psychiatric drugs	Prazepam	0.03	99.97	
Psychiatric drugs	Promazine	99.63	0.37	
Psychiatric drugs	Protriptyline	99.98	0.02	
Psychiatric drugs	Quetiapine	35.46	64.54	
Psychiatric drugs	Risperidone	92.16	7.84	
Psychiatric drugs	<i>Ritalinic acid</i>	0.03	99.94	0.03
Psychiatric drugs	Secobarbital		86.59	13.41
Psychiatric drugs	Sertraline	99.66	0.34	
Psychiatric drugs	Temazepam		100	
Psychiatric drugs	Topiramate		99.40	0.60
Psychiatric drugs	Trazodone	76.81	23.19	
Psychiatric drugs	Triazolam			100
Psychiatric drugs	Trimipramine	99.58	0.42	
Psychiatric drugs	Venlafaxine	99.45	0.55	
Psychiatric drugs	Zolpidem	37.06	62.94	
Psychiatric drugs	Zopiclone	33.39	66.61	
Psychiatric drugs	<i>α-Hydroxyalprazolam</i>		100	
Psychiatric drugs	<i>α-Hydroxymidazolam</i>	0.04	99.96	
Psychiatric drugs	<i>α-Hydroxytriazolam</i>		100	
Receptor antagonists	Atropine	99.90	0.10	
Receptor antagonists	Flumazenil		100	
Stimulants	Caffeine		100	
Stimulants	<i>Cotinine</i>	0.52	99.48	
Stimulants	Phentermine	99.89	0.11	
UV filter	Octinoxate	--	--	--

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Veterinary drugs	Carprofen		0.69	99.31
Veterinary drugs	Diaveridine	56.30	43.70	
Veterinary drugs	Difloxacin	9.62	65.06	25.31
Veterinary drugs	Dimetridazole	0.01	99.99	
Veterinary drugs	Enrofloxacin	18.65	69.30	12.04
Veterinary drugs	Flunixin		0.63	99.37
Veterinary drugs	Furaltadone	13.41	86.59	
Veterinary drugs	Ipronidazole		100	
Veterinary drugs	Marbofloxacin	6.70	64.03	29.27
Veterinary drugs	Monensin		0.18	99.82
Veterinary drugs	Orbifloxacin	18.15	79.23	2.62
Veterinary drugs	Oxibendazole	6.47	93.51	0.02
Veterinary drugs	Ronidazole		100	
Veterinary drugs	Salinomycin		0.23	99.77
Veterinary drugs	Sarafloxacin	12.65	85.56	1.79
Veterinary drugs	Sulfachlorpyridazine		7.36	92.64
Veterinary drugs	Sulfaclozine		0.67	99.33
Veterinary drugs	Sulfadoxine		12.63	87.37
Veterinary drugs	Sulfamonomethoxine	0.00	31.87	68.13
Veterinary drugs	Sulfanitran		72.45	27.55
Veterinary drugs	Sulfaquinolaxline		4.28	95.72
Veterinary drugs	Tilmicosin	99.74	0.26	
X-ray contrast medium	Iopromide		99.98	0.02

Legend

“n.a.” The charge was not calculated due to unavailable pK_a values from the CAS SciFinder[®].

Table S4. Calculated percentage of ionic forms of the non-target OMPs at pH = 7. The transformation products are written in italics.

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Analgesics/anti-inflammatories	<i>2,6-Xylidine / Lidocaine-M / Dimethylaniline</i>	0.20	99.80	
Analgesics/anti-inflammatories	Azelastine	99.31	0.69	
Analgesics/anti-inflammatories	Benzocaine		100	
Analgesics/anti-inflammatories	<i>Depropionylbezitramide</i>	94.19	5.81	
Analgesics/anti-inflammatories	<i>Dimethylaminophenazone</i>	0.32	99.68	

Table S3. (continued)

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Analgesics/anti-inflammatories	Fenoprofen		0.16	99.84
Analgesics/anti-inflammatories	Metaxalone		100	
Analgesics/anti-inflammatories	Niflumic acid		0.51	99.49
Analgesics/anti-inflammatories	Parsalimide	0.09	99.91	
Analgesics/anti-inflammatories	Propacetamol	92.32	7.68	
Analgesics/anti-inflammatories	Tapentadol	99.65	0.35	
Analgesics/anti-inflammatories	<i>Tramadol-N-oxide</i>	0.55	99.45	
Antiacids	Lansoprazole	0.04	99.68	0.27
Antiacids	Omeprazole	0.51	97.86	1.62
Antiacids	Troxipide	99.52	0.48	
Antiarrhythmic agent	Flecainide	99.80	0.20	
Antibiotics	<i>2-Hydroxyquinoline</i>		100	
Antibiotics	<i>Azithromycin 3'-N-oxide</i>	97.49	2.51	
Antibiotics	<i>Azithromycin N'-(Desmethyl)</i>	99.16	0.84	
Antibiotics	Cefalexin	0.01	40.89	59.10
Antibiotics	Cefoxitin			100
Antibiotics	<i>Clarithromycin-N-oxide</i>	0.13	99.87	
Antibiotics	<i>Erythromycin A enol ether</i>	93.10	6.90	
Antibiotics	Gatifloxacin	20.89	77.63	1.48
Antibiotics	Moxifloxacin	21.20	78.78	0.02
Antibiotics	N4-Acetylsulfamethoxazole		3.83	96.17
Antibiotics	Pazufloxacin	0.61	54.26	45.13
Antibiotics	Rifaximin		3.83	96.17
Anti-cancer drug	Cyclophosphamide	0.01	99.99	
Anti-cancer drug	Cytarabine	0.18	99.82	
Anti-cancer drug	Flutamide		100	
Anti-cancer drug	Lapatinib	17.95	82.05	
Antidiabetic drug	Metformin	100		
Antidiabetic drug	Sitagliptin	61.31	38.69	
Antiemetic	Metoclopramide	99.18	0.82	
Antigout preparation	Allopurinol		99.37	0.63
Antihistamine	Fexofenadine	0.27	99.35	0.38
Antihypertensives	Candesartan		3.83	96.17
Antihypertensives	Irbesartan		0.14	99.86
Antihypertensives	Losartan		0.24	99.75
Antihypertensives	Nitrendipin	0.01	99.99	
Antihypertensives	Olmesartan		0.35	99.65
Antihypertensives	Sotalol	94.99	4.99	0.02
Antihypertensives	Telmisartan		1.01	98.99
Antihypertensives	Valsartan		0.04	99.96
Antiparasitics	Hydroxychloroquine	98.67	1.33	
Antiseptics	4-Chloroaniline	0.09	99.91	

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Antiseptics	Chlorhexidine	100		
Antithrombotics	Clopidogrel	0.36	99.64	
Antithrombotics	Dabigatran	0.15	99.85	
Beta-blockers	<i>Desacetylmepipranolol</i>	99.79	0.21	
Beta-blockers	<i>Metoprolol acid</i>	0.26	99.39	0.35
Bronchodilators	Terbutaline	99.23	0.77	0.00
Bronchodilators	Theophylline		97.55	2.45
Food additives	Methylsalicylate		99.83	0.17
Food additives	Triethyl citrate		100	
Hormones	Boldione			
Hormones	Paramethasone acetate		100	
Illicit drug	<i>Norcocaine</i>	0.02	99.96	0.02
Lipid regulators	Atorvastatin		0.19	99.81
Lipid regulators	Bezafibrate		0.02	99.98
Other	1,2-Benzisothiazolinone		99.94	0.06
Other	1-Methylimidazole	100		
Other	1-Naphthylamine	0.16	99.84	
Other	2,2'-Oxamido bis-[ethyl-3-(3,5-di-t-butyl-4-hydroxyphenyl) propionate]		100	
Other	Indole		100	
Other	MIT / Methylisothiazolinone		100	
Other	NDEA / Nitrosodiethylamine		100	
Other	Nicopholine	0.13	99.87	
Other	Picaridin / Bayrepel / Icaridin		100	
Pesticide	DEET / Diethyltoluamide		100	
Plastic additive	5-Methyl-1H-benzotriazole		98.21	1.79
Psychiatric drugs	<i>10,11-Dihydro-10-hydroxycarbamazepine</i>		100	
Psychiatric drugs	Acridine / Carbamazepine-M	3.50	96.50	
Psychiatric drugs	<i>Carbamazepine 10,11-epoxide</i>		100	
Psychiatric drugs	Levetiracetam	n.a.	n.a.	n.a.
Psychiatric drugs	<i>Norcitalopram / Desmethylcitalopram</i>	99.97	0.03	
Psychiatric drugs	Pregabalin	0.17	99.83	
Psychiatric drugs	Propyperone	89.05	10.95	
Psychiatric drugs	Sulpiride	98.94	1.06	
Stimulants	<i>3-Hydroxycotinine</i>	0.52	99.48	
Stimulants	Nicotine	90.91	9.09	
Stimulants	<i>Paraxanthine</i>		96.93	3.07
Stimulants	Theobromine		99.87	0.13

Table S3. (continued)

Class	Compound	cationic form (%)	neutral/zwitterionic form (%)	anionic form (%)
Synthetic musks	AHDI / Phantolide	n.a.	n.a.	n.a.
Synthetic musks	Ceolestolide	n.a.	n.a.	n.a.
UV filter	Dioxybenzone / Benzophenone-8		56.30	43.70
X-ray contrast media	Diatrizoate / Amidotrizoic acid			100
X-ray contrast media	Iohexol		100	
X-ray contrast media	Iopamidol		99.99	0.01

Legend

"n.a." The charge was not calculated due to unavailable pK_a values from the CAS SciFinder[®].

Table S5. List of conventional parameters analyzed and corresponding analytical methods.

Parameter	Unit	Analytical method
<i>Wastewater</i>		
COD	mg/L	ISO 15705 par 10.2:2002
BOD ₅	mg/L	APHA Standard Methods for the Examination of Water and Wastewater ed 23 rd 2017 5210 D
DOC	mg/L	APHA Standard Methods for the Examination of Water and Wastewater ed 23 rd 2017 5310 B
UV ₂₅₄ absorbance	ABS/cm	APHA Standard Methods for the Examination of Water and Wastewater ed 23 rd 2017 5910 A B
Total suspended solids (TSS)	g/L	CNR IRSA 1A Q 64 Vol. 2 1984
Volatile suspended solids (VSS)	% of TSS	CNR IRSA 1A Q 64 Vol. 2 1984
N-NH ₄ ⁺	mg/L	APAT CNR IRSA 4030 A1 Man 29 2003
N-NO ₃ ⁻	mg/L	APAT CNR IRSA 4020 Man 29 2003
N-NO ₂ ⁻	mg/L	APAT CNR IRSA 4050 Man 29 2003
Total nitrogen (N _{tot})	mg/L	UNI EN 12260:2004
Total phosphorous (P _{tot})	mg/L	UNI EN ISO 6878:2004
Anionic surfactants (MBAS assay)	mg/L	M10R759.0 rev. 0 2015
Non-anionic surfactants (BIAS procedure)	mg/L	M10R759.0 rev. 0 2015
Cationic surfactants	mg/L	M10R759.0 rev. 0 2015
Total surfactants	mg/L	M10R759.0 rev. 0 2015
Acute Toxicity Test with <i>Daphnia magna</i>	Mortality (%)	APAT CNR IRSA 8020 B Man 29 2003
<i>Escherichia coli</i>	UFC/100 mL	M10P509.0 rev 4 2015 and APAT CNR IRSA 7030 D Man 29 2003
<i>Mixed liquor</i>		
Total suspended solids (TSS)	g/L	CNR IRSA 1A Q 64 Vol. 2 1984
DOC	mg/L	APHA Standard Methods for the Examination of Water and Wastewater ed 23 rd 2017 5310 B
UV ₂₅₄ absorbance	ABS/cm	APHA Standard Methods for the Examination of Water and Wastewater ed 23 rd 2017 5910 A B

Table S6. Compound method for the 232 OMP target analytes. ^A = Stipaničev et al. (2017).

Name	CAS#	Formula	Transition	Transition 1	Transition 2	LOD (ng/L)	LOQ (ng/L)	CF R2	RT	Mass Accuracy
2-NP-AOZ	19687-73-1	C10H9N3O4	236.0666	134.0243	236.0688	1	6.64	0.9970	8.81	5.55
4-Acetylaminoantipyrine	83-15-8	C13H15N3O2	246.1237	205.1155	204.1124	1.92	6.41	0.9998	6.56	6.44
4-FormylAminoAntipyrine	1672-58-8	C12H13N3O2	232.1081	214.0975	215.0994	1.17	3.90	0.9969	6.39	0.08
6-Acetylmorphine	2784-73-8	C19H21NO4	328.1543	165.0699	181.0648	1.33	4.43	0.9997	6.04	2.84
7-Aminoclonazepam	4959-17-5	C15H12ClN3O	284.1194	135.0917	226.0901	0.81	2.70	0.9994	9.18	7.82
7-Aminoflunitrazepam	34084-50-9	C16H14FN3O	284.1194	240.0932	256.1240	0.81	2.70	0.9996	9.18	7.82
10-Hydroxycarbazepine	29331-92-8	C15H14N2O2	255.1128	194.0964	179.0730	1.34 ^A	4.48 ^A	0.9977	10.31	1.00
Acetaminophen	103-90-2	C8H9NO2	152.0706	65.0386	109.0522	5.09	16.98	0.9997	4.54	-0.32
Acetylcodeine	6703-27-1	C20H23NO4	342.1700	225.0910	282.1489	1.90	6.34	0.9994	8.23	3.17
Albendazole	54965-21-8	C12H15N3O2S	266.0958	234.0696	191.0148	1.42	4.73	0.9977	13.86	1.79
Alfentanil	71195-58-9	C21H32N6O3	417.2609	268.1768	197.1285	0.80	2.68	0.9990	11.33	2.49
alpha-Hydroxyalprazolam	37115-43-8	C17H13ClN4O	325.0851	216.0808	243.0917	2.61	8.71	0.9978	12.74	-0.31
alpha-Hydroxymidazolam	59468-90-5	C18H13ClFN3O	342.0804	168.0682	203.0366	0.70	2.34	0.9998	12.77	1.33
alpha-Hydroxytriazolam	37115-45-0	C17H12Cl2N4O	359.0461	331.0274	250.0418	1.80	6.00	0.9992	12.46	0.79
Alprazolam	28981-97-7	C17H13ClN4	309.0902	281.0714	205.0761	1.56	5.21	0.9994	13.23	3.84
Aminopyrine	58-15-1	C13H17N3O	232.1444	56.0495	98.0839	3.81	12.71	0.9990	6.21	-0.78
Amiodarone	1951-25-3	C25H29I2NO3	646.0310	100.1121	86.0964	2.72	9.05	0.9988	17.08	2.57
Amisulpride	71675-85-9	C17H27N3O4S	370.1795	242.0482	112.1121	1.49	4.97	0.9994	6.62	3.16
Amitriptyline	50-48-6	C20H23N	278.1903	233.1325	91.0542	1.32	4.39	0.9995	12.98	3.68
Amoxapine	14028-44-5	C17H16ClN3O	314.1055	271.0633	193.0522	1.85	6.18	0.9987	12.63	1.64
Amoxicillin	61336-70-7	C16H19N3O5S	366.1118	114.0008	134.0600	2.04	6.79	0.9982	6.04	-4.02
Amphetamine	300-62-9	C9H13N	136.1121	91.0542	65.0386	2.03	6.78	0.9979	6.27	-0.75
Acetylsalicylic acid	50-78-2	C9H8O4	181.0495	149.0236	150.0267	3.39	11.31	0.9953	8.03	3.54
Atenolol	29122-68-7	C14H22N2O3	267.1703	145.0648	56.0495	1.20	3.99	0.9993	4.66	4.16
Atropine	51-55-8	C17H23NO3	290.1751	93.0699	124.1121	2.04	6.81	0.9994	7.21	6.06
Azithromycin	83905-01-5	C38H72N2O12	749.5158	158.1176	591.4215	2.80	9.33	0.9963	10.82	-0.40
Benzoylcegonine	519-09-5	C16H19NO4	290.1387	168.1019	105.0335	1.93	6.42	0.9986	7.61	7.50
Betamethasone 17,21-dipropionate	5593-20-4	C28H37FO7	505.2596	209.0819	453.2053	2.52	8.39	0.9991	16.53	0.71
Bisoprolol	66722-44-9	C18H31NO4	326.2326	74.0600	56.0495	2.58	8.59	0.9971	10.53	4.59
Bromazepam	1812-30-2	C14H10BrN3O	318.0061	182.0839	209.0947	1.89	6.30	0.9996	11.82	-0.25
BTA / Benzotriazole	95-14-7	C6H5N3	120.0556	65.0386	92.0495	1.65	5.50	0.9995	4.85	-2.46
Buprenorphine	52485-79-7	C29H41NO4	468.3108	414.2639	396.2169	0.97	3.25	0.9995	11.98	2.83
Buprenorphine glucuronide	101224-22-0	C35H49NO10	644.3429	468.3108	414.2639	3.71	12.38	0.9994	9.82	-0.62
Caffeine	58-08-2	C8H10N4O2	195.0877	138.0662	110.0713	1.54	5.14	0.9990	6.83	0.03
Carbamazepine	298-46-4	C15H12N2O	237.1022	193.0886	179.0730	0.79	2.64	0.9982	12.25	7.27
Carisoprodol	78-44-4	C12H24N2O4	261.1809	55.0542	62.0237	3.11	10.35	0.9975	12.96	-0.48
Carprofen	53716-49-7	C15H12ClNO2	274.0629	228.0586	190.0662	1.86	6.20	0.9981	15.82	5.77
CBN / Cannabinol	521-35-7	C21H26O2	311.2006	208.0883	179.0855	4.55	15.16	0.9983	18.31	1.29
Chlordiazepoxide	58-25-3	C16H14ClN3O	300.0898	282.0793	227.0496	2.16	7.19	0.9994	12.46	0.90
Chlorprothixene	113-59-7	C18H18ClNS	316.0921	231.0030	271.0343	3.32	11.05	0.9985	14.12	3.13
Cinoxacin	28657-80-9	C12H10N2O5	263.0662	245.0557	189.0295	1.12	3.72	0.9994	9.46	1.16
Ciprofloxacin	85721-33-1	C17H18FN3O3	332.1405	294.1237	314.1299	3.19	10.64	0.9986	7.70	1.31

Table S6. (continued)

Name	CAS#	Formula	Transition	Transition 1	Transition 2	LOD (ng/L)	LOQ (ng/L)	CF R2	RT	Mass Accuracy
Citalopram	59729-33-8	C20H21FN2O	325.1711	109.0448	234.0714	2.36	7.86	0.9994	11.09	6.82
Clarithromycin	81103-11-9	C38H69NO13	748.4842	158.1176	590.3899	2.27	7.55	0.9968	14.43	1.87
Clobazam	22316-47-8	C16H13CIN2O2	301.0738	224.0944	259.0633	1.35	4.51	0.9983	12.88	2.43
Clomipramine	303-49-1	C19H23CIN2	315.1623	86.0964	58.0651	1.67	5.57	0.9971	14.17	3.16
Clonazepam	1622-61-3	C15H10CIN3O3	316.0483	270.0554	207.0917	2.41	8.04	0.9986	12.34	1.13
Clonidine	4205-90-7	C9H9Cl2N3	230.0246	159.9715	144.9606	0.26	0.88	0.9983	5.82	1.68
Clorazepate	23887-31-2	C16H13CIN2O4	333.0637	126.0108	156.0771	3.16	10.55	0.9992	7.92	-0.82
Clozapine	5786-21-0	C18H19CIN4	327.1371	270.0793	84.0809	1.16	3.88	0.9985	11.62	4.19
Cocaethylene	529-38-4	C23H32O5	318.1700	82.0651	105.0335	0.53	1.77	0.9964	9.68	2.76
Cocaine	50-36-2	C29H47NO6	304.1543	82.0651	182.1176	3.02	10.05	0.9988	8.54	1.96
Codeine	76-57-3	C18H21NO3	300.1594	199.0757	171.0804	1.69	5.63	0.9990	5.23	3.69
Cotinine	486-56-6	C14H12O2	177.1022	80.0495	98.0600	2.20	7.33	0.9951	3.66	2.13
Desalkylflurazepam	2886-65-9	C15H10ClFN2O	289.0538	140.0257	165.0209	0.86	2.87	0.9997	13.42	1.76
Desipramine	50-47-5	C18H22N2	267.1856	72.0808	193.0886	4.02	13.38	0.9974	13.06	3.83
Dexametasone	382-67-2	C22H29FO4	393.2072	237.1274	147.0804	3.20	10.68	0.9954	16.53	-2.57
Diaveridine	5355-16-8	C13H16N4O2	261.1346	123.0665	245.1033	1.64	5.47	0.9968	6.28	7.20
Diazepam	439-14-5	C16H13CIN2O	285.0789	193.0886	154.0417	1.48	4.94	0.9974	14.44	7.16
Diclofenac	15307-79-6	C14H11Cl2NO2	296.0240	214.0418	180.0808	0.89	2.97	0.9963	15.61	1.02
Difloxacin	98106-17-3	C21H19F2N3O3	400.1467	382.1362	299.0991	4.00	13.34	0.9986	8.31	1.36
Digitoxin	71-63-6	C41H64O13	787.4239	97.0648	113.0597	6.15	20.52	0.9974	16.31	-1.57
Dimetridazole	551-92-8	C5H7N3O2	142.0611	78.0338	96.0682	1.09	3.64	0.9984	14.21	6.21
Diphenhydramine	58-73-1	C17H21NO	256.1696	165.0699	152.0621	1.78	5.93	0.9985	11.28	0.67
Dothiepin	113-53-1	C19H21NS	296.1467	221.0420	203.0855	2.40	8.02	0.9992	12.36	3.56
Doxepin	1668-19-5	C19H21NO	280.1696	115.0542	107.0491	1.66	5.52	0.9991	11.57	2.82
Doxycycline	24390-14-5	C22H24N2O8	445.1605	98.0600	267.0652	1.47	4.88	0.9981	13.73	8.00
Dextromethorphan	125-71-3	C18H25NO	272.2009	171.0804	147.0804	1.58	5.28	0.9957	11.30	3.33
Ecgonine methyl ester	7143-09-1	C10H17NO3	200.1281	91.0542	94.0651	3.78	12.61	0.9990	17.19	6.71
EDDP	30223-73-5	C11H17O3PS	278.1913	234.1277	186.1277	0.79	2.65	0.9984	11.24	0.41
Enoxacin	74011-58-8	C15H17FN4O3	321.1357	303.1252	234.1038	2.71	9.02	0.9989	7.29	2.43
Enrofloxacin	93106-60-6	C19H22FN3O3	360.1718	316.1820	245.1084	2.14	7.12	0.9954	7.90	5.33
Erythromycin A	114-07-8	C37H67NO13	734.4685	233.1536	576.3742	2.75	9.16	0.9989	13.19	0.31
Etodolac	41340-25-4	C17H21NO3	286.1594	181.0897	212.1418	1.70	5.65	0.9996	3.44	-3.20
Felbamate	25451-15-4	C11H14N2O4	261.0846	115.0542	117.0699	1.79	5.98	0.9990	8.49	0.89
Phenazepam	51753-57-2	C15H10BrCIN2O	350.9716	242.0605	183.9756	2.94	9.80	0.9992	14.01	1.81
Fentanyl	437-38-7	C22H28N2O	337.2274	105.0699	188.1434	1.10 ^A	3.67 ^A	0.9981	10.72	2.27
Flubendazole	31430-15-6	C16H12FN3O3	314.0935	282.0673	123.0241	3.26	10.86	0.9994	13.31	1.73
Fludrocortisone-acetate	514-36-3	C23H31FO6	423.2177	181.1012	143.0855	3.81	12.69	0.9961	13.73	0.40
Flumazenil	78755-81-4	C15H14FN3O3	326.0911	258.0673	217.0396	3.87	12.89	0.9997	10.75	0.74
Flumequine	42835-25-6	C14H12FNO3	262.0874	244.0768	202.0287	1.83	6.09	0.9987	11.86	2.50
Flumethasone	2135-17-3	C22H28F2O5	411.1978	277.1587	275.1430	2.97	9.90	0.9989	16.54	6.20
Flunixin	38677-85-9	C14H11F3N2O2	297.0845	264.0505	279.0740	1.75	5.83	0.9964	14.62	7.73
Fluoxetine	54910-89-3	C17H18F3NO	310.1413	199.1842	149.0236	1.77	5.91	0.9969	13.35	2.20
Flupentixol	2709-56-0	C23H25F3N2OS	435.1712	305.0606	265.0293	1.59	5.30	0.9976	15.23	4.30

Table S6. (continued)

Name	CAS#	Formula	Transition	Transition 1	Transition 2	LOD (ng/L)	LOQ (ng/L)	CF R2	RT	Mass Accuracy
Flurazepam	17617-23-1	C21H23ClFN3O	388.1586	315.0695	317.0851	1.03	3.42	0.9985	11.29	2.96
Fluvoxamine	54739-18-3	C15H21F3N2O2	319.1628	71.0503	200.0682	1.44	4.80	0.9972	13.23	2.22
Furaltadone	139-91-3	C13H16N4O6	325.1143	100.0757	128.1070	2.82	9.41	0.9962	5.01	0.01
Furazolidon	67-45-8	C8H7N3O5	226.0458	67.0417	122.0111	1.68	5.60	0.9995	6.40	1.37
Gabapentin	60142-96-3	C9H17NO2	172.1332	67.0542	91.0542	0.88	2.92	0.9988	5.96	-1.18
Haloperidol	52-86-8	C21H23ClFNO2	376.1474	165.0710	123.0241	1.23	4.08	0.9984	11.84	3.41
Hydrocodone	125-29-1	C18H21NO3	300.1594	199.0754	171.0804	1.66	5.53	0.9957	5.22	3.27
Hydrocortisone	50-23-7	C21H30O5	363.2166	121.0648	97.0648	1.56	5.20	0.9987	12.67	0.06
Hydromorphone	466-99-9	C17H19NO3	286.1438	185.0597	157.0648	1.72	5.73	0.9998	3.44	1.32
Ibuprofen	15687-27-1	C13H18O2	207.1380	105.0707	162.1352	1.84 ^A	6.12 ^A	0.9974	9.52	8.18
Imipramine	50-49-7	C19H24N2	281.2012	58.0651	86.0964	0.49	1.64	0.9971	12.91	3.03
Iopromide	73334-07-3	C18H24I3N3O8	791.8770	558.8850	572.9007	1.01	3.35	0.9952	5.12	-0.57
Iprnidazole	14885-29-1	C7H11N3O2	170.0924	124.0995	109.0760	1.11	3.71	0.9991	7.08	7.44
Ketamine	6740-88-1	C13H16ClNO	238.0993	125.0153	128.0621	1.96	6.54	0.9966	8.02	2.21
Ketoprofen	22071-15-4	C16H14O3	255.1016	77.0386	103.0542	4.02	13.40	0.9983	13.64	-0.02
Lamotrigine	84057-84-1	C9H7Cl2N5	256.0151	156.9606	58.0400	1.14	3.79	0.9988	8.79	3.82
Levamisole	14769-73-4	C11H12N2S	205.0794	178.0685	91.0542	3.15	10.50	0.9994	5.67	0.35
Lidocaine	137-58-6	C14H22N2O	235.1805	86.0964	58.0651	1.29	4.30	0.9984	7.34	1.85
Lomefloxacin	98079-51-7	C17H19F2N3O3	352.1467	265.1147	334.1362	2.39	7.96	0.9991	8.04	1.50
Lorazepam	846-49-1	C15H10Cl2N2O2	321.0192	229.0527	275.0137	2.00	6.66	0.9962	13.11	1.02
Maprotiline	10262-69-8	C20H23N	278.1903	234.1283	186.1277	0.98	3.28	0.9984	11.24	3.94
Marbofloxacin	115550-35-1	C17H19FN4O4	363.1463	72.0781	345.1358	3.59	11.95	0.9966	6.75	1.25
MDA	4764-17-4	C10H13NO2	180.1019	79.0542	77.0386	3.56	11.86	0.9979	6.48	-0.45
MDEA (MDE)	82801-81-8	C12H17NO2	208.1332	105.0699	135.0441	1.69	5.63	0.9988	7.22	1.90
MDMA	42542-10-9	C11H15NO2	194.1176	77.0386	79.0542	1.42	4.73	0.9969	6.60	0.30
Mebendazole	31431-39-7	C16H13N3O3	296.1030	191.0862	134.0966	1.26	4.19	0.9993	12.92	1.98
Medazepam	2898-12-6	C16H15ClN2	271.0997	207.1043	242.0731	2.95	9.84	0.9995	11.96	0.76
Meloxicam	71125-38-7	C14H13N3O4S2	352.0420	115.0324	141.0117	2.04	6.79	0.9989	13.31	1.93
Memantine	19982-08-2	C12H21N	180.1747	91.0542	107.0855	1.91	6.38	0.9997	11.61	-0.29
Pethidine	57-42-1	C15H21NO2	248.1645	70.0651	91.0542	1.17	3.91	0.9985	9.16	4.68
Methadone	76-99-3	C11H15NO2	310.2165	105.0335	77.0386	3.19	10.62	0.9997	13.09	5.86
Methamphetamine	537-46-2	C10H15N	150.1277	91.0542	65.0386	0.96	3.18	0.9989	6.49	0.71
Methylphenidate	113-45-1	C14H19NO2	234.1489	84.0808	56.0495	4.20	13.99	0.9972	8.71	0.39
Methylprednisolone	83-43-2	C22H30O5	375.2166	161.0961	135.0804	5.07	16.90	0.9975	13.68	-0.38
Metoprolol	37350-58-6	C15H25NO3	268.1907	72.0808	56.0495	1.62	5.41	0.9970	13.06	-6.04
Metronidazole	443-48-1	C6H9N3O3	172.0717	128.0455	82.0526	1.46	4.87	0.9996	4.73	0.18
Mianserin	24219-97-4	C18H20N2	265.1699	58.0651	208.1121	1.50	5.01	0.9986	11.33	2.47
Minocycline	13614-98-7	C23H27N3O7	458.1922	337.0945	283.0839	3.47	11.57	0.9955	13.75	3.35
Mirtazapine	61337-67-5	C17H19N3	266.1652	195.0917	72.0808	2.05 ^A	6.83 ^A	0.9974	9.07	2.09
Mometasone furoate	83919-23-7	C27H30Cl2O6	543.1312	278.1665	355.1459	2.02	6.73	0.9969	15.90	0.18
Monensin	17090-79-8	C36H62O11	693.4184	675.4079	461.2820	2.44	8.14	0.9955	19.15	0.99
Morphine-6-β-D-glucuronide	20290-10-2	C23H27NO9	462.1759	286.1438	58.0651	1.20	3.98	0.9991	3.15	-0.67
Morphine	57-27-2	C17H19NO3	286.1438	165.0699	153.0699	1.72	5.73	0.9998	3.44	1.32

Table S6. (continued)

Name	CAS#	Formula	Transition	Transition 1	Transition 2	LOD (ng/L)	LOQ (ng/L)	CF R2	RT	Mass Accuracy
Nalidixic acid	389-08-2	C12H12N2O3	233.0921	159.0553	104.0495	3.53	11.76	0.9977	11.57	2.09
Naltrexone	16590-41-3	C20H23NO4	342.1700	55.0542	267.1254	2.40	7.99	0.9998	5.75	2.20
Naproxen	22204-53-1	C14H14O3	231.1016	185.0961	141.0699	1.19	3.96	0.9959	4.14	-6.86
N-Desmethyldiclozapine	6104-71-8	C17H17ClN4	313.1215	253.0523	192.0682	2.47	8.23	0.9969	11.58	2.59
Nitrazepam	146-22-5	C15H11N3O3	282.0873	236.0944	207.0917	2.99	9.96	0.9987	12.29	0.35
Nitrofurantoin	59-87-0	C6H6N4O4	199.0462	54.0100	69.0447	2.15	7.17	0.9997	6.44	-0.52
Norbuprenorphine	78715-23-8	C25H35NO4	414.2639	101.0961	83.0855	4.91	16.36	0.9972	10.61	-1.04
Nordiazepam	1088-11-5	C15H11ClN2O	271.0633	140.0257	165.0209	1.10	3.66	0.9987	15.82	1.10
Norfentanyl	1609-66-1	C14H20N2O	233.1648	84.0808	55.0542	1.19	3.96	0.9972	8.11	4.17
Norfloxacin	70458-96-7	C16H18FN3O3	320.1405	302.1299	276.1504	2.43	8.11	0.9962	7.46	0.51
Norpethidine	77-17-8	C14H19NO2	234.1489	56.0495	84.0808	1.73	5.77	0.9994	11.25	-8.16
Norpropoxyphene	3376-94-1	C21H27NO2	326.2121	91.0694	128.0842	1.73	5.76	0.9998	10.53	6.45
Nortriptyline	72-69-5	C19H21N	264.1747	91.0542	203.0855	1.47	4.89	0.9968	12.98	5.44
Octinoxate	5466-77-3	C18H26O3	291.1955	133.0635	79.0542	1.74	5.81	0.9997	7.21	-5.90
Desvenlafaxine	93413-62-8	C16H25NO2	264.1958	133.0648	107.0491	0.96	3.21	0.9959	8.17	2.05
O-Desmethyltramadol	73986-53-5	C15H23NO2	250.1802	58.0651	232.1696	1.22	4.07	0.9996	6.61	3.84
Ofloxacin	82419-36-1	C18H20FN3O4	362.1511	318.1612	261.1033	3.72	12.40	0.9990	7.24	1.51
Olanzapine	132539-06-1	C17H20N4S	313.1481	256.0903	198.0246	3.39	11.31	0.9954	6.88	1.03
Oleandomycin	3922-90-5	C35H61NO12	688.4267	158.1176	544.3453	2.11	7.03	0.9992	12.01	1.17
Opipramol	315-72-0	C23H29N3O	364.2383	143.1179	100.0757	1.29	4.29	0.9972	12.63	4.35
Orbifloxacin	113617-63-3	C19H20FN3O3	396.1530	352.1631	378.1424	2.31	7.71	0.9970	8.19	2.08
OTC / Oxytetracycline	2058-46-0	C22H24N2O9	461.1555	283.0561	201.0506	4.28	14.27	0.9993	13.71	3.31
Oxazepam	604-75-1	C15H11ClN2O2	287.0582	241.0527	104.0495	1.06	3.54	0.9988	14.45	64.57
Oxcarbazepine	28721-07-5	C15H12N2O2	253.0972	236.0706	180.0808	1.83	6.09	0.9989	11.78	-69.19
Oxibendazole	20559-55-1	C12H15N3O3	250.1186	176.0455	218.0924	0.96	3.21	0.9998	11.89	6.11
Oxolinic acid	14698-29-4	C13H11NO5	262.0710	160.0393	216.0291	1.50	5.00	0.9992	10.08	2.30
Oxycodone	76-42-6	C18H21NO4	316.1543	80.0498	298.1438	1.59	5.29	0.9989	5.59	1.97
Oxymorphone	76-41-5	C17H19NO4	302.1387	227.0941	198.0913	1.95	6.52	0.9992	3.72	0.62
Paliperidone	144598-75-4	C23H27FN4O3	427.2140	207.1128	110.0598	1.40	4.67	0.9955	9.51	3.16
Paroxetine	61869-08-7	C19H20FNO3	330.1500	192.1183	151.0390	3.02	10.07	0.9952	12.49	2.61
Phencyclidine	77-10-1	C17H25N	244.2060	91.0542	86.0964	3.80	12.67	0.9989	10.40	0.09
Penicillin G	113-98-4	C16H18N2O4S	335.1060	176.0706	160.0427	8.97	29.92	0.9958	15.13	27.92
Pentazocine	359-83-1	C19H27NO	286.2165	69.0699	218.1539	1.26	4.20	0.9984	10.01	8.68
Phenazepam	51753-57-2	C15H10BrClN2O	348.9738	206.0839	183.9756	2.50	8.33	0.9994	14.02	0.74
Phentermine	122-09-8	C10H15N	150.1277	91.0542	65.0386	2.55	8.51	0.9989	6.49	0.71
Phenylbutazone	50-33-9	C19H20N2O2	309.1598	92.0495	77.0386	1.72	5.72	0.9984	9.48	2.55
Phenytoin	57-41-0	C15H12N2O2	253.0972	180.0808	208.0757	4.89	16.29	0.9990	11.00	0.29
Pipamperone	1893-33-0	C21H30FN3O2	376.2395	165.0710	98.0600	2.08	6.95	0.9976	9.10	2.47
Pipemidic acid	51940-44-4	C14H17N5O3	304.1404	286.1299	217.1085	3.22	10.74	0.9978	6.48	1.50
Prazepam	2955-38-6	C19H17ClN2O	325.1102	271.0633	140.0261	1.19	3.96	0.9991	15.81	7.39
Praziquantel	55268-74-1	C19H24N2O2	313.1911	55.0542	83.0855	2.64	8.81	0.9974	14.43	1.50
Prednicarbate	73771-04-7	C27H36O8	511.2302	289.1587	307.1693	3.78	12.60	0.9996	16.09	-0.98
Prednisolone	50-24-8	C21H28O5	395.1631	147.0804	67.0542	6.51	21.69	0.9950	10.92	0.26

Table S6. (continued)

Name	CAS#	Formula	Transition	Transition 1	Transition 2	LOD (ng/L)	LOQ (ng/L)	CF R2	RT	Mass Accuracy
Procaine (Novocaine)	59-46-1	C13H20N2O2	237.1598	100.1121	120.0444	1.28	4.28	0.9988	4.86	2.17
Promazine	58-40-2	C17H20N2S	285.1420	86.0964	58.0651	3.92	13.07	0.9984	12.62	2.49
Promethazine	60-87-7	C17H20N2S	285.1420	198.0372	86.0964	2.97	9.91	0.9972	12.34	1.84
Propafenone	53-16-7	C18H22O2	342.2064	72.0808	116.1070	0.95	3.18	0.9967	12.85	6.91
Dextropropoxyphene	469-62-5	C22H29NO2	340.2271	58.0651	91.0542	5.15	17.16	0.9993	12.74	0.48
Protriptyline	438-60-8	C19H21N	264.1747	191.0855	91.0545	1.23	4.11	0.9989	13.00	5.58
p-Toluenesulfonamide	70-55-3	C7H9NO2S	172.0427	91.0542	119.0604	2.49	8.29	0.9988	10.07	3.96
Quetiapine	111974-69-7	C21H25N3O2S	384.1740	221.1073	253.0794	1.45	4.85	0.9993	11.78	5.03
Risperidone	106266-06-2	C23H27FN4O2	411.2191	191.1179	192.1236	1.48	4.93	0.9956	10.25	4.09
Ritalinic acid	19395-41-6	C13H17NO2	220.1332	84.0808	56.0495	2.29	7.62	0.9989	7.67	1.19
Ronidazole	7681-76-7	C6H8N4O4	223.0438	55.0417	140.0455	2.65	8.85	0.9972	4.58	-0.35
Roxithromycin	80214-83-1	C41H76N2O15	837.5319	679.4382	158.1176	4.19	13.97	0.9977	14.60	1.95
Salinomycin	53003-10-4	C42H70O11	768.5256	733.4888	531.3260	8.14	27.12	0.9960	12.73	-5.16
Sarafloxacin	98105-99-8	C20H17F2N3O3	386.1311	368.1205	342.1439	3.87	12.90	0.9986	8.49	0.84
Secobarbital	76-73-3	C12H18N2O3	256.1656	91.0552	176.1442	1.73	5.75	0.9964	11.28	1.28
Sertraline	79617-96-2	C17H17Cl2N	306.0811	158.9763	129.0699	2.79	9.32	0.9985	13.95	0.84
Spiramycin	8025-81-8	C43H74N2O14	843.5213	174.1125	101.0597	7.86	26.20	0.9966	10.29	0.06
Strophanthidin	66-28-4	C23H32O6	405.2310	145.0997	125.0589	3.96	13.20	0.9954	10.97	-9.97
Strophanthin	11005-63-3	C36H54O14	549.3065	405.2273	387.2164	4.44	14.81	0.9991	16.54	-1.82
Sulfabenzamide	127-71-9	C13H12N2O3S	277.0641	92.0495	65.0386	3.22	10.75	0.9986	8.49	-1.13
Sulfacetamide	144-80-9	C8H10N2O3S	237.0304	94.9895	65.0386	1.74	5.81	0.9977	3.92	0.64
Sulfachlorpyridazine	80-32-0	C10H9ClN4O2S	285.0208	157.0150	156.0118	1.10	3.65	0.9975	7.29	0.54
Sulfaclozine	102-65-8	C10H9ClN4O2S	285.0208	156.0118	108.0457	1.26	4.20	0.9976	7.29	0.54
Sulfadiazine	68-35-9	C10H10N4O2S	251.0597	92.0495	65.0386	2.29	7.63	0.9990	4.74	1.35
Sulfadimethoxine	122-11-2	C12H14N4O4S	311.0809	92.0495	108.0444	2.10	7.01	0.9971	7.92	3.98
Sulfadimidine	57-68-1	C12H14N4O2S	279.0910	124.0869	186.0332	1.97	6.56	0.9986	6.83	2.07
Sulfadoxine	2447-57-6	C12H14N4O4S	311.0809	140.0455	154.0611	2.74	9.12	0.9999	7.93	4.03
Sulfafurazole	127-69-5	C11H13N3O3S	268.0750	65.0386	113.0709	3.80	12.68	0.9996	7.87	2.44
Sulfaguandine	57-67-0	C7H10N4O2S	215.0597	65.0386	92.0495	1.42	4.75	0.9959	6.47	-3.22
Sulfamerazine	127-79-7	C11H12N4O2S	265.0754	92.0495	108.0430	2.05	6.82	0.9996	5.83	0.88
Sulfamethoxydiazine	651-06-9	C11H12N4O3S	281.0703	215.0930	156.0122	3.81	12.70	0.9998	6.44	0.47
Sulfamethizole	144-82-1	C9H10N4O2S2	271.0318	108.0444	92.0495	3.75 ^A	12.50 ^A	0.9978	6.56	0.86
Sulfamethoxazole	723-46-6	C10H11N3O3S	254.0594	65.0386	92.0468	1.81	6.04	0.9997	7.40	1.70
Sulfamethoxypridazine	80-35-3	C11H12N4O3S	281.0703	108.0444	92.0495	1.12	3.73	0.9998	6.44	0.47
Sulfamonomethoxine	1220-83-3	C11H12N4O3S	281.0703	126.0662	156.0100	1.67	5.57	0.9989	6.97	1.72
Sulfanilamide	63-74-1	C6H8N2O2S	173.0379	93.0573	65.0386	3.31	11.04	0.9976	10.07	1.31
Sulfanitran	122-16-7	C14H13N3O5S	336.0649	93.0335	65.0386	2.19	7.32	0.9959	13.32	3.41
Sulfaphenazole	526-08-9	C15H14N4O2S	315.0910	158.0713	92.0495	2.65	8.82	0.9993	8.95	1.02
Sulfapyridine	144-83-2	C11H11N3O2S	250.0645	156.0114	108.0444	1.68	5.59	0.9997	5.50	1.19
Sulfaquinoxaline	59-40-5	C14H12N4O2S	301.0754	108.0444	156.0114	1.49	4.97	0.9963	9.80	-0.31
Sulfathiazole	72-14-0	C9H9N3O2S2	256.0209	92.0495	108.0444	1.71	5.71	0.9984	8.79	-1.74
Tiabendazole	148-79-8	C10H7N3S	202.0433	131.0604	175.0325	0.68	2.26	0.9959	8.28	4.24
Temazepam	846-50-4	C16H13ClN2O2	301.0738	255.0684	177.0209	1.89	6.30	0.9990	13.51	1.78

Table S6. (continued)

Name	CAS#	Formula	Transition	Transition 1	Transition 2	LOD (ng/L)	LOQ (ng/L)	CF R2	RT	Mass Accuracy
Terbinafine	91161-71-6	C21H25N	292.2060	141.0699	115.0542	1.50	5.01	0.9970	14.21	4.02
THC	1972-08-3	C13H19NO2S	315.2319	123.0441	193.1223	2.91	9.71	0.9976	17.51	1.13
Tilmicosin	108050-54-0	C46H80N2O13	869.5733	174.1125	870.5847	3.83	12.76	0.9974	11.77	0.76
Tinidazole	19387-91-8	C8H13N3O4S	248.0700	82.0526	121.0318	2.12	7.08	0.9997	5.76	0.70
Tolfenamic acid	13710-19-5	C14H12ClNO2	262.0629	244.0524	229.0289	1.29	4.31	0.9966	10.08	3.13
Topiramate	97240-79-4	C12H21NO8S	340.1061	59.0491	55.0178	2.31	7.70	0.9972	5.20	2.71
Torsemide	56211-40-6	C16H20N4O3S	349.1329	183.0910	264.0798	2.41	8.03	0.9975	11.16	0.86
Tramadol	27203-92-5	C16H25NO2	264.1958	58.0651	58.0654	1.02 ^A	3.40 ^A	0.9969	8.55	4.57
Trazodone	19794-93-5	C19H22ClN5O	372.1586	176.0818	148.0524	1.87	6.24	0.9993	10.04	2.32
Triamcinolone	124-94-7	C21H27FO6	395.1864	147.0816	121.0648	0.99	3.30	0.9988	10.92	1.24
Triamcinolone acetonide	76-25-5	C24H31FO6	435.2177	147.0804	213.1274	1.92	6.42	0.9989	13.75	0.51
Triazolam	28911-01-5	C17H12Cl2N4	343.0512	308.0823	239.0389	1.23	4.11	0.9985	13.18	3.38
Triclabendazole	68786-66-3	C14H9Cl3N2O5	360.9545	273.9962	343.9339	1.00	3.32	0.9985	16.80	2.93
Trimethoprim	738-70-5	C14H18N4O3	291.1452	110.0587	81.0447	1.13	3.78	0.9988	6.64	6.84
Trimipramine	739-71-9	C20H26N2	295.2169	58.0651	100.1121	2.95	9.85	0.9961	13.37	3.95
Venlafaxine	93413-69-5	C17H27NO2	278.2115	58.0652	165.0714	0.76	2.54	0.9997	11.24	-1.88
Verapamil	52-53-9	C27H38N2O4	455.2904	165.0910	150.0675	1.17	3.90	0.9967	12.17	4.40
Zolpidem	82626-48-0	C19H21N3O	308.1757	235.1230	236.1308	1.15	3.82	0.9988	9.48	4.86
Zopiclone	43200-80-2	C17H17ClN6O3	411.0943	245.0220	217.0271	3.77	12.58	0.9996	8.25	-0.43

Legend

LOD = Limit of detection; LOQ = Limit of quantification; CF R2 = ; RT = Retention time

Table S7. Compound method for the 90 non-target analytes in the non-target screening (NTS).

Name	CAS#	Formula	Product Ion	Qualifier 1	Qualifier 2	RT
1,2-Benzisothiazolinone	2634-33-5	C7H5NOS	152.0165	-109.0107	-134.0059	9.05
10,11-Dihydro-10-hydroxycarbamazepine	29331-92-8	C15H14N2O2	255.1128	-114	-113.1077	12.78
1-Methylimidazole	616-47-7	C4H6N2	83.0604	-69	-68.0365	6.63
1-Naphthylamine	134-32-7	C10H9N	144.0808	-55	-91.0542	6.92
2,2'-Oxamido bis-[ethyl-3-(3,5-di-t-butyl-4-hydroxyphenyl) propionate	70331-94-1	C40H60N2O8	697.4422	-246	-229.1588	11.00
2,6-Xylidine / Lidocaine-M / Dimethylaniline	87-62-7	C8H11N	122.0964	-77	-105.0699	5.61
2-Hydroxyquinoline	59-31-4	C9H7NO	146.0600	-91	-118.0651	9.98
3-Hydroxycotinine	34834-67-8	C10H12N2O2	193.0972	-134	-78.0337	3.18
4-Chloroaniline	106-47-8	C6H6ClN	128.0262	-93	-110.9994	13.35
5-Methyl-1H-benzotriazole	136-85-6	C7H7N3	134.0713	-791	-106.0651	10.67
Acridine / Carbamazepine-M	260-94-6	C13H9N	180.0808	-69	-79.0541	10.97
AHDI / Phantolide	15323-35-0	C17H24O	245.1900	-189.126	-175.1098	17.01
Allopurinol	315-30-0	C5H4N4O	137.0458	-110	-119.0352	3.87
Atorvastatin	134523-00-5	C33H35FN2O5	559.2603	-440	-250.1027	15.99
Azelastine	58581-89-8	C22H24ClN3O	382.1681	-275	-294.1058	4.03
Azithromycin 3'-N-oxide	90503-06-3	C38H72N2O13	765.5107	-417	-83.0491	11.51
Azithromycin N'-(Desmethyl)	172617-84-4	C37H70N2O12	735.5002	-573	-158.1176	12.07

Name	CAS#	Formula	Product Ion	Qualifier 1	Qualifier 2	RT
Benzocaine	94-09-7	C9H11NO2	166.0863	-77	-120.0808	4.43
Bezafibrate	41859-67-0	C19H20CINO4	362.1154	-344	-276.0775	4.16
Boldione	897-06-3	C19H24O2	285.1849	-121	-91.0542	14.49
Candesartan	139481-59-7	C24H20N6O3	441.1670	-263	-352.1094	14.60
Carbamazepine 10,11-epoxide	36507-30-9	C15H12N2O2	253.0972	-180	-210.0913	11.16
Cefalexin	15686-71-2	C16H17N3O4S	370.0832	-140	-158.027	12.29
Cefoxitin	35607-66-0	C16H17N3O7S2	450.0400	-208	-304.0732	10.95
Celestolide	13171-00-1	C17H24O	245.1901	-189.126	-175.1098	17.10
Chlorhexidine	55-56-1	C22H30Cl2N10	505.2105	-184	-336.1698	13.43
Clarithromycin-N-oxide	118074-07-0	C38H69NO14	764.4791	-606	-606.3848	13.66
Clopidogrel	113665-84-2	C16H16ClNO2S	322.0663	-155	-155.0258	17.17
Cyclophosphamide	50-18-0	C7H15Cl2N2O2P	261.0321	-142	-62.9996	11.09
Cytarabine	147-94-4	C9H13N3O5	244.0928	-112	-95.024	2.25
Dabigatran	211914-51-1	C25H25N7O3	472.2092	-318	-261.1037	8.28
DEET / Diethyltoluamide	134-62-3	C12H17NO	192.1383	-119.0491	-91.0542	14.34
Desacetylmepitranolol	57193-14-3	C15H25NO3	268.1907	-116	-72.0808	9.46
Despropionylbezitramide	83898-28-6	C28H28N4O	437.2336	-89	-133.0865	7.73
Diatrizoate / Amidotrizoic acid	117-96-4	C11H9I3N2O4	614.7769	-361	-233.0557	3.94
Dimethylaminophenazone	58-15-1	C13H17N3O	232.1444	-133	-144.0806	6.64
Dioxybenzone / Benzophenone-8	131-53-3	C14H12O4	245.0808	-133	-144.0806	14.18
Erythromycin A enol ether	33396-29-1	C37H65NO12	716.4580	-558	-500.3961	14.63
Fenoprofen	31879-05-7	C15H14O3	243.1016	-91	-89.0597	5.39
Fexofenadine	83799-24-0	C32H39NO4	502.2952	-171	-466.2741	13.10
Flecainide	54143-55-4	C17H20F6N2O3	415.1451	-398	-301.0294	14.09
Flutamide	13311-84-7	C11H11F3N2O3	294.1060	-159	-137.0459	3.92
Gatifloxacin	112811-59-3	C19H22FN3O4	376.1667	-318	-261.1037	8.07
Hydroxychloroquine	118-42-3	C18H26ClN3O	336.1837	-247	-158.1539	7.08
Indole	120-72-9	C8H7N	118.0651	-91	-65.0386	10.03
Iohexol	66108-95-0	C19H26I3N3O9	821.8876	-804	-602.9099	4.35
Iopamidol	60166-93-0	C17H22I3N3O8	777.8614	-559	-541.8828	3.64
Irbesartan	138402-11-6	C25H28N6O	429.2397	-195	-386.2217	15.22
Lansoprazole	103577-45-3	C16H14F3N3O2S	370.0832	-136	-205.0731	12.21
Lapatinib	231277-92-2	C29H26ClFN4O4S	581.1420	-458	-365.0779	10.45
Levetiracetam	102767-28-2	C8H14N2O2	171.1126	-69	-126.0913	6.10
Losartan	114798-26-4	C22H23ClN6O	423.1695	-207	-206.084	14.40
Metaxalone	1665-48-1	C12H15NO3	222.1125	-91	-161.0961	10.33
Metformin	657-24-9	C4H11N5	130.1087	-71	-68.0243	2.06
Methylsalicylate	119-36-8	C8H8O3	153.0546	-65	-149.0233	14.19
Metoclopramide	364-62-5	C14H22ClN3O2	300.1473	-227	-184.016	9.56
Metoprolol acid	56392-14-4	C14H21NO4	268.1543	-133		7.23
MIT / Methylisothiazolinone	2682-20-4	C4H5NOS	116.0165	-70	-71.99	3.42
Moxifloxacin	354812-41-2	C21H24FN3O4	402.1824	-384	-358.1925	10.45
N4-Acetylsulfamethoxazole	21312-10-7	C12H13N3O4S	296.0707	-134	-188.0807	9.91
NDEA / Nitrosodiethylamine	55-18-5	C4H10N2O	103.0866	-62	-57.0695	2.86
Nicopholine	492-85-3	C10H12N2O2	193.0972	-179	-163.0866	3.18
Nicotine	54-11-5	C10H14N2	163.1230	-84	-130.0651	3.30
Niflumic acid	4394-00-7	C13H9F3N2O2	283.0689	-265	-245.0521	16.70
Nitrendipin	39562-70-4	C18H20N2O6	361.1394	-165	-143.0816	10.32
Norcitalopram / Desmethylcitalopram	62498-67-3	C19H19FN2O	311.1554	-109	-262.1027	12.03
Norcocaine	129944-99-6	C16H19NO5	290.1387	-68	-136.0757	8.46
Olmesartan	144689-63-4	C24H26N6O3	447.2139	-207	-235.0979	11.17
Omeprazole	73590-58-6	C17H19N3O3S	346.1220	-180	-198.0583	12.23
Paramethasone acetate	1597-82-6	C24H31FO6	435.2177	-119	-135.0804	16.27
Paraxanthine	611-59-6	C7H8N4O2	181.0720	-124	-69.0447	6.34
Parsamide	30653-83-9	C14H18N2O2	247.1441	-180	-210.0912	7.24
Pazufloxacin	127045-41-4	C16H15FN2O	271.1241	-105	-91.0543	15.63
Picaridin / Bayrepel / Icaridin	119515-38-7	C12H23NO3	230.1751	-130	-84.0808	14.58
Pregabalin	148553-50-8	C8H17NO2	160.1332	-55	-97.1012	6.74
Propacetamol	66532-85-2	C14H20N2O3	265.1547	-89	-133.0864	7.05
Propyperone	3781-28-0	C23H33FN2O2	389.2599	-89	-371.2281	8.24
Rifaximin	80621-81-4	C43H51N3O11	786.3596	-334	-336.2512	16.11
Sitagliptin	486460-32-6	C16H15F6N5O	408.1254	-193	-235.0801	9.70
Sotalol	3930-20-9	C12H20N2O3S	273.1267	-133	-213.0692	4.86
Sulpiride	15676-16-1	C15H23N3O4S	342.1482	-112	-214.0168	5.12
Tapentadol	175591-23-8	C14H23NO	222.1852	-107	-121.0648	9.81
Telmisartan	144701-48-4	C33H30N4O2	515.2442	-497	-276.1369	16.02
Terbutaline	23031-25-6	C12H19NO3	226.1438	-77	-107.0491	10.23

Name	CAS#	Formula	Product Ion	Qualifier 1	Qualifier 2	RT
Theobromine	83-67-0	C7H8N4O2	181.0720	-138	-110.0713	5.48
Theophylline	58-55-9	C7H8N4O2	181.0720	-124	-69.0447	6.38
Tramadol-N-oxide	147441-56-3	C16H25NO3	280.1907	-58	107.0491	7.17
Triethyl citrate	77-93-0	C12H20O7	277.1282	-157	-68.9971	12.37
Troxipide	30751-05-4	C15H22N2O4	295.1652	-138	-195.088	6.61
Valsartan	137862-53-4	C24H29N5O3	436.2343	-291	-235.0965	15.29

Legend

RT = Retention time

3. Wastewater and flow rate characteristics

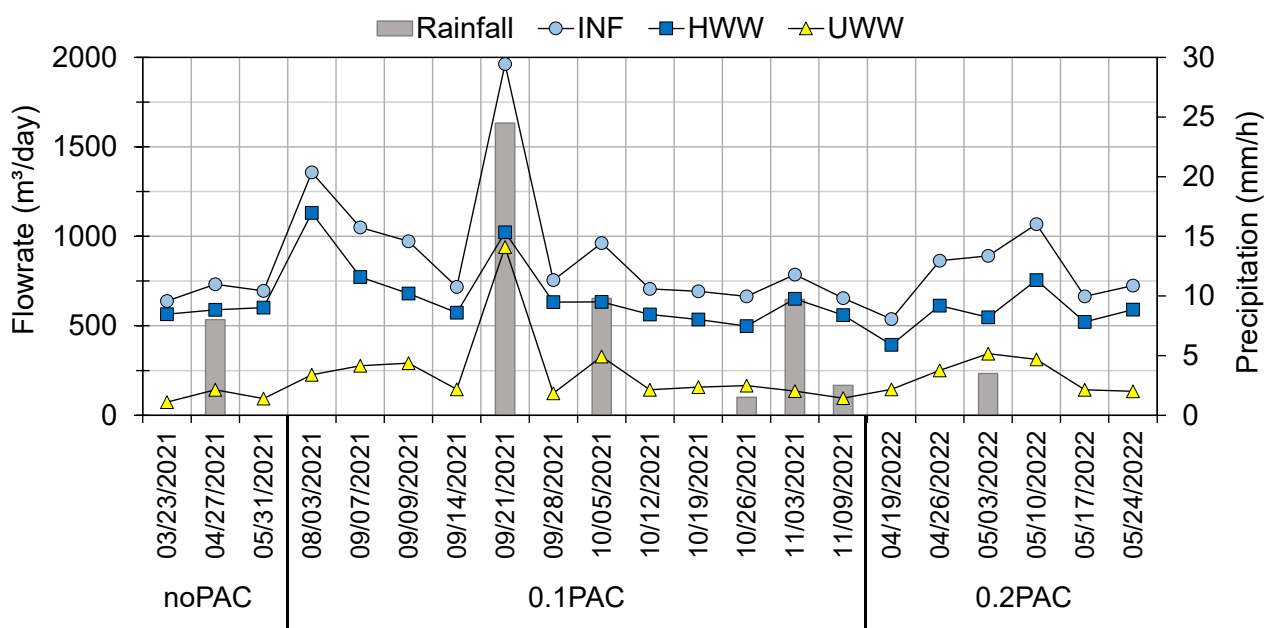


Figure S1. Average flow rates of HWW, UWW and INF as well as precipitation (mm/h) during the sampling days of each experimental campaign.

Table S8. Characterization of the HWW and INF for a set of conventional parameters as well as EFF concentration and removal efficiencies for the noPAC and 0.1PAC campaigns. n: number of samples. SD: Standard deviation.

Parameter	HWW			INF			noPAC			0.1PAC		
	n	Range	Average ± SD	n	Range	Average ± SD	n	EFF	Rem. eff.(%) Average ± SD	n	EFF	Rem. eff.(%) Average ± SD
COD (mg/L)	10	131 - 351	225.5 ± 65.1	12	104 - 242	178.7 ± 38.1	2	29 ± 5.7	78 ± 14	10	22.5 ± 7	87 ± 5
BOD ₅ (mg/L)	8	50 - 135	92.1 ± 27.6	10	46 - 105	79.3 ± 20.5	2	12 ± 2.8	83 ± 5	8	10 ± 0	87 ± 4
TSS (mg/L)	10	35 - 188	92 ± 43.1	12	42 - 330	102.9 ± 74.3	2	6 ± 1.4	90 ± 3	7	5.4 ± 0.53	93 ± 2
VSS (% TSS)	7	79.2 - 89.8	83.7 ± 3.5	7	37.9 - 89	76.2 ± 18.2			n.a.			n.a.
NH ₄ ⁺ (mg/L)	7	24.3 - 42.5	32.4 ± 7.1	9	22.6 - 42	32.4 ± 6.7	2	< 1	97 ± 1	7	0.2 ± 0.04	93 ± 4
N _{tot} (mg/L)	7	21.3 - 38.7	29.2 ± 6.5	9	21.3 - 39.2	29.3 ± 6.7	2	9.9 ± 0.3	64 ± 16	7	7.1 ± 2.05	73 ± 14
NO ₃ ⁻ (mg/L)	7	< 0.5	< 0.5	7	< 0.5	< 0.5			n.a.	7	5.3 ± 3.3	
NO ₂ ⁻ (mg/L)	7	0.04 - 0.06	0.04 ± 0.01	7	0.04 - 0.07	0.04 ± 0.01			n.a.	7	0.3 ± 0.3	
P _{tot} (mg/L)	7	2.4 - 4.3	3.5 ± 0.7	9	2.3 - 6.2	4.1 ± 1.4	2	3.3 ± 1.1	4 ± 6	7	3.2 ± 0.37	19 ± 24
Anionic surfactants (mg/L)	5	1 - 3.1	2 ± 1	5	1.7 - 3.2	2.4 ± 0.6			n.a.	5	< 0.2	91 ± 2
Non anionic surfactants (mg/L)	5	0.7 - 2.1	1.4 ± 0.5	5	0.9 - 1.5	1.1 ± 0.2			n.a.	5	< 0.2	87 ± 4
Cationic surfactants (mg/L)	5	0.3 - 0.4	0.4 ± 0.1	5	0.3 - 0.5	0.4 ± 0.1			n.a.	5	< 0.2	42 ± 12
Total surfactants (mg/L)	5	2.7 - 5.6	3.7 ± 1.1	6	2.3 - 5.2	3.6 ± 1			n.a.	5	< 0.2	93 ± 1
<i>D. magna</i> (% mortality)	3	6.6 - 20	12.2 ± 7	3	3.3 - 20	8.9 ± 9.6			n.a.	3	< 3.3	
<i>E. coli</i> (UFC/mL)	3	5.8·10 ⁵ - 9.8·10 ⁵	7.6·10 ⁵ ± 2.0·10 ⁵	3	9.1·10 ⁵ - 1.0·10 ⁶	9.5·10 ⁵ ± 4.7·10 ⁵			n.a.	3	< 2	99.9999

Legend

n.a.: data not available

Text S4. Analysis of the average loads, the frequency of detection, the range of variability and the average concentrations of the target OMPs in the HWW and the INF.

During the sampling periods, the WWTP treated on average 855 m³/d, from which 221 m³/d are from UWW and 634 m³/d from HWW, representing approximately 25% and 75% of the total flow rate, respectively. HWW varied between 393 m³/d and 1,131 m³/d (standard deviation, SD = 170), the UWW between 73 m³/d and 940 m³/d (SD = 184) and the INF between 538 m³/d and 1,963 m³/d (SD = 317) (Figure S1). Since the hospital has a capacity of 900 beds, the corresponding specific consumption is 705 L/bed/day, in agreement with the literature (Verlicchi et al., 2010).

Overall, the OMP load of the HWW represents 78.6% of the total load arriving at the WWTP. Seven out of the twenty OMP classes are the main contributors to the OMP load in the INF. As reported in Table S9: analgesics/anti-inflammatories (27%), antibiotics (20%), X-ray contrast media (18%), psychiatric drugs (11%), plastic additives (10%), stimulants (6%) and illicit drugs (3%), whereas the remaining 13 classes represent less than 4% of the total load.

During the noPAC (March – August 2021) and 0.1PAC (September – November 2021) campaigns, the average load of OMPs in both HWW and INF was significantly higher compared to the 0.2PAC campaign (April – May 2022) (Figure S2A). The first two campaigns were conducted during the Covid-19 pandemic which, in the face of the trend of infection steadily decreasing by 2022, led to the end of the state of emergency in Italy before the beginning of the 0.2PAC treatment. The analgesics/anti-inflammatories average load decreased from 23.3 g/d during noPAC to 12.1 g/d in 0.1PAC and 6.1 g/d in 0.2PAC, whereas antibiotics were on average 11.7 g/d and 11.4 g/d during the noPAC and 0.1PAC campaigns, respectively, and decreased to 3.8 g/d during 0.2PAC campaign (Table S9). Antibiotics were frequently prescribed to patients with Covid-19 and related post-structural lung damage due to their increased vulnerability to microbial infections (Knight et al., 2021). Furthermore, the use of scanning tools to determine the degree of infection is one of the main techniques used in the diagnosis and aftercare of Covid-19 patients (Abuzaid et al., 2023), which can be outlined by the high average load of X-ray contrast media during the 0.1PAC campaign (12 g/d) (Table S9).

Water sampling was not carried out during rainy events, as the precipitation collected in the combined urban sewer may alter OMP and macroparameter quantification. Yet on two occasions during the 0.1PAC treatment (September 21, 2021 and October 5, 2021), the rain collected in the accumulation tank (see Figure 1) increased the flow rate of the UWW arriving at the WWTP (Figure S1), which considerably increased the total load of OMPs in the INF compared to the HWW (Figure S2B). Higher HWW loads observed on August 3, 2021 and April 26, 2022 (Figure S2B) and average loads per OMP class (Table S9) may be due to uncertainties related to the sampling mode (i.e., 24-h time proportional instead of flow proportional composite sampling), OMP quantification (i.e., influence of the water matrix) and most significantly the presence of the accumulation tank (Figure 1). Most of these issues are described in detail in section 4.3.

Table S10 shows the frequency of detection, range of variability and average concentration of the 232 target OMPs analyzed and grouped according to their class in both HWW and INF, considering the whole experimental period. Regarding the frequency of detection in the INF, it emerges that target OMPs may be categorized into four main groups, with each group accounting for roughly one-quarter of the total number of compounds: 63 highly detected ($Freq > 75\%$), 44 moderately detected ($25\% < Freq \leq 75\%$), 59 slightly detected ($0\% < Freq \leq 25\%$) and 66 non-detected ($Freq = 0\%$). A similar distribution of frequencies was found in HWW. In both HWW and INF, 28% of the target compounds were not detected.

Regarding OMP concentrations (Table S10), it emerges that in the INF 11 compounds show an average concentration higher than 1 $\mu\text{g/L}$, namely iopromide (7.14 $\mu\text{g/L}$), acetaminophen (4.99 $\mu\text{g/L}$), benzotriazole (4.64 $\mu\text{g/L}$), gabapentin (3.38 $\mu\text{g/L}$), azithromycin (3.08 $\mu\text{g/L}$), caffeine (2.64 $\mu\text{g/L}$), naproxen (2.09 $\mu\text{g/L}$), ketoprofen (1.68 $\mu\text{g/L}$), ciprofloxacin (1.27 $\mu\text{g/L}$), ofloxacin (1.21 $\mu\text{g/L}$) and diclofenac (1.04 $\mu\text{g/L}$), with all of them having a frequency of detection of 100% except naproxen ($Freq = 11\%$). Among them, four OMPs reached maximum concentrations above 10 $\mu\text{g/L}$, i.e., iopromide (44.48 $\mu\text{g/L}$), naproxen (19.62 $\mu\text{g/L}$), diclofenac (15.49 $\mu\text{g/L}$) and benzotriazole (10.50 $\mu\text{g/L}$). On the other hand, 85 OMPs were found, on average, below the < LOD.

Comparing INF and HWW, it emerges that for 85 out of 232 target compounds, HWW have higher average concentrations than INF (corresponding to the 60% of the detected OMPs). The highest differences were found for iopromide (11.9 $\mu\text{g/L}$ in HWW and 7.14 $\mu\text{g/L}$ in INF) and albendazole (0.13 $\mu\text{g/L}$ in HWW and 0.003 $\mu\text{g/L}$ in INF). However, on some occasions, the concentration was higher in the INF compared to the HWW, which was the case for diclofenac (1.04 $\mu\text{g/L}$ versus 0.08 $\mu\text{g/L}$, respectively) and the psychiatric drug amisulpride (0.12 $\mu\text{g/L}$ versus 0.01 $\mu\text{g/L}$).

Table S11 reports the range of variability and the average load of all the target compounds. A total of 10 OMPs stood out due to their high average loads (> 1 g/d) in the INF: three analgesics/anti-inflammatories, namely acetaminophen (4.4 g/d), naproxen (2.2 g/d) and ketoprofen (1.4 g/d); three antibiotics, azithromycin (2.4 g/d), ciprofloxacin (1.1 g/d) and ofloxacin (1 g/d); one plastic additive, benzotriazole (4.2 g/d); one psychiatric drug, gabapentin (3 g/d); one stimulant, caffeine (2.3 g/d), and the contrast media, iopromide (6.4 g/d). In some cases, discrepancies between the OMP loads, in particular concerning HWW and INF, are found. An effort to interpret these results is made in section 4.1.

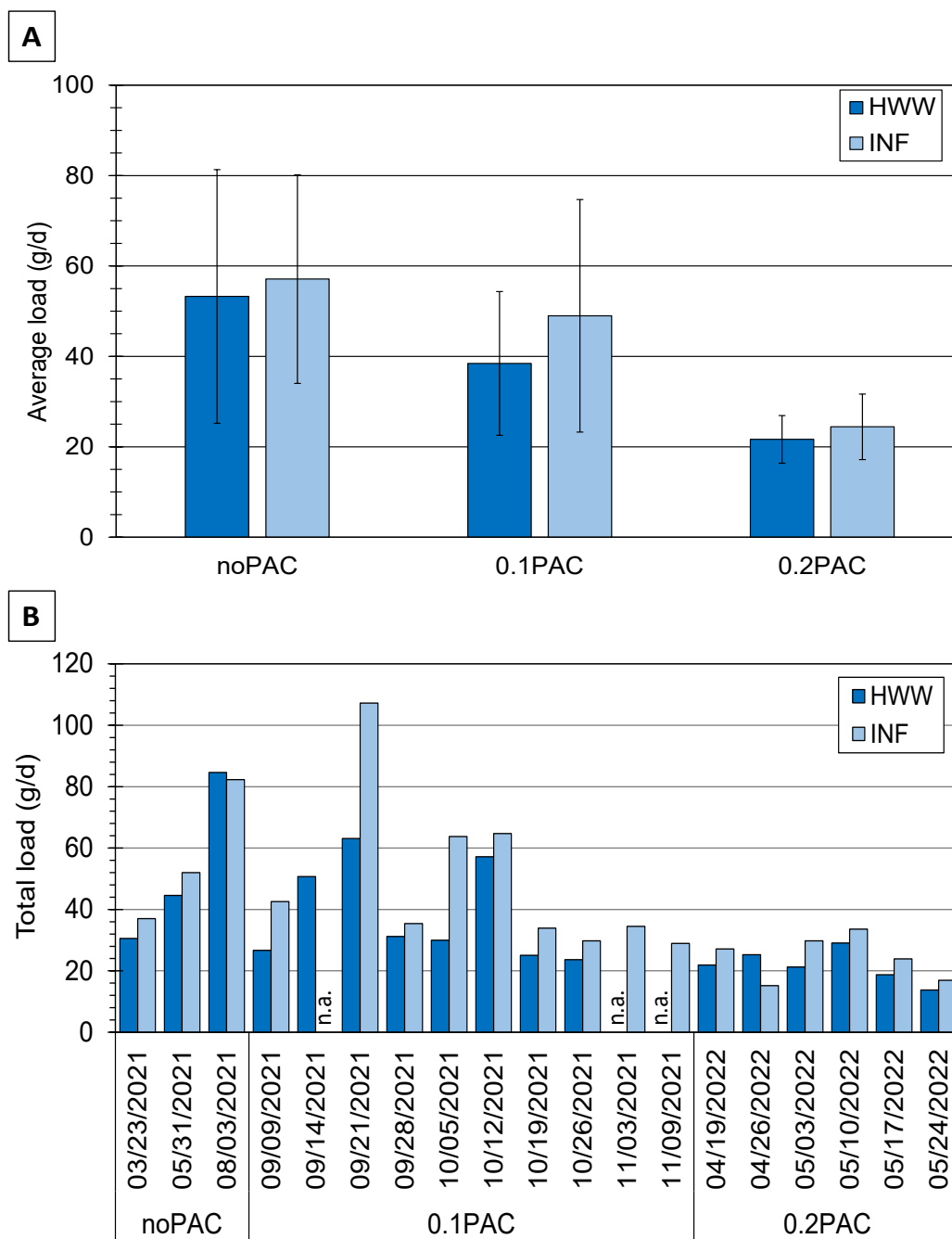


Figure S2. OMP load distribution in HWW and INF during three experimental campaigns (i.e., noPAC, 0.1PAC and 0.2PAC). A) Average load (g/d) and SD of all the target OMPs; B) total load (g/d) (sum of the individual OMP loads) per sampling day and campaign. n.a. = data not available.

Table S9. Average load and contribution to the load (%) of each class of target OMPs in HWW and INF during the three experimental campaigns and referring to the whole period. In between brackets, the number of OMPs pertaining to each class.

OMP class	noPAC		0.1PAC		0.2PAC		Whole period									
	HWW (n=3)		INF (n = 3)		HWW (n=8)		INF (n = 9)		HWW (n=6)		INF (n = 6)		HWW (n=17)		INF (n = 18)	
	Average load (mg/d)	% load	Average load (mg/d)	% load	Average load (mg/d)	% load	Average load (mg/d)	% load	Average load (mg/d)	% load	Average load (mg/d)	% load	Average load (mg/d)	% load	Average load (mg/d)	% load
Analgesics/anti-inflammatory (39)	19,006	35.7	23,322	40.8	6,998	16.7	12,055	23.0	5,078	23.5	6,091	24.9	8,439	23.0	11,945	27.3
Antiarrhythmic agents (5)	57	0.1	69	0.1	35	<0.1	47	<0.1	36	0.2	53	0.2	39	<0.1	53	0.1
Antibiotics (41)	13,086	24.6	11,668	20.4	10,186	24.3	11,381	21.7	3,942	18.2	3,790	15.5	8,494	23.1	8,899	20.3
Antifungals (3)	2	<0.1	1.8	<0.1	1.3	<0.1	2	<0.1	1.1	<0.1	1.5	<0.1	1.3	<0.1	1.8	<0.1
Antihistamines (2)	1.8	<0.1	2.1	<0.1	1.5	<0.1	2.2	<0.1	1.3	<0.1	1.8	<0.1	1.5	<0.1	2	<0.1
Antihypertensive (1)	0.4	<0.1	0.5	<0.1	0.5	<0.1	0.5	<0.1	0.1	<0.1	0.1	<0.1	0.4	<0.1	0.4	<0.1
Antiparasitics (6)	68	0.1	122	0.2	314	0.7	82	0.2	52	0.2	54	0.2	178	0.5	79	0.2
Antiseptic (1)	32	<0.1	39	<0.1	116	0.3	142	0.3	0.6	<0.1	0.8	<0.1	60	0.2	78	0.2
Beta-blockers (3)	433	0.8	679	1.2	437	1.0	696	1.3	308	1.4	448	1.8	391	1.1	611	1.4
Calcium channel blocker (1)	60	0.1	31	<0.1	33	<0.1	61	0.1	11	<0.1	17	<0.1	30	<0.1	41	<0.1
Diuretic (1)	0.9	<0.1	1.1	<0.1	0.8	<0.1	1.1	<0.1	0.7	<0.1	0.9	<0.1	0.8	<0.1	1	<0.1
Hormones (9)	235	0.4	188	0.3	137	0.3	175	0.3	29	0.1	11	<0.1	116	0.3	122	0.3
Illicit drugs (13)	6,986	13.1	2,985	5.2	1,000	2.4	1,544	3.0	427	2.0	413	1.7	1,854	5.0	1,407	3.2
Plastic additives (2)	5,745	10.8	6,854	12.0	2,758	6.6	3,820	7.3	2,689	12.4	3,450	14.1	3,261	8.9	4,202	9.6
Psychiatric drugs (76)	3,145	5.9	4,664	8.2	3,370	8.0	5,957	11.4	1,973	9.1	2,942	12.0	2,837	7.7	4,736	10.8
Receptor antagonists (2)	2.3	<0.1	2.6	<0.1	3.6	<0.1	3.7	<0.1	1.6	<0.1	2.3	<0.1	2.7	<0.1	3.1	<0.1
Stimulants (3)	2,149	4.0	2,874	5.0	2,090	5.0	3,508	6.7	1,274	5.9	1,748	7.2	1,812	4.9	2,815	6.4
UV filter (1)	59	0.1	127	0.2	49	0.1	105	0.2	17	<0.1	30	0.1	39	0.1	83	0.2
Veterinary drugs (22)	989	1.9	1,045	1.8	631	1.5	793	1.5	208	1.0	267	1.1	545	1.5	660	1.5
X-ray contrast medium (1)	1,207	2.3	2,423	4.2	13,750	32.8	11,953	22.8	5,596	25.9	5,100	20.9	8,659	23.6	8,080	18.4

Table S10. Frequency of detection, range of variability and average occurrence of the 232 target OMPs analyzed in HWW and INF considering the three experimental campaigns together: noPAC, March – August 2021 ($n = 3$); 0.1PAC September – November 2021 ($n = 8$, HWW and $n = 9$, INF); 0.2PAC April – May 2022 ($n = 6$). Transformation products are written in italics. SD: standard deviation. LOD: Limit of detection. n : number of samples.

Compound	HWW ($n = 17$)			INF ($n = 18$)		
	Freq (%)	Range ($\mu\text{g/L}$)	Average \pm SD ($\mu\text{g/L}$)	Freq (%)	Range ($\mu\text{g/L}$)	Average \pm SD ($\mu\text{g/L}$)
Analgesics/Anti-inflammatories						
<i>4-Acetylaminoantipyrine</i>	82	<LOD - 0.193	0.052 \pm 0.054	94	<LOD - 0.176	0.054 \pm 0.048
<i>4-FormylAminoAntipyrine</i>	88	<LOD - 0.147	0.044 \pm 0.04	94	<LOD - 0.134	0.05 \pm 0.04
<i>6-Acetylmorphine</i>	88	<LOD - 0.686	0.099 \pm 0.215	72	<LOD - 0.665	0.068 \pm 0.172
Acetaminophen	100	0.134 - 6.504	5.156 \pm 1.806	100	0.095 - 7.256	4.985 \pm 1.91
<i>Acetylcodeine</i>	41	<LOD - 0.017	0.005 \pm 0.006	33	<LOD - 0.019	0.005 \pm 0.006
Acetylsalicylic acid	100	0.136 - 1.212	0.516 \pm 0.272	100	0.053 - 0.776	0.506 \pm 0.24
Alfentanil	35	<LOD - 0.04	0.007 \pm 0.012	28	<LOD - 0.065	0.006 \pm 0.015
Aminopyrine	53	<LOD - 0.725	0.243 \pm 0.257	56	<LOD - 1.299	0.312 \pm 0.391
Betamethasone 17,21-dipropionate	59	<LOD - 0.026	0.009 \pm 0.008	56	<LOD - 0.033	0.01 \pm 0.009
Buprenorphine	82	<LOD - 0.185	0.089 \pm 0.052	67	<LOD - 0.18	0.078 \pm 0.064
<i>Buprenorphine glucuronide</i>	47	<LOD - 0.414	0.122 \pm 0.147	33	<LOD - 0.528	0.107 \pm 0.177
Carisoprodol	6	<LOD - 0.195	0.013 \pm 0.047	6	<LOD - 0.091	0.007 \pm 0.021
Codeine	100	0.059 - 0.417	0.258 \pm 0.093	100	0.076 - 0.407	0.248 \pm 0.105
Dextromethorphan	0	<LOD	<LOD	6	<LOD - 0.008	<LOD
Dextropropoxyphene	0	<LOD	<LOD	0	<LOD	<LOD
Diclofenac	100	0.026 - 0.207	0.082 \pm 0.048	100	0.05 - 15.491	1.04 \pm 3.607
Etodolac	0	<LOD	<LOD	0	<LOD	<LOD
Fentanyl	0	<LOD	<LOD	0	<LOD	<LOD
Hydrocodone	88	<LOD - 0.39	0.212 \pm 0.115	94	<LOD - 0.38	0.22 \pm 0.109
Hydromorphone	100	0.045 - 0.371	0.153 \pm 0.096	100	0.041 - 0.327	0.138 \pm 0.086
Ibuprofen	94	<LOD - 1.092	0.579 \pm 0.361	100	0.067 - 1.449	0.596 \pm 0.406
Ketoprofen	100	0.52 - 2.34	1.55 \pm 0.519	100	0.659 - 3.828	1.683 \pm 0.729
Lidocaine	100	0.105 - 0.403	0.223 \pm 0.09	100	0.084 - 0.384	0.211 \pm 0.1
Meloxicam	6	<LOD - 0.002	<LOD	0	<LOD	<LOD
Morphine	100	0.045 - 0.371	0.155 \pm 0.095	100	0.041 - 0.327	0.139 \pm 0.085
<i>Morphine-6-β-D-glucuronide</i>	35	<LOD - 0.153	0.032 \pm 0.052	22	<LOD - 0.156	0.022 \pm 0.049
Naproxen	12	<LOD - 23.256	1.929 \pm 5.96	11	<LOD - 19.621	2.091 \pm 6.09
<i>Norfentanyl</i>	94	<LOD - 0.105	0.029 \pm 0.026	89	<LOD - 0.085	0.026 \pm 0.02
<i>Norpethidine</i>	88	<LOD - 0.076	0.03 \pm 0.019	78	<LOD - 0.074	0.023 \pm 0.019
<i>Norpropoxyphene</i>	6	<LOD - 0.024	0.002 \pm 0.006	0	<LOD	<LOD
<i>O-Desmethyltramadol</i>	100	0.058 - 0.436	0.198 \pm 0.144	100	0.108 - 0.479	0.265 \pm 0.12
Oxycodone	82	<LOD - 0.058	0.027 \pm 0.018	83	<LOD - 0.044	0.021 \pm 0.013
Oxymorphone	94	<LOD - 0.066	0.034 \pm 0.016	94	<LOD - 0.081	0.038 \pm 0.023
Pentazocine	0	<LOD	<LOD	0	<LOD	<LOD
Pethidine	18	<LOD - 0.008	0.002 \pm 0.002	22	<LOD - 0.01	0.002 \pm 0.003
Phenylbutazone	18	<LOD - 0.019	0.004 \pm 0.007	11	<LOD - 0.029	0.003 \pm 0.007
Procaine	94	<LOD - 0.235	0.039 \pm 0.059	89	<LOD - 0.135	0.038 \pm 0.045
Tolfenamic acid	6	<LOD - 0.007	<LOD	6	<LOD - 0.007	<LOD
Tramadol	100	0.047 - 0.452	0.292 \pm 0.104	100	0.21 - 0.482	0.299 \pm 0.079

Table S10. (continued)

Antiarrhythmic agents						
Amiodarone	0	<LOD	<LOD	0	<LOD	<LOD
Digitoxin	0	<LOD	<LOD	0	<LOD	<LOD
Propafenone	100	0.018 - 0.111	0.056 ± 0.034	94	<LOD - 0.201	0.043 ± 0.044
Strophanthidin	0	<LOD	<LOD	6	<LOD - 0.069	0.006 ± 0.016
Strophanthin	0	<LOD	<LOD	6	<LOD - 0.203	0.013 ± 0.047
Antibiotics						
2-NP-AOZ	0	<LOD	<LOD	0	<LOD	<LOD
Amoxicillin	94	<LOD - 0.447	0.101 ± 0.099	89	<LOD - 0.219	0.082 ± 0.059
Azithromycin	100	1.379 - 10.483	4.005 ± 2.213	100	1.064 - 9.873	3.082 ± 2.043
Cinoxacin	18	<LOD - 0.006	0.001 ± 0.002	17	<LOD - 0.008	0.002 ± 0.003
Ciprofloxacin	100	0.345 - 2.884	1.639 ± 0.802	100	0.236 - 2.834	1.266 ± 0.733
Clarithromycin	100	0.013 - 0.562	0.245 ± 0.148	100	0.026 - 0.498	0.178 ± 0.112
Doxycycline	59	<LOD - 2.533	0.639 ± 0.823	61	<LOD - 1.947	0.484 ± 0.569
Enoxacin	24	<LOD - 0.653	0.064 ± 0.164	17	<LOD - 0.529	0.065 ± 0.155
Erythromycin	100	0.068 - 1.897	0.565 ± 0.426	89	<LOD - 1.441	0.396 ± 0.353
Flumequine	0	<LOD	<LOD	0	<LOD	<LOD
Furazolidon	0	<LOD	<LOD	6	<LOD - 0.01	<LOD
Lomefloxacin	76	<LOD - 0.185	0.086 ± 0.062	72	<LOD - 0.169	0.085 ± 0.062
Metronidazole	94	<LOD - 0.883	0.304 ± 0.269	100	0.008 - 0.556	0.152 ± 0.145
Minocycline	76	<LOD - 0.473	0.204 ± 0.143	56	<LOD - 0.787	0.201 ± 0.224
Nalidixic acid	6	<LOD - 0.026	<LOD	6	<LOD - 0.036	0.004 ± 0.008
Norfloxacin	76	<LOD - 0.317	0.075 ± 0.078	61	<LOD - 0.284	0.061 ± 0.076
Ofloxacin	100	0.494 - 2.485	1.304 ± 0.561	100	0.504 - 1.922	1.213 ± 0.49
Oleandomycin	76	<LOD - 1.481	0.538 ± 0.458	78	<LOD - 1.176	0.472 ± 0.419
Oxolinic acid	0	<LOD	<LOD	0	<LOD	<LOD
Oxytetracycline	65	<LOD - 0.6	0.112 ± 0.146	50	<LOD - 0.315	0.089 ± 0.108
Penicillin G	6	<LOD - 0.102	0.01 ± 0.024	6	<LOD - 0.163	0.013 ± 0.037
Pipemidic acid	0	<LOD	<LOD	0	<LOD	<LOD
Roxithromycin	94	<LOD - 0.991	0.477 ± 0.312	89	<LOD - 1.236	0.469 ± 0.286
Silvadene	35	<LOD - 1.167	0.149 ± 0.363	44	<LOD - 1.075	0.096 ± 0.267
Spiramycin	47	<LOD - 4.439	1.24 ± 1.505	39	<LOD - 2.668	0.752 ± 1.036
Sulfabenzamide	47	<LOD - 1.524	0.464 ± 0.554	39	<LOD - 1.677	0.501 ± 0.676
Sulfadimethoxine	0	<LOD	<LOD	0	<LOD	<LOD
Sulfadimidine	18	<LOD - 0.06	0.01 ± 0.02	17	<LOD - 0.097	0.013 ± 0.029
Sulfafurazole	0	<LOD	<LOD	0	<LOD	<LOD
Sulfaguanidine	24	<LOD - 0.226	0.033 ± 0.066	22	<LOD - 0.142	0.027 ± 0.051
Sulfamerazine	35	<LOD - 1.766	0.206 ± 0.568	28	<LOD - 1.37	0.135 ± 0.39
Sulfamethizole	12	<LOD - 0.132	0.011 ± 0.032	17	<LOD - 0.087	0.011 ± 0.024
Sulfamethoxazole	100	0.151 - 1.315	0.505 ± 0.302	100	0.108 - 1.23	0.417 ± 0.259
Sulfamethoxydiazine	0	<LOD	<LOD	0	<LOD	<LOD
Sulfamethoxypridazine	6	<LOD - 0.055	0.004 ± 0.013	6	<LOD - 0.006	<LOD
Sulfanilamide	0	<LOD	<LOD	0	<LOD	<LOD
Sulfaphenazole	0	<LOD	<LOD	0	<LOD	<LOD
Sulfapyridine	94	<LOD - 0.32	0.07 ± 0.079	83	<LOD - 0.211	0.057 ± 0.058
Sulfathiazole	65	<LOD - 0.361	0.141 ± 0.135	50	<LOD - 0.441	0.161 ± 0.179
Tinidazole	6	<LOD - 1.208	0.072 ± 0.293	6	<LOD - 1.567	0.088 ± 0.369
Trimethoprim	100	0.07 - 0.541	0.211 ± 0.125	100	0.065 - 0.388	0.172 ± 0.087
Antifungals						

Table S10. (continued)

Sulfacetamide	0	<LOD	<LOD	0	<LOD	<LOD
Terbinafine	0	<LOD	<LOD	0	<LOD	<LOD
Tiabendazole	100	<LOD - 0.003	<LOD	100	<LOD - 0.003	<LOD
Antihistamines						
Diphenhydramine	0	<LOD	<LOD	0	<LOD	<LOD
Promethazine	0	<LOD	<LOD	0	<LOD	<LOD
Antihypertensive						
Clonidine	29	<LOD - 0.002	0.001 ± 0.001	22	<LOD - 0.002	0 ± 0.001
Antiparasitics						
Albendazole	41	<LOD - 1.972	0.132 ± 0.476	17	<LOD - 0.031	0.003 ± 0.008
Flubendazole	0	<LOD	<LOD	0	<LOD	<LOD
Levamisole	24	<LOD - 0.146	0.019 ± 0.045	17	<LOD - 0.101	0.016 ± 0.034
Mebendazole	24	<LOD - 1.489	0.092 ± 0.36	11	<LOD - 0.031	0.003 ± 0.007
Praziquantel	59	<LOD - 0.206	0.056 ± 0.062	61	<LOD - 0.172	0.065 ± 0.059
Triclabendazole	0	<LOD	<LOD	0	<LOD	<LOD
Antiseptic						
Nitrofurantoin	12	<LOD - 1.453	0.096 ± 0.352	11	<LOD - 1.686	0.105 ± 0.397
Beta-blockers						
Atenolol	100	0.196 - 0.6	0.438 ± 0.13	100	0.155 - 0.841	0.524 ± 0.184
Bisoprolol	100	0.057 - 0.152	0.097 ± 0.027	100	0.051 - 0.165	0.101 ± 0.034
Metoprolol	100	0.007 - 0.214	0.086 ± 0.065	94	<LOD - 0.221	0.084 ± 0.072
Calcium channel blocker						
Verapamil	71	<LOD - 0.113	0.046 ± 0.042	89	<LOD - 0.112	0.047 ± 0.035
Diuretic						
Torsemide	0	<LOD	<LOD	0	<LOD	<LOD
Hormones						
Fludrocortisone-acetate	0	<LOD	<LOD	0	<LOD	<LOD
Flumethasone	0	<LOD	<LOD	0	<LOD	<LOD
Hydrocortisone	65	<LOD - 0.357	0.126 ± 0.128	56	<LOD - 0.438	0.101 ± 0.138
Methylprednisolone	0	<LOD	<LOD	0	<LOD	<LOD
Mometasone furoate	0	<LOD	<LOD	0	<LOD	<LOD
Prednicarbate	0	<LOD	<LOD	0	<LOD	<LOD
Prednisolone	12	<LOD - 0.187	0.019 ± 0.048	0	<LOD	<LOD
Triamcinolone	0	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone acetonide	24	<LOD - 0.155	0.029 ± 0.055	22	<LOD - 0.215	0.032 ± 0.063
Illicit drugs						
Amphetamine	94	<LOD - 11.258	1.27 ± 3.264	100	0.025 - 1.634	0.287 ± 0.402
<i>Benzoyllecgonine</i>	100	0.071 - 0.421	0.242 ± 0.114	100	0.104 - 0.403	0.267 ± 0.083
Cannabinol	35	<LOD - 0.057	0.013 ± 0.018	28	<LOD - 0.024	0.005 ± 0.006
<i>Cocaethylene</i>	53	<LOD - 0.099	0.035 ± 0.04	44	<LOD - 0.111	0.029 ± 0.038
Cocaine	29	<LOD - 0.053	0.012 ± 0.019	44	<LOD - 0.073	0.017 ± 0.023
<i>Ecgonine methyl ester</i>	100	<LOD - 0.485	0.096 ± 0.148	100	<LOD - 0.253	0.048 ± 0.074
Ketamine	18	<LOD - 0.021	0.003 ± 0.006	17	<LOD - 0.018	0.003 ± 0.005
MDA	100	0.022 - 2.234	0.79 ± 0.787	78	<LOD - 2.293	0.911 ± 0.79
MDEA	59	<LOD - 0.117	0.017 ± 0.028	44	<LOD - 0.033	0.008 ± 0.011
MDMA	76	<LOD - 0.198	0.027 ± 0.049	50	<LOD - 0.289	0.037 ± 0.074
Methamphetamine	6	<LOD - 0.014	0.001 ± 0.003	11	<LOD - 0.013	0.002 ± 0.004
Phencyclidine	0	<LOD	<LOD	0	<LOD	<LOD
THC	76	<LOD - 0.11	0.03 ± 0.026	50	<LOD - 0.247	0.037 ± 0.061

Table S10. (continued)

Plastic additives						
Benzotriazole	100	1.212 - 9.191	4.847 ± 2.181	100	0.891 - 10.5	4.643 ± 2.724
p-Toluenesulfonamide	59	<LOD - 0.386	0.068 ± 0.096	39	<LOD - 0.233	0.036 ± 0.062
Psychiatric drugs						
<i>10-Hydroxycarbazepine</i>	82	<LOD - 1.663	0.619 ± 0.526	78	<LOD - 1.503	0.602 ± 0.469
<i>7-Aminoclonazepam</i>	0	<LOD	<LOD	0	<LOD	<LOD
<i>7-Aminoflunitrazepam</i>	0	<LOD	<LOD	0	<LOD	<LOD
Alprazolam	0	<LOD	<LOD	0	<LOD	<LOD
Amisulpride	53	<LOD - 0.08	0.013 ± 0.021	83	<LOD - 0.937	0.117 ± 0.298
Amitriptyline	47	<LOD - 0.19	0.022 ± 0.05	39	<LOD - 0.149	0.011 ± 0.035
Amoxapine	0	<LOD	<LOD	0	<LOD	<LOD
Bromazepam	0	<LOD	<LOD	11	<LOD - 0.49	0.028 ± 0.115
Carbamazepine	100	0.043 - 0.264	0.129 ± 0.058	100	0.106 - 0.29	0.192 ± 0.062
Chlordiazepoxide	0	<LOD	<LOD	0	<LOD	<LOD
Chlorprothixene	0	<LOD	<LOD	0	<LOD	<LOD
Citalopram	100	0.02 - 0.098	0.031 ± 0.018	89	<LOD - 0.054	0.023 ± 0.013
Clobazam	12	<LOD - 0.005	<LOD	0	<LOD	<LOD
Clomipramine	18	<LOD - 0.036	0.005 ± 0.01	11	<LOD - 0.136	0.01 ± 0.032
Clonazepam	0	<LOD	<LOD	6	<LOD - 0.02	<LOD
Clorazepate	0	<LOD	<LOD	0	<LOD	<LOD
Clozapine	41	<LOD - 0.059	0.011 ± 0.018	33	<LOD - 0.036	0.006 ± 0.01
<i>Desalkylflurazepam</i>	12	<LOD - 0.006	0.001 ± 0.001	6	<LOD - 0.006	<LOD
Desipramine	6	<LOD - 0.17	0.012 ± 0.041	0	<LOD	<LOD
Desvenlafaxine	100	0.014 - 0.07	0.034 ± 0.016	100	0.029 - 0.103	0.054 ± 0.02
Dexametasone	18	<LOD - 0.405	0.053 ± 0.127	6	<LOD - 0.304	0.018 ± 0.071
Diazepam	6	<LOD - 0.006	<LOD	0	<LOD	<LOD
Dothiepin	24	<LOD - 0.13	0.023 ± 0.043	17	<LOD - 0.104	0.016 ± 0.035
Doxepin	0	<LOD	<LOD	0	<LOD	<LOD
<i>EDDP</i>	94	<LOD - 0.085	0.03 ± 0.019	89	<LOD - 0.067	0.022 ± 0.016
Felbamate	6	<LOD - 0.173	0.011 ± 0.042	6	<LOD - 0.204	0.012 ± 0.048
Fluoxetine	76	<LOD - 0.038	0.016 ± 0.01	78	<LOD - 0.029	0.016 ± 0.01
Flupentixol	0	<LOD	<LOD	0	<LOD	<LOD
Flurazepam	0	<LOD	<LOD	6	<LOD - 0.009	<LOD
Fluvoxamine	65	<LOD - 0.103	0.033 ± 0.034	56	<LOD - 0.102	0.031 ± 0.035
Gabapentin	100	0.501 - 5.065	2.611 ± 1.375	100	1.259 - 5.332	3.376 ± 1.226
Haloperidol	0	<LOD	<LOD	0	<LOD	<LOD
Imipramine	0	<LOD	<LOD	0	<LOD	<LOD
Lamotrigine	100	0.051 - 0.324	0.187 ± 0.095	100	0.131 - 0.435	0.262 ± 0.098
Lorazepam	82	<LOD - 0.166	0.088 ± 0.053	72	<LOD - 0.132	0.072 ± 0.048
Maprotiline	88	<LOD - 0.082	0.027 ± 0.019	89	<LOD - 0.062	0.019 ± 0.014
Medazepam	0	<LOD	<LOD	0	<LOD	<LOD
Memantine	88	<LOD - 0.068	0.016 ± 0.015	94	<LOD - 0.057	0.021 ± 0.016
Methodone	47	<LOD - 0.085	0.016 ± 0.022	33	<LOD - 0.056	0.012 ± 0.017
Methylphenidate	47	<LOD - 0.02	0.009 ± 0.008	44	<LOD - 0.023	0.009 ± 0.008
Mianserin	0	<LOD	<LOD	0	<LOD	<LOD
Mirtazapine	59	<LOD - 0.018	0.007 ± 0.006	50	<LOD - 0.019	0.007 ± 0.007
Naltrexone	18	<LOD - 0.024	0.004 ± 0.008	17	<LOD - 0.026	0.005 ± 0.008
<i>N-Desmethylclozapine</i>	12	<LOD - 0.013	<LOD	6	<LOD - 0.01	<LOD
Nitrazepam	47	<LOD - 0.097	0.029 ± 0.032	39	<LOD - 0.097	0.027 ± 0.035

Table S10. (continued)

<i>Norbuprenorphine</i>	59	<LOD - 0.576	0.059 ± 0.136	50	<LOD - 1.139	0.089 ± 0.266
Nordiazepam	6	<LOD - 0.004	<LOD	11	<LOD - 0.004	<LOD
Nortriptyline	0	<LOD	<LOD	0	<LOD	<LOD
Olanzapine	35	<LOD - 0.148	0.027 ± 0.043	33	<LOD - 0.069	0.018 ± 0.025
Opipramol	12	<LOD - 0.022	0.003 ± 0.006	11	<LOD - 0.017	0.002 ± 0.005
Oxazepam	0	<LOD	<LOD	0	<LOD	<LOD
Oxcarbazepine	71	<LOD - 0.141	0.025 ± 0.035	56	<LOD - 0.055	0.016 ± 0.018
Paliperidone	6	<LOD - 0.158	0.01 ± 0.038	6	<LOD - 0.114	0.007 ± 0.027
Paroxetine	0	<LOD	<LOD	0	<LOD	<LOD
Phenazepam	24	<LOD - 0.426	0.053 ± 0.116	11	<LOD - 0.441	0.031 ± 0.105
Phenytoin	65	<LOD - 0.21	0.061 ± 0.06	67	<LOD - 0.165	0.073 ± 0.061
Pipamperone	6	<LOD - 0.009	<LOD	6	<LOD - 0.009	<LOD
Prazepam	0	<LOD	<LOD	0	<LOD	<LOD
Promazine	0	<LOD	<LOD	0	<LOD	<LOD
Protriptyline	0	<LOD	<LOD	0	<LOD	<LOD
Quetiapine	94	<LOD - 0.048	0.023 ± 0.01	100	0.007 - 0.04	0.02 ± 0.01
Risperidone	47	<LOD - 0.107	0.025 ± 0.042	33	<LOD - 0.127	0.025 ± 0.046
<i>Ritalinic acid</i>	29	<LOD - 0.228	0.033 ± 0.07	44	<LOD - 0.108	0.02 ± 0.034
Secobarbital	0	<LOD	<LOD	0	<LOD	<LOD
Sertraline	6	<LOD - 0.006	<LOD	0	<LOD	<LOD
Temazepam	35	<LOD - 0.032	0.006 ± 0.009	39	<LOD - 0.048	0.008 ± 0.012
Topiramate	6	<LOD - 0.054	0.004 ± 0.013	11	<LOD - 0.032	0.003 ± 0.007
Trazodone	94	<LOD - 0.076	0.033 ± 0.019	94	<LOD - 0.084	0.03 ± 0.019
Triazolam	0	<LOD	<LOD	0	<LOD	<LOD
Trimipramine	6	<LOD - 0.249	0.016 ± 0.06	6	<LOD - 0.058	0.005 ± 0.013
Venlafaxine	100	0.015 - 0.086	0.046 ± 0.025	100	0.026 - 0.119	0.056 ± 0.026
Zolpidem	0	<LOD	<LOD	0	<LOD	<LOD
Zopiclone	6	<LOD - 0.032	<LOD	0	<LOD	<LOD
<i>α-Hydroxyalprazolam</i>	6	<LOD - 0.018	<LOD	6	<LOD - 0.024	<LOD
<i>α-Hydroxymidazolam</i>	100	0.005 - 0.052	0.014 ± 0.012	100	0.004 - 0.043	0.013 ± 0.009
<i>α-Hydroxytriazolam</i>	12	<LOD - 0.109	0.009 ± 0.027	11	<LOD - 0.042	0.004 ± 0.01
Receptor antagonists						
Atropine	6	<LOD - 0.009	<LOD	0	<LOD	<LOD
Flumazenil	6	<LOD - 0.016	<LOD	6	<LOD - 0.014	<LOD
Stimulants						
Caffeine	100	1.652 - 3.976	2.301 ± 0.594	100	1.648 - 5.971	2.637 ± 1.221
<i>Cotinine</i>	100	0.424 - 0.701	0.553 ± 0.095	100	0.434 - 0.838	0.626 ± 0.114
Phentermine	0	<LOD	<LOD	0	<LOD	<LOD
UV filter						
Octinoxate	88	<LOD - 0.11	0.06 ± 0.031	94	<LOD - 0.22	0.098 ± 0.053
Veterinary drugs						
Carprofen	18	<LOD - 0.135	0.013 ± 0.034	17	<LOD - 0.132	0.016 ± 0.036
Diaveridine	94	<LOD - 0.773	0.378 ± 0.163	94	<LOD - 0.657	0.405 ± 0.161
Difloxacin	12	<LOD - 0.022	<LOD	17	<LOD - 0.014	<LOD
Dimetridazole	0	<LOD	<LOD	0	<LOD	<LOD
Enrofloxacin	18	<LOD - 0.013	0.003 ± 0.004	6	<LOD - 0.003	<LOD
Flunixin	59	<LOD - 0.017	0.009 ± 0.007	50	<LOD - 0.022	0.009 ± 0.009
Furaltadone	71	<LOD - 0.115	0.055 ± 0.04	61	<LOD - 0.111	0.047 ± 0.041

Table S10. (continued)

Iprnidazole	6	<LOD - 0.006	<LOD	6	<LOD - 0.002	<LOD
Marbofloxacin	59	<LOD - 1.462	0.297 ± 0.423	50	<LOD - 0.777	0.191 ± 0.251
Monensin	0	<LOD	<LOD	0	<LOD	<LOD
Orbifloxacin	0	<LOD	<LOD	6	<LOD - 0.008	<LOD
Oxibendazole	6	<LOD - 0.004	<LOD	6	<LOD - 0.005	<LOD
Ronidazole	6	<LOD - 0.034	0.003 ± 0.008	6	<LOD - 0.029	0.003 ± 0.007
Salinomycin	6	<LOD - 0.552	0.036 ± 0.133	6	<LOD - 0.5	0.032 ± 0.117
Sarafloxacin	0	<LOD	<LOD	0	<LOD	<LOD
Sulfachlorpyridazine	24	<LOD - 0.065	0.011 ± 0.021	22	<LOD - 0.049	0.008 ± 0.015
Sulfaclozine	6	<LOD - 0.046	0.003 ± 0.011	11	<LOD - 0.076	0.007 ± 0.02
Sulfadoxine	100	<LOD	<LOD	100	<LOD	<LOD
Sulfamonomethoxine	0	<LOD	<LOD	0	<LOD	<LOD
Sulfanitran	0	<LOD	<LOD	0	<LOD	<LOD
Sulfaquinoxaline	18	<LOD - 0.06	0.009 ± 0.02	6	<LOD - 0.152	0.009 ± 0.036
Tilmicosin	6	<LOD - 0.335	0.021 ± 0.081	6	<LOD - 0.178	0.012 ± 0.042
X-ray contrast medium						
Iopromide	100	0.294 - 50.728	11.896 ± 15.428	100	0.221 - 44.481	7.143 ± 10.26

Table S11. Ranges of variability and average load of the 232 target OMPs analyzed in HWW and INF considering the three experimental campaigns together: noPAC, March – August 2021 ($n = 3$); 0.1PAC September – November 2021 ($n = 8$, HWW and $n = 9$, INF); 0.2PAC April – May 2022 ($n = 6$). The compounds in italics correspond to the transformation products. SD: Standard deviation. n : number of samples.

Compound	HWW ($n = 17$)		INF ($n = 18$)	
	Range (mg/day)	Average ± SD (mg/day)	Range (mg/day)	Average ± SD (mg/day)
Analgesics/anti-inflammatories				
<i>4-Acetylaminoantipyrine</i>	0.5 - 76	30 ± 27	0.64 - 117	43 ± 33
<i>4-FormylAminoAntipyrine</i>	0.31 - 73	28 ± 25	0.39 - 174	45 ± 44
<i>6-Acetylmorphine</i>	0.35 - 450	61 ± 137	0.44 - 593	56 ± 147
Acetaminophen	67 - 6,810	3,327 ± 1,606	63 - 11,500	4,399 ± 2,489
<i>Acetylcodeine</i>	0.37 - 10	3.3 ± 3.7	0.51 - 14	4.1 ± 5.2
Acetylsalicylic acid	74 - 745	328 ± 187	35 - 1,410	454 ± 324
Alfentanil	0.16 - 25	4.9 ± 8	0.22 - 62	6.2 ± 15
Aminopyrine	0.75 - 820	172 ± 218	1 - 902	239 ± 277
Betamethasone 17,21-dipropionate	0.49 - 15	5.8 ± 4.8	0.68 - 23	8.3 ± 7.7
Buprenorphine	0.24 - 117	56 ± 35	0.26 - 353	76 ± 84
<i>Buprenorphine glucuronide</i>	0.93 - 274	79 ± 101	1 - 415	90 ± 141
Carisoprodol	0.61 - 220	14 ± 53	0.84 - 123	8.1 ± 29
Codeine	31 - 309	160 ± 65	50 - 455	207 ± 97
Dextromethorphan	0.31 - 0.9	0.5 ± 0.15	0.43 - 11	1.2 ± 2.5
Dextropropoxyphene	1 - 2.9	1.6 ± 0.48	1.4 - 5.1	2.2 ± 0.87
Diclofenac	13 - 141	54 ± 37	33 - 14,905	985 ± 3,476
Etodolac	0.33 - 0.96	0.54 ± 0.16	0.46 - 1.7	0.73 ± 0.29
Fentanyl	0.22 - 0.62	0.35 ± 0.1	0.3 - 1.1	0.47 ± 0.19
Hydrocodone	0.49 - 283	131 ± 77	0.89 - 416	181 ± 99
Hydromorphone	24 - 209	93 ± 53	27 - 252	112 ± 66
Ibuprofen	0.54 - 856	377 ± 255	44 - 1,616	526 ± 414
Ketoprofen	306 - 1,554	968 ± 366	478 - 3,228	1,411 ± 688
Lidocaine	41 - 222	140 ± 57	46 - 292	171 ± 71
Meloxicam	0.4 - 1.2	0.68 ± 0.22	0.55 - 2	0.88 ± 0.34

Compound	HWW (n = 17)		INF (n = 18)	
	Range (mg/day)	Average ± SD (mg/day)	Range (mg/day)	Average ± SD (mg/day)
Morphine	24 - 209	95 ± 52	27 - 252	113 ± 65
<i>Morphine-6-β-D-glucuronide</i>	0.23 - 82	22 ± 33	0.32 - 212	23 ± 58
Naproxen	0.23 - 26,311	1,885 ± 6,445	0.32 - 26,625	2,174 ± 6,775
<i>Norfentanyl</i>	0.31 - 52	18 ± 14	0.32 - 60	22 ± 17
<i>Norpethidine</i>	0.45 - 46	20 ± 14	0.57 - 47	20 ± 16
<i>Norpropoxyphene</i>	0.34 - 14	1.4 ± 3.4	0.46 - 1.7	0.74 ± 0.29
<i>O-Desmethyltramadol</i>	34 - 240	115 ± 74	72 - 495	224 ± 121
Oxycodone	0.41 - 33	17 ± 11	0.52 - 31	17 ± 11
Oxymorphone	0.74 - 46	21 ± 12	0.64 - 85	33 ± 22
Pentazocine	0.25 - 0.71	0.4 ± 0.12	0.34 - 1.2	0.54 ± 0.21
Pethidine	0.23 - 7.4	1.2 ± 1.9	0.32 - 19	2.2 ± 4.4
Phenylbutazone	0.34 - 20	3.3 ± 6.4	0.46 - 39	4.4 ± 11
Procaine	0.73 - 117	21 ± 30	0.42 - 90	29 ± 32
Tolfenamic acid	0.25 - 4	0.62 ± 0.88	0.35 - 5	0.81 ± 1.1
Tramadol	28 - 351	182 ± 76	136 - 502	253 ± 100
Antiarrhythmic agents				
Amiodarone	0.53 - 1.5	0.86 ± 0.25	0.73 - 2.7	1.2 ± 0.46
Digitoxin	1.2 - 3.5	1.9 ± 0.57	1.7 - 6	2.6 ± 1
Propafenone	11 - 63	33 ± 18	0.35 - 128	33 ± 29
Strophanthidin	0.78 - 2.2	1.3 ± 0.37	1.1 - 67	5.3 ± 15
Strophanthin	0.87 - 2.5	1.4 ± 0.41	1.2 - 147	10 ± 34
Antibiotics				
<i>2-NP-AOZ</i>	0.39 - 1.1	0.63 ± 0.19	0.54 - 2	0.86 ± 0.34
Amoxicillin	0.4 - 253	64 ± 57	0.55 - 189	71 ± 51
Azithromycin	899 - 5,923	2,459 ± 1,279	783 - 6,303	2,431 ± 1,306
Cinoxacin	0.22 - 5.8	0.89 ± 1.5	0.3 - 11	1.6 ± 2.9
Ciprofloxacin	204 - 1,940	1,029 ± 536	171 - 2,656	1,060 ± 673
Clarithromycin	7.5 - 356	152 ± 98	18 - 481	152 ± 116
Doxycycline	0.29 - 1,583	413 ± 539	0.39 - 2,279	451 ± 609
Enoxacin	0.53 - 357	41 ± 96	0.73 - 472	66 ± 155
Erythromycin	39 - 1,141	348 ± 262	0.74 - 943	322 ± 258
Flumequine	0.36 - 1	0.58 ± 0.17	0.49 - 1.8	0.79 ± 0.31
Furazolidon	0.33 - 0.95	0.53 ± 0.16	0.45 - 6.3	1 ± 1.3
Lomefloxacin	0.47 - 166	58 ± 47	0.64 - 305	76 ± 75
Metronidazole	0.42 - 507	183 ± 157	5.9 - 386	125 ± 111
Minocycline	0.68 - 236	130 ± 82	0.93 - 502	168 ± 170
Nalidixic acid	0.69 - 16	2 ± 3.5	0.95 - 25	2.8 ± 5.5
Norfloxacin	0.48 - 174	49 ± 49	0.65 - 253	57 ± 73
Ofloxacin	248 - 2,020	828 ± 448	335 - 2,148	1,032 ± 544
Oleandomycin	0.41 - 899	355 ± 315	0.57 - 1,724	415 ± 436
Oxolinic acid	0.29 - 0.85	0.47 ± 0.14	0.4 - 1.5	0.64 ± 0.25
Oxytetracycline	0.84 - 299	69 ± 82	1.2 - 288	73 ± 91
Penicillin G	1.8 - 58	6.1 ± 13	2.4 - 104	9.5 ± 24
Pipemidic acid	0.63 - 1.8	1 ± 0.3	0.87 - 3.2	1.4 ± 0.54
Roxithromycin	0.82 - 807	320 ± 248	1.1 - 844	386 ± 222
Silvadene	0.45 - 669	93 ± 217	0.62 - 1,035	86 ± 248
Spiramycin	1.5 - 2,670	796 ± 969	2.1 - 2,014	605 ± 827

Compound	HWW (n = 17)		INF (n = 18)	
	Range (mg/day)	Average ± SD (mg/day)	Range (mg/day)	Average ± SD (mg/day)
Sulfabenzamide	0.63 - 816	270 ± 318	0.87 - 1,337	377 ± 507
Sulfadimethoxine	0.41 - 1.2	0.66 ± 0.2	0.57 - 2.1	0.9 ± 0.35
Sulfadimidine	0.39 - 61	7 ± 16	0.53 - 143	14 ± 36
Sulfafurazole	0.75 - 2.2	1.2 ± 0.35	1 - 3.7	1.6 ± 0.64
Sulfaguanidine	0.28 - 256	30 ± 67	0.38 - 193	32 ± 63
Sulfamerazine	0.4 - 945	113 ± 312	0.55 - 950	91 ± 263
Sulfamethizole	0.74 - 66	6.1 ± 16	1 - 58	8.6 ± 17
Sulfamethoxazole	85 - 1,488	348 ± 336	77 - 1,669	378 ± 355
Sulfamethoxydiazine	0.75 - 2.2	1.2 ± 0.36	1 - 3.7	1.6 ± 0.64
Sulfamethoxypyridazine	0.22 - 32	2.2 ± 7.6	0.3 - 4.6	0.71 ± 0.98
Sulfanilamide	0.65 - 1.9	1 ± 0.31	0.89 - 3.2	1.4 ± 0.56
Sulfaphenazole	0.52 - 1.5	0.84 ± 0.25	0.71 - 2.6	1.1 ± 0.45
Sulfapyridine	0.5 - 160	40 ± 41	0.54 - 153	44 ± 41
Sulfathiazole	0.43 - 301	88 ± 94	0.56 - 577	135 ± 167
Tinidazole	0.42 - 680	41 ± 165	0.57 - 1,106	62 ± 260
Trimethoprim	42 - 612	146 ± 138	47 - 527	155 ± 117
Antifungals				
Sulfacetamide	0.34 - 0.99	0.55 ± 0.16	0.47 - 1.7	0.75 ± 0.29
Terbinafine	0.3 - 0.85	0.47 ± 0.14	0.4 - 1.5	0.65 ± 0.25
Tiabendazole	0.13 - 1.6	0.3 ± 0.34	0.18 - 2.1	0.39 ± 0.45
Antihistamines				
Diphenhydramine	0.35 - 1	0.56 ± 0.17	0.48 - 1.7	0.76 ± 0.3
Promethazine	0.58 - 1.7	0.94 ± 0.28	0.8 - 2.9	1.3 ± 0.5
Antihypertensives				
Clonidine	0.05 - 1.2	0.36 ± 0.45	0.07 - 1.9	0.37 ± 0.53
Antiparasitics				
Albendazole	0.28 - 1,110	76 ± 268	0.38 - 61	4.7 ± 14
Flubendazole	0.64 - 1.8	1 ± 0.3	0.88 - 3.2	1.4 ± 0.55
Levamisole	0.62 - 84	12 ± 27	0.85 - 107	17 ± 37
Mebendazole	0.25 - 838	53 ± 203	0.34 - 61	4.1 ± 14
Praziquantel	0.52 - 155	36 ± 43	0.71 - 129	52 ± 46
Triclabendazole	0.2 - 0.56	0.32 ± 0.09	0.27 - 0.98	0.43 ± 0.17
Antiseptic				
Nitrofurantoin	0.42 - 919	60 ± 223	0.58 - 1,272	78 ± 299
Beta-blockers				
Atenolol	102 - 599	279 ± 121	112 - 1,344	456 ± 264
Bisoprolol	28 - 103	61 ± 22	28 - 175	85 ± 35
Metoprolol	4.5 - 129	51 ± 37	0.64 - 186	69 ± 56
Calcium channel blocker				
Verapamil	0.23 - 89	30 ± 28	0.43 - 109	41 ± 33
Diuretic				
Torsemide	0.47 - 1.4	0.76 ± 0.22	0.65 - 2.4	1 ± 0.41
Hormones				
Fludrocortisone-acetate	0.75 - 2.2	1.2 ± 0.36	1 - 3.7	1.6 ± 0.64
Flumethasone	0.58 - 1.7	0.94 ± 0.28	0.8 - 2.9	1.3 ± 0.5
Hydrocortisone	0.39 - 297	84 ± 92	0.42 - 426	87 ± 122

Compound	HWW (n = 17)		INF (n = 18)	
	Range (mg/day)	Average ± SD (mg/day)	Range (mg/day)	Average ± SD (mg/day)
Methylprednisolone	1 - 2.9	1.6 ± 0.47	1.4 - 5	2.2 ± 0.86
Mometasone furoate	0.4 - 1.1	0.64 ± 0.19	0.54 - 2	0.87 ± 0.34
Prednicarbate	0.74 - 2.1	1.2 ± 0.35	1 - 3.7	1.6 ± 0.64
Prednisolone	1.6 - 73	9.2 ± 20	1.8 - 6.4	2.8 ± 1.1
Triamcinolone	0.19 - 0.56	0.31 ± 0.09	0.27 - 0.97	0.43 ± 0.17
Triamcinolone acetonide	0.38 - 106	17 ± 33	0.52 - 149	24 ± 48
Illicit drugs				
Amphetamine	0.51 - 9,524	1,027 ± 2,724	17 - 2,217	282 ± 511
<i>Benzoylcegonine</i>	36 - 383	158 ± 98	76 - 543	233 ± 123
Cannabinol	0.89 - 36	8.3 ± 12	1.2 - 33	4.9 ± 7.5
<i>Cocaehtylene</i>	0.1 - 95	24 ± 30	0.14 - 97	27 ± 34
Cocaine	0.59 - 34	7 ± 12	0.81 - 57	14 ± 19
<i>Ecgonine methyl ester</i>	0.95 - 373	70 ± 114	1.2 - 333	48 ± 90
Ketamine	0.39 - 12	2.1 ± 3.6	0.53 - 16	2.7 ± 4.5
MDA	14 - 1,609	509 ± 536	1.3 - 1,464	730 ± 595
MDEA	0.33 - 66	10 ± 16	0.45 - 64	8.4 ± 16
MDMA	0.38 - 112	17 ± 28	0.38 - 185	27 ± 49
Methamphetamine	0.19 - 8	0.76 ± 1.9	0.26 - 11	1.5 ± 3.2
Phencyclidine	0.75 - 2.2	1.2 ± 0.35	1 - 3.7	1.6 ± 0.64
THC	0.57 - 66	19 ± 16	0.78 - 171	28 ± 42
Plastic additives				
Benzotriazole	476 - 8,555	3,221 ± 2,005	480 - 9,867	4,169 ± 2,973
p-Toluenesulfonamide	0.49 - 207	40 ± 51	0.67 - 173	33 ± 55
Psychiatric drugs				
<i>10-Hydroxycarbazepine</i>	0.35 - 1,132	394 ± 354	0.36 - 2,040	552 ± 541
<i>7-Aminoclonazepam</i>	0.16 - 0.46	0.26 ± 0.08	0.22 - 0.79	0.35 ± 0.14
<i>7-Aminoflunitrazepam</i>	0.16 - 0.46	0.26 ± 0.08	0.22 - 0.79	0.35 ± 0.14
Alprazolam	0.31 - 0.88	0.49 ± 0.15	0.42 - 1.5	0.67 ± 0.26
Amisulpride	0.39 - 47	9.1 ± 14	0.5 - 737	88 ± 215
Amitriptyline	0.26 - 107	13 ± 28	0.35 - 95	8 ± 22
Amoxapine	0.36 - 1	0.59 ± 0.17	0.5 - 1.8	0.8 ± 0.31
Bromazepam	0.37 - 1.1	0.6 ± 0.18	0.51 - 472	27 ± 111
Carbamazepine	22 - 161	81 ± 42	57 - 365	163 ± 78
Chlordiazepoxide	0.42 - 1.2	0.68 ± 0.2	0.58 - 2.1	0.93 ± 0.36
Chlorprothixene	0.65 - 1.9	1 ± 0.31	0.89 - 3.3	1.4 ± 0.56
Citalopram	11 - 59	20 ± 12	0.85 - 44	19 ± 11
Clobazam	0.27 - 3.3	0.65 ± 0.73	0.36 - 1.3	0.58 ± 0.23
Clomipramine	0.33 - 22	2.9 ± 5.8	0.45 - 95	6.9 ± 22
Clonazepam	0.47 - 1.4	0.76 ± 0.22	0.65 - 14	1.8 ± 3.2
Clorazepate	0.62 - 1.8	1 ± 0.29	0.85 - 3.1	1.4 ± 0.53
Clozapine	0.23 - 35	7 ± 11	0.31 - 35	6 ± 11
<i>Desalkylflurazepam</i>	0.17 - 3	0.53 ± 0.74	0.23 - 3.9	0.57 ± 0.86
Desipramine	0.79 - 96	6.8 ± 23	1.1 - 3.9	1.7 ± 0.68
Desvenlafaxine	5.6 - 39	22 ± 11	15 - 106	46 ± 22
Dexametasone	0.63 - 364	38 ± 98	0.86 - 202	13 ± 47
Diazepam	0.29 - 3.4	0.64 ± 0.72	0.4 - 1.5	0.64 ± 0.25
Dothiepin	0.47 - 73	15 ± 27	0.65 - 156	17 ± 40

Compound	HWW (n = 17)		INF (n = 18)	
	Range (mg/day)	Average ± SD (mg/day)	Range (mg/day)	Average ± SD (mg/day)
Doxepin	0.33 - 0.94	0.52 ± 0.15	0.45 - 1.6	0.71 ± 0.28
<i>EDDP</i>	0.23 - 48	19 ± 13	0.21 - 65	20 ± 16
Felbamate	0.35 - 98	6.3 ± 24	0.48 - 131	8 ± 31
Fluoxetine	0.46 - 21	10 ± 6.9	0.57 - 43	14 ± 11
Flupentixol	0.31 - 0.9	0.5 ± 0.15	0.43 - 1.6	0.68 ± 0.27
Flurazepam	0.2 - 0.58	0.32 ± 0.1	0.28 - 18	1.4 ± 4.1
Fluvoxamine	0.28 - 70	23 ± 25	0.39 - 121	31 ± 40
Gabapentin	250 - 3,370	1,630 ± 878	836 - 8,558	2,958 ± 1,734
Haloperidol	0.24 - 0.69	0.39 ± 0.11	0.33 - 1.2	0.53 ± 0.21
Imipramine	0.1 - 0.28	0.16 ± 0.05	0.13 - 0.48	0.21 ± 0.08
Lamotrigine	29 - 270	121 ± 74	76 - 517	227 ± 117
Lorazepam	0.57 - 126	53 ± 33	0.54 - 116	59 ± 40
Maprotiline	0.29 - 46	18 ± 13	0.36 - 57	17 ± 14
Medazepam	0.58 - 1.7	0.93 ± 0.28	0.79 - 2.9	1.3 ± 0.5
Memantine	0.5 - 43	10 ± 9.7	0.69 - 75	20 ± 19
Methadone	0.63 - 48	9 ± 12	0.86 - 36	8.7 ± 12
Methylphenidate	0.82 - 18	6.2 ± 5.8	1.1 - 24	7.2 ± 7
Mianserin	0.3 - 0.85	0.47 ± 0.14	0.4 - 1.5	0.65 ± 0.25
Mirtazapine	0.54 - 12	4.7 ± 4	0.55 - 18	6.4 ± 6.5
Naltrexone	0.47 - 14	2.6 ± 4.2	0.64 - 18	3.7 ± 6.2
<i>N-Desmethyloclozapine</i>	0.49 - 7.5	1.4 ± 1.9	0.66 - 6.5	1.4 ± 1.3
Nitrazepam	0.59 - 55	17 ± 18	0.8 - 68	20 ± 26
<i>Norbuprenorphine</i>	0.96 - 324	35 ± 77	1.3 - 804	70 ± 189
Nordiazepam	0.22 - 2.2	0.46 ± 0.46	0.3 - 2.6	0.65 ± 0.56
Nortriptyline	0.29 - 0.83	0.46 ± 0.14	0.39 - 1.4	0.63 ± 0.25
Olanzapine	0.67 - 81	17 ± 27	0.91 - 73	16 ± 24
Opipramol	0.25 - 11	1.6 ± 3.5	0.35 - 16	2 ± 4.3
Oxazepam	0.21 - 0.6	0.34 ± 0.1	0.29 - 1	0.46 ± 0.18
Oxcarbazepine	0.36 - 71	14 ± 18	0.49 - 51	14 ± 16
Paliperidone	0.28 - 95	6 ± 23	0.38 - 79	5 ± 19
Paroxetine	0.59 - 1.7	0.96 ± 0.28	0.81 - 3	1.3 ± 0.51
Phenazepam	0.49 - 244	30 ± 67	0.67 - 428	29 ± 101
Phenytoin	0.96 - 120	39 ± 38	1.3 - 297	69 ± 75
Pipamperone	0.41 - 9.9	1.2 ± 2.3	0.56 - 13	1.5 ± 2.8
Prazepam	0.23 - 0.67	0.38 ± 0.11	0.32 - 1.2	0.51 ± 0.2
Promazine	0.77 - 2.2	1.2 ± 0.37	1.1 - 3.8	1.7 ± 0.66
Protriptyline	0.24 - 0.7	0.39 ± 0.12	0.33 - 1.2	0.53 ± 0.21
Quetiapine	0.38 - 29	15 ± 7.5	4.1 - 38	17 ± 9.2
Risperidone	0.29 - 85	17 ± 28	0.4 - 154	22 ± 44
<i>Ritalinic acid</i>	0.45 - 129	20 ± 40	0.61 - 75	15 ± 23
Secobarbital	0.34 - 0.98	0.55 ± 0.16	0.46 - 1.7	0.74 ± 0.29
Sertraline	0.55 - 7	1.2 ± 1.5	0.75 - 2.7	1.2 ± 0.47
Temazepam	0.37 - 18	3.6 ± 4.9	0.51 - 52	8 ± 14
Topiramate	0.45 - 30	2.5 ± 7.2	0.62 - 20	2.5 ± 4.8
Trazodone	0.49 - 48	20 ± 12	0.68 - 81	26 ± 18
Triazolam	0.24 - 0.7	0.39 ± 0.11	0.33 - 1.2	0.53 ± 0.21
Trimipramine	0.58 - 150	9.7 ± 36	0.79 - 40	3.5 ± 9.2

Compound	HWW (n = 17)		INF (n = 18)	
	Range (mg/day)	Average ± SD (mg/day)	Range (mg/day)	Average ± SD (mg/day)
Venlafaxine	6 - 54	29 ± 16	14 - 95	47 ± 22
Zolpidem	0.23 - 0.65	0.36 ± 0.11	0.31 - 1.1	0.49 ± 0.19
Zopiclone	0.74 - 19	2.3 ± 4.4	1 - 3.7	1.6 ± 0.64
<i>α</i> -Hydroxyalprazolam	0.51 - 12	1.5 ± 2.6	0.7 - 18	2.1 ± 4
<i>α</i> -Hydroxymidazolam	2.2 - 33	9.1 ± 8	3.1 - 32	11 ± 7.9
<i>α</i> -Hydroxytriazolam	0.35 - 62	5.3 ± 15	0.48 - 29	3.7 ± 8.7
Receptor antagonists				
Atropine	0.4 - 5.4	0.93 ± 1.2	0.55 - 2	0.88 ± 0.34
Flumazenil	0.76 - 10	1.7 ± 2.2	1 - 11	2.2 ± 2.3
Stimulants				
Caffeine	726 - 2,518	1,458 ± 547	916 - 5,745	2,274 ± 1,351
<i>Cotinine</i>	168 - 655	354 ± 130	233 - 1,343	540 ± 240
Phentermine	0.5 - 1.4	0.81 ± 0.24	0.69 - 2.5	1.1 ± 0.43
UV filter				
Octinoxate	0.45 - 79	39 ± 23	0.58 - 210	83 ± 52
Veterinary drugs				
Carprofen	0.37 - 76	7.7 ± 19	0.5 - 92	11 ± 26
Diaveridine	0.32 - 570	244 ± 131	0.44 - 1,184	364 ± 247
Difloxacin	0.79 - 23	2.6 ± 5.2	1.1 - 28	4.2 ± 7.4
Dimetridazole	0.21 - 0.62	0.34 ± 0.1	0.29 - 1.1	0.47 ± 0.18
Enrofloxacin	0.42 - 11	1.9 ± 2.9	0.57 - 4.6	1.1 ± 0.95
Flunixin	0.34 - 16	6.2 ± 5.5	0.47 - 36	9.3 ± 11
Furaltadone	0.55 - 93	37 ± 30	0.76 - 110	40 ± 36
Iprnidazole	0.22 - 7.1	0.74 ± 1.7	0.3 - 2.3	0.56 ± 0.46
Marbofloxacin	0.7 - 729	189 ± 240	0.96 - 635	170 ± 220
Monensin	0.48 - 1.4	0.77 ± 0.23	0.66 - 2.4	1 ± 0.41
Orbifloxacin	0.45 - 1.3	0.73 ± 0.22	0.62 - 7.9	1.4 ± 1.7
Oxibendazole	0.19 - 2.4	0.43 ± 0.51	0.26 - 3.3	0.58 ± 0.7
Ronidazole	0.52 - 22	2.1 ± 5.1	0.71 - 28	2.6 ± 6.4
Salinomycin	1.6 - 312	21 ± 75	2.2 - 319	21 ± 74
Sarafloxacin	0.76 - 2.2	1.2 ± 0.36	1 - 3.8	1.7 ± 0.65
Sulfachlorpyridazine	0.22 - 35	5.9 ± 11	0.29 - 34	5.8 ± 11
Sulfaclozine	0.25 - 23	1.7 ± 5.4	0.34 - 53	5.1 ± 14
Sulfadoxine	0.54 - 1.5	0.86 ± 0.26	0.74 - 2.7	1.2 ± 0.46
Sulfamonomethoxine	0.33 - 0.95	0.53 ± 0.16	0.45 - 1.6	0.72 ± 0.28
Sulfanitran	0.43 - 1.2	0.69 ± 0.2	0.59 - 2.2	0.94 ± 0.37
Sulfaquinoxaline	0.29 - 41	6.1 ± 13	0.4 - 148	8.8 ± 35
Tilmicosin	0.75 - 201	13 ± 49	1 - 124	8.4 ± 29
X-ray contrast medium				
Iopromide	166 - 28,550	7,025 ± 9,057	141 - 31,829	6,406 ± 9,447

Table S12. Scores attributed to each OMP for frequency (F), average occurrence (O_{av}), maximum occurrence (O_{max}) and load (L) criteria in HWW and INF as well as bioaccumulation (B) and toxicity (T). The final score S of FO_{av}BT, FO_{max}BT and FLBT approaches for HWW and INF are displayed. The final scores $S \geq 14$ are in bold. The transformation products are in italics.

Compound	HWW				INF				B	T	HWW			INF		
	F	O_{av}	O_{max}	L	F	O_{av}	O_{max}	L			Final score S			Final score S		
											FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT
Analgesics/anti-inflammatory																
<i>4-Acetylaminoantipyrine</i>	5	2	3	1	5	2	3	1	1	2	10	11	9	10	11	9
<i>4-FormylAminoAntipyrine</i>	5	2	3	1	5	2	3	1	1	1	9	10	8	9	10	8
<i>6-Acetylmorphine</i>	5	2	4	2	4	2	4	2	2	3	12	14	12	11	13	11
Acetaminophen	5	5	5	5	5	5	5	5	1	1	12	12	12	12	12	12
<i>Acetylcodeine</i>	3	1	2	1	2	1	2	1	3	3	10	11	10	9	10	9
Acetylsalicylic acid	5	4	5	3	5	4	4	3	2	2	13	14	12	13	13	12
Alfentanil	2	1	2	1	2	1	2	1	3	4	10	11	10	10	11	10
Aminopyrine	3	3	4	3	3	3	5	3	1	2	9	10	9	9	11	9
Betamethasone 17,21-dipropionate	3	1	2	1	3	1	2	1	4	3	11	12	11	11	12	11
Buprenorphine	5	2	3	2	4	2	3	2	3	4	14	15	14	13	14	13
<i>Buprenorphine glucuronide</i>	3	3	3	2	2	3	4	2	1	4	11	11	10	10	11	9
Carisoprodol	1	2	3	1	1	1	2	1	3	2	8	9	7	7	8	7
Codeine	5	3	3	3	5	3	3	3	2	3	13	13	13	13	13	13
Dextromethorphan	1	1	1	1	1	1	1	1	4	3	9	9	9	9	9	9
Dextropropoxyphene	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Diclofenac	5	2	3	2	5	5	5	4	5	5	17	18	17	20	20	19
Etodolac	1	1	1	1	1	1	1	1	4	3	9	9	9	9	9	9
Fentanyl	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Hydrocodone	5	3	3	3	5	3	3	3	3	3	14	14	14	14	14	14
Hydromorphone	5	3	3	2	5	3	3	3	3	3	14	14	13	14	14	14
Ibuprofen	5	4	5	3	5	4	5	4	4	5	18	19	17	18	19	18
Ketoprofen	5	5	5	4	5	5	5	5	3	3	16	16	15	16	16	16
Lidocaine	5	3	3	3	5	3	3	3	3	3	14	14	14	14	14	14
Meloxicam	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Morphine	5	3	3	2	5	3	3	3	1	3	12	12	11	12	12	12
<i>Morphine-6-β-D-glucuronide</i>	2	2	3	1	2	2	3	1	1	3	8	9	7	8	9	7
Naproxen	1	5	5	5	1	5	5	5	3	3	12	12	12	12	12	12
<i>Norfentanyl</i>	5	2	3	1	5	2	2	1	2	2	11	12	10	11	11	10
<i>Norpethidine</i>	5	2	2	1	4	2	2	1	2	2	11	11	10	10	10	9
<i>Norpropoxyphene</i>	1	1	2	1	1	1	1	1	4	3	9	10	9	9	9	9
<i>O-Desmethyltramadol</i>	5	3	3	3	5	3	3	3	2	2	12	12	12	12	12	12
Oxycodone	5	2	2	1	5	2	2	1	2	3	12	12	11	12	12	11
Oxymorphone	5	2	2	1	5	2	2	1	2	3	12	12	11	12	12	11
Pentazocine	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Pethidine	1	1	1	1	2	1	1	1	3	2	7	7	7	8	8	8
Phenylbutazone	1	1	2	1	1	1	2	1	4	3	9	10	9	9	10	9
Procaine	5	2	3	1	5	2	3	1	3	3	13	14	12	13	14	12
Tolfenamic acid	1	1	1	1	1	1	1	1	5	4	11	11	11	11	11	11
Tramadol	5	3	3	3	5	3	3	3	3	3	14	14	14	14	14	14

Table S12. (continued)

Compound	HWW				INF				B T		HWW			INF		
	F	O _{av}	O _{max}	L	F	O _{av}	O _{max}	L			Final score S			Final score S		
									FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT		
Antiarrhythmic agents																
Amiodarone	1	1	1	1	1	1	1	1	5	5	12	12	12	12	12	12
Digitoxin	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Propafenone	5	2	3	1	5	2	3	1	4	4	15	16	14	15	16	14
Strophanthidin	1	1	1	1	1	1	2	1	1	2	5	5	5	5	6	5
Strophanthin	1	1	1	1	1	2	3	1	1	2	5	5	5	6	7	5
Antibiotics																
2-NP-AOZ	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Amoxicillin	5	3	3	2	5	2	3	2	1	5	14	14	13	13	14	13
Azithromycin	5	5	5	5	5	5	5	5	3	5	18	18	18	18	18	18
Cinoxacin	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Ciprofloxacin	5	5	5	5	5	5	5	5	2	5	17	17	17	17	17	17
Clarithromycin	5	3	4	3	5	3	3	3	3	4	15	16	15	15	15	15
Doxycycline	3	4	5	3	4	3	5	3	2	4	13	14	12	13	15	13
Enoxacin	2	2	4	1	1	2	4	2	2	3	9	11	8	8	10	8
Erythromycin	5	4	5	3	5	3	5	3	2	4	15	16	14	14	16	14
Flumequine	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Furazolidon	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Lomefloxacin	4	2	3	2	4	2	3	2	3	4	13	14	13	13	14	13
Metronidazole	5	3	4	3	5	3	4	3	1	2	11	12	11	11	12	11
Minocycline	4	3	3	3	3	3	4	3	3	5	15	15	15	14	15	14
Nalidixic Acid	1	1	2	1	1	1	2	1	1	3	6	7	6	6	7	6
Norfloxacin	4	2	3	1	4	2	3	2	2	4	12	13	11	12	13	12
Ofloxacin	5	5	5	4	5	5	5	5	2	4	16	16	15	16	16	16
Oleandomycin	4	4	5	3	4	3	5	3	3	4	15	16	14	14	16	14
Oxolinic acid	1	1	1	1	1	1	1	1	1	2	5	5	5	5	5	5
Oxytetracycline	4	3	4	2	3	2	3	2	1	4	12	14	11	10	11	10
Penicillin G	1	2	3	1	1	2	3	1	2	5	10	11	9	10	11	9
Pipemidic acid	1	1	1	1	1	1	1	1	1	4	7	7	7	7	7	7
Roxithromycin	5	3	4	3	5	3	5	3	3	5	16	17	16	16	18	16
Silvadene	2	3	5	2	3	2	5	2	1	3	9	11	8	9	12	9
Spiramycin	3	5	5	4	2	4	5	4	3	4	15	15	14	13	14	13
Sulfabenzamide	3	3	5	3	2	4	5	3	2	3	11	13	11	11	12	10
Sulfadimethoxine	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Sulfadimidine	1	1	2	1	1	2	2	1	1	3	6	7	6	7	7	6
Sulfafurazole	1	1	1	1	1	1	1	1	2	3	7	7	7	7	7	7
Sulfaguandine	2	2	3	1	2	2	3	1	1	2	7	8	6	7	8	6
Sulfamerazine	2	3	5	3	2	3	5	2	1	3	9	11	9	9	11	8
Sulfamethizole	1	2	3	1	1	2	2	1	1	3	7	8	6	7	7	6
Sulfamethoxazole	5	4	5	3	5	3	5	3	1	4	14	15	13	13	15	13
Sulfamethoxydiazine	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Sulfamethoxypyridazine	1	1	2	1	1	1	1	1	1	3	6	7	6	6	6	6
Sulfanilamide	1	1	1	1	1	1	1	1	1	2	5	5	5	5	5	5
Sulfaphenazole	1	1	1	1	1	1	1	1	2	4	8	8	8	8	8	8
Sulfapyridine	5	2	3	1	5	2	3	1	1	3	11	12	10	11	12	10
Sulfathiazole	4	3	3	2	3	3	3	3	1	3	11	12	10	10	10	10

Table S12. (continued)

Compound	HWW				INF						HWW			INF		
	F	O _{av}	O _{max}	L	F	O _{av}	O _{max}	L	B	T	Final score S			Final score S		
											FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT
Tinidazole	1	2	5	1	1	2	5	2	1	2	6	9	5	6	9	6
Trimethoprim	5	3	4	3	5	3	3	3	1	2	11	12	11	11	11	11
Antifungals																
Sulfacetamide	1	1	1	1	1	1	1	1	1	2	5	5	5	5	5	5
Terbinafine	1	1	1	1	1	1	1	1	5	5	12	12	12	12	12	12
Tiabendazole	5	1	1	1	5	1	1	1	3	3	12	12	12	12	12	12
Antihistamines																
Diphenhydramine	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Promethazine	1	1	1	1	1	1	1	1	5	4	11	11	11	11	11	11
Antihypertensives																
Clonidine	2	1	1	1	2	1	1	1	3	3	9	9	9	9	9	9
Antiparasitics																
Albendazole	3	3	5	2	1	1	2	1	4	4	14	16	13	10	11	10
Flubendazole	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Levamisole	2	2	3	1	1	2	3	1	2	3	9	10	8	8	9	7
Mebendazole	2	2	5	2	1	1	2	1	3	4	11	14	11	9	10	9
Praziquantel	3	2	3	1	4	2	3	2	3	3	11	12	10	12	13	12
Triclabendazole	1	1	1	1	1	1	1	1	5	5	12	12	12	12	12	12
Antiseptic																
Nitrofurantoin	1	2	5	2	1	3	5	2	1	3	7	10	7	8	10	7
Beta-blockers																
Atenolol	5	3	4	3	5	4	4	3	1	1	10	11	10	11	11	10
Bisoprolol	5	2	3	2	5	3	3	2	2	3	12	13	12	13	13	12
Metoprolol	5	2	3	2	5	2	3	2	2	3	12	13	12	12	13	12
Calcium channel blockers																
Verapamil	4	2	3	1	5	2	3	1	4	3	13	14	12	14	15	13
Diuretics																
Torsemide	1	1	1	1	1	1	1	1	2	4	8	8	8	8	8	8
Hormones																
Fludrocortisone-Acetate	1	1	1	1	1	1	1	1	3	2	7	7	7	7	7	7
Flumethasone	1	1	1	1	1	1	1	1	2	2	6	6	6	6	6	6
Hydrocortisone	4	3	3	2	3	3	3	2	2	2	11	12	10	10	10	9
Methylprednisolone	1	1	1	1	1	1	1	1	3	2	7	7	7	7	7	7
Mometasone furoate	1	1	1	1	1	1	1	1	4	3	9	9	9	9	9	9
Prednicarbate	1	1	1	1	1	1	1	1	3	3	8	8	8	8	8	8
Prednisolone	1	2	3	1	1	1	1	1	2	2	7	8	6	6	6	6
Triamcinolone	1	1	1	1	1	1	1	1	1	2	5	5	5	5	5	5
Triamcinolone Acetonide	2	2	3	1	2	2	3	1	3	2	9	10	8	9	10	8
Illicit drugs																
Amphetamine	5	5	5	5	5	3	5	3	2	2	14	14	14	12	14	12
Benzoyllecgonine	5	3	3	3	5	3	3	3	3	5	16	16	16	16	16	16
Cannabinol	2	2	2	1	2	1	2	1	5	5	14	14	13	13	14	13
Cocaethylene	3	2	2	1	3	2	3	1	3	3	11	11	10	11	12	10
Cocaine	2	2	2	1	3	2	2	1	3	3	10	10	9	11	11	10
Ecgonine methyl ester	5	2	3	2	5	2	3	1	1	2	10	11	10	10	11	9
Ketamine	1	1	2	1	1	1	2	1	4	3	9	10	9	9	10	9

Table S12. (continued)

Compound	HWW				INF				B T		HWW			INF		
	F	O _{av}	O _{max}	L	F	O _{av}	O _{max}	L			Final score S			Final score S		
									FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT		
MDA	5	4	5	4	4	4	5	4	2	2	13	14	13	12	13	12
MDEA	3	2	3	1	3	1	2	1	3	2	10	11	9	9	10	9
MDMA	4	2	3	1	3	2	3	1	3	2	11	12	10	10	11	9
Methamphetamine	1	1	2	1	1	1	2	1	3	3	8	9	8	8	9	8
Phencyclidine	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
THC	4	2	3	1	3	2	3	1	5	5	16	17	15	15	16	14
Plastic additives																
Benzotriazole	5	5	5	5	5	5	5	5	2	3	15	15	15	15	15	15
p-Toluenesulfonamide	3	2	3	1	2	2	3	1	1	1	7	8	6	6	7	5
Psychiatric drugs																
10-Hydroxycarbazepine	5	4	5	3	4	4	5	4	1	3	13	14	12	12	13	12
7-Aminoclonazepam	1	1	1	1	1	1	1	1	2	4	8	8	8	8	8	8
7-Aminoflunitrazepam	1	1	1	1	1	1	1	1	2	4	8	8	8	8	8	8
Alprazolam	1	1	1	1	1	1	1	1	2	5	9	9	9	9	9	9
Amisulpride	3	2	2	1	5	3	4	2	2	3	10	10	9	13	14	12
Amitriptyline	3	2	3	1	2	2	3	1	4	4	13	14	12	12	13	11
Amoxapine	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Bromazepam	1	1	1	1	1	2	3	1	3	4	9	9	9	10	11	9
Carbamazepine	5	3	3	2	5	3	3	3	2	5	15	15	14	15	15	15
Chlordiazepoxide	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Chlorprothixene	1	1	1	1	1	1	1	1	5	5	12	12	12	12	12	12
Citalopram	5	2	2	1	5	2	2	1	4	2	13	13	12	13	13	12
Clobazam	1	1	1	1	1	1	1	1	2	3	7	7	7	7	7	7
Clomipramine	1	1	2	1	1	1	3	1	5	4	11	12	11	11	13	11
Clonazepam	1	1	1	1	1	1	2	1	3	4	9	9	9	9	10	9
Clorazepate	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Clozapine	3	2	2	1	2	1	2	1	4	4	13	13	12	11	12	11
Desalkylflurazepam	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Desipramine	1	2	3	1	1	1	1	1	4	4	11	12	10	10	10	10
Desvenlafaxine	5	2	2	1	5	2	3	1	2	3	12	12	11	12	13	11
Dexametasone	1	2	3	1	1	2	3	1	3	2	8	9	7	8	9	7
Diazepam	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Dothiepin	2	2	3	1	1	2	3	1	4	4	12	13	11	11	12	10
Doxepin	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
EDDP	5	2	2	1	5	2	2	1	5	4	16	16	15	16	16	15
Felbamate	1	2	3	1	1	2	3	1	1	2	6	7	5	6	7	5
Fluoxetine	4	2	2	1	4	2	2	1	4	5	15	15	14	15	15	14
Flupentixol	1	1	1	1	1	1	1	1	4	5	11	11	11	11	11	11
Flurazepam	1	1	1	1	1	1	1	1	5	5	12	12	12	12	12	12
Fluvoxamine	4	2	3	1	3	2	3	1	4	3	13	15	12	12	13	11
Gabapentin	5	5	5	5	5	5	5	5	2	3	15	15	15	15	15	15
Haloperidol	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Imipramine	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Lamotrigine	5	3	3	3	5	3	3	3	2	3	13	13	13	13	13	13
Lorazepam	5	2	3	2	4	2	3	2	3	5	15	16	15	14	15	14
Maprotiline	5	2	2	1	5	2	2	1	4	4	15	15	14	15	15	14

Table S12. (continued)

Compound	HWW				INF				B T		HWW			INF		
	F	O _{av}	O _{max}	L	F	O _{av}	O _{max}	L			Final score S			Final score S		
									FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT		
Medazepam	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Memantine	5	2	2	1	5	2	2	1	4	3	14	14	13	14	14	13
Methadone	3	2	2	1	2	2	2	1	4	4	13	13	12	12	12	11
Methylphenidate	3	1	2	1	3	1	2	1	3	2	9	10	9	9	10	9
Mianserin	1	1	1	1	1	1	1	1	2	4	8	8	8	8	8	8
Mirtazapine	3	1	2	1	3	1	2	1	1	4	9	10	9	9	10	9
Naltrexone	1	1	2	1	1	1	2	1	3	3	8	9	8	8	9	8
<i>N-Desmethylclozapine</i>	1	1	2	1	1	1	2	1	4	5	11	12	11	11	12	11
Nitrazepam	3	2	2	1	2	2	2	1	3	4	12	12	11	11	11	10
<i>Norbuprenorphine</i>	3	2	4	1	3	2	5	2	2	3	10	12	9	10	13	10
Nordiazepam	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Nortriptyline	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Olanzapine	2	2	3	1	2	2	2	1	4	5	13	14	12	13	13	12
Opipramol	1	1	2	1	1	1	2	1	4	4	10	11	10	10	11	10
Oxazepam	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Oxcarbazepine	4	2	3	1	3	2	2	1	2	3	11	12	10	10	10	9
Paliperidone	1	1	3	1	1	1	3	1	2	4	8	10	8	8	10	8
Paroxetine	1	1	1	1	1	1	1	1	4	3	9	9	9	9	9	9
Phenazepam	2	2	3	1	1	2	3	1	4	4	12	13	11	11	12	10
Phenytoin	4	2	3	1	4	2	3	2	2	4	12	14	11	12	13	12
Pipamperone	1	1	1	1	1	1	1	1	3	3	8	8	8	8	8	8
Prazepam	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Promazine	1	1	1	1	1	1	1	1	5	4	11	11	11	11	11	11
Protriptyline	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Quetiapine	5	2	2	1	5	2	2	1	3	4	14	14	13	14	14	13
Risperidone	3	2	3	1	2	2	3	1	3	4	12	13	11	11	12	10
<i>Ritalinic acid</i>	2	2	3	1	3	2	3	1	2	2	8	9	7	9	10	8
Secobarbital	1	1	1	1	1	1	1	1	3	3	8	8	8	8	8	8
Sertraline	1	1	1	1	1	1	1	1	5	5	12	12	12	12	12	12
Temazepam	2	1	2	1	2	1	2	1	3	5	11	12	11	11	12	11
Topiramate	1	1	2	1	1	1	2	1	3	2	7	8	7	7	8	7
Trazodone	5	2	2	1	5	2	2	1	3	5	15	15	14	15	15	14
Triazolam	1	1	1	1	1	1	1	1	3	5	10	10	10	10	10	10
Trimipramine	1	2	3	1	1	1	2	1	5	4	12	13	11	11	12	11
Venlafaxine	5	2	2	1	5	2	3	1	3	5	15	15	14	15	16	14
Zolpidem	1	1	1	1	1	1	1	1	4	4	10	10	10	10	10	10
Zopiclone	1	1	2	1	1	1	1	1	3	5	10	11	10	10	10	10
<i>α-Hydroxyalprazolam</i>	1	1	2	1	1	1	2	1	1	4	7	8	7	7	8	7
<i>α-Hydroxymidazolam</i>	5	2	2	1	5	2	2	1	3	4	14	14	13	14	14	13
<i>α-Hydroxytriazolam</i>	1	1	3	1	1	1	2	1	1	5	8	10	8	8	9	8
Receptor antagonists																
Atropine	1	1	1	1	1	1	1	1	2	2	6	6	6	6	6	6
Flumazenil	1	1	2	1	1	1	2	1	3	3	8	9	8	8	9	8
Stimulants																
Caffeine	5	5	5	5	5	5	5	5	1	3	14	14	14	14	14	14
<i>Cotinine</i>	5	4	4	3	5	4	4	4	1	3	13	13	12	13	13	13

Table S12. (continued)

Compound	HWW				INF				B T		HWW			INF		
	F	O _{av}	O _{max}	L	F	O _{av}	O _{max}	L			Final score S			Final score S		
											FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT
Phentermine	1	1	1	1	1	1	1	1	3	2	7	7	7	7	7	7
UV filters																
Octinoxate	5	2	3	1	5	2	3	2	5	5	17	18	16	17	18	17
Veterinary drugs																
Carprofen	1	2	3	1	1	2	3	1	4	4	11	12	10	11	12	10
Diaveridine	5	3	4	3	5	3	4	3	1	4	13	14	13	13	14	13
Difloxacin	1	1	2	1	1	1	2	1	1	3	6	7	6	6	7	6
Dimetridazole	1	1	1	1	1	1	1	1	1	2	5	5	5	5	5	5
Enrofloxacin	1	1	2	1	1	1	1	1	3	3	8	9	8	8	8	8
Flunixin	3	1	2	1	3	1	2	1	5	4	13	14	13	13	14	13
Furaltadone	4	2	3	1	4	2	3	1	1	2	9	10	8	9	10	8
Iprnidazole	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Marbofloxacin	3	3	5	3	3	3	4	3	1	3	10	12	10	10	11	10
Monensin	1	1	1	1	1	1	1	1	4	3	9	9	9	9	9	9
Orbifloxacin	1	1	1	1	1	1	1	1	3	5	10	10	10	10	10	10
Oxibendazole	1	1	1	1	1	1	1	1	3	3	8	8	8	8	8	8
Ronidazole	1	1	2	1	1	1	2	1	1	2	5	6	5	5	6	5
Salinomycin	1	2	4	1	1	2	4	1	5	4	12	14	11	12	14	11
Sarafloxacin	1	1	1	1	1	1	1	1	1	3	6	6	6	6	6	6
Sulfachlorpyridazine	2	2	2	1	2	1	2	1	1	4	9	9	8	8	9	8
Sulfaclozine	1	1	2	1	1	1	2	1	1	3	6	7	6	6	7	6
Sulfadoxine	5	1	1	1	5	1	1	1	1	3	10	10	10	10	10	10
Sulfamonomethoxine	1	1	1	1	1	1	1	1	2	3	7	7	7	7	7	7
Sulfanitran	1	1	1	1	1	1	1	1	3	4	9	9	9	9	9	9
Sulfaquinoxaline	1	1	2	1	1	1	3	1	2	4	8	9	8	8	10	8
Tilmicosin	1	2	3	1	1	2	3	1	4	5	12	13	11	12	13	11
X-ray contrast media																
Iopromide	5	5	5	5	5	5	5	5	1	4	15	15	15	15	15	15
											HWW			INF		
											FO _{av} BT	FO _{max} BT	FLBT	FO _{av} BT	FO _{max} BT	FLBT
Number of OMPs selected (S ≥ 14)											40	57	34	34	47	30

Text S5. Analysis of the contribution of the different criteria to the FO_{av}BT final score *S* in the selection of the key OMPs.

The following analysis refers to Figure 2 in the manuscript.

The eight analgesics/anti-inflammatories selected as key OMPs were: buprenorphine, diclofenac, hydrocodone, hydromorphone, ibuprofen, ketoprofen, lidocaine and tramadol. They present a high frequency of detection in the HWW (82% – 100%) and a high bioaccumulation potential ($\log K_{ow} \geq 2.127$). Among them ibuprofen, which has an average concentration of 0.579 $\mu\text{g/L}$, is the compound with the highest score in the OMP class (18 out of 20). Diclofenac obtained a final score of 17 since it had a maximum score (5) in three criteria: *Freq* = 100%; $\log K_{ow}$ = 4.55; PNEC = 0.05 $\mu\text{g/L}$ and a score of 2 for *O_{av}*, with an average HWW concentration of 0.082 $\mu\text{g/L}$. It is worth noting that the INF average concentration of 1.04 $\mu\text{g/L}$ leads to the maximum score of 20 when applying the FO_{av}BT to INF. Diclofenac and ibuprofen are compounds that have been included in prioritization lists in previous studies (Daouk et al., 2015).

Amoxicillin, azithromycin, ciprofloxacin, clarithromycin, erythromycin, minocycline, ofloxacin, oleandomycin, roxithromycin, spiramycin and sulfamethoxazole are the compounds among the antibiotics to be ranked in the FO_{av}BT analysis. They are characterized by high toxicity (PNEC in the range 0.019 – 0.87 $\mu\text{g/L}$), and many of them are found at concentrations higher than 1 $\mu\text{g/L}$ in HWW: azithromycin (4.005 $\mu\text{g/L}$), ciprofloxacin (1.639 $\mu\text{g/L}$), ofloxacin (1.304 $\mu\text{g/L}$) and spiramycin (1.240 $\mu\text{g/L}$), with the latter being the only compound in the antibiotics with a significantly lower frequency of detection (47%).

Among the psychiatric drugs, nine OMPs (carbamazepine, fluoxetine, gabapentin, lorazepam, maprotiline, memantine, quetiapine, trazodone and venlafaxine) and two transformation products, EDDP (major metabolite of methadone) and α -hydroxymidazolam (linked to midazolam), are selected. As for antibiotics, the psychiatric drugs selected present quite low PNEC values (in the range of 0.016 – 0.3 $\mu\text{g/L}$) except for memantine (1.84 $\mu\text{g/L}$) and gabapentin (10 $\mu\text{g/L}$). These compounds show high frequencies of detection in HWW ($\geq 76\%$), although their average occurrence could be considered low ($\leq 0.129 \mu\text{g/L}$) except for gabapentin (2.611 $\mu\text{g/L}$), a pharmaceutical primarily used to treat seizures and neuropathic pain.

Among the 4 illicit drugs selected, only amphetamine obtained a score of 5 in both the *F* (*Freq* = 94%) and *O_{av}* ($c = 1.27 \mu\text{g/L}$) criteria. Cannabinol and THC are selected due to their high potential for bioaccumulation ($\log K_{ow} \geq 6.8$) and their toxicity (PNEC of 0.072 and 0.08 $\mu\text{g/L}$ for THC and cannabinol, respectively). Benzoylecgonine, a metabolite of cocaine (which was not among the key OMPs) is selected due to 100% frequency of detection and the lack of a PNEC value which, according to a precautionary principle, implies a score of 5 for the toxicity criterion.

Only one compound was selected for the rest of the OMP classes, propafenone (antiarrhythmic agent), albendazole (antiparasitic), verapamil (calcium channel blocker), benzotriazole (plastic additive), caffeine (stimulant), octinoxate (UV filter) and iopromide (X-ray contrast medium). Among them, three compounds are selected due to their high frequency of detection (100%) and average concentration in HWW, namely

benzotriazole (4.847 µg/L), caffeine (2.301 µg/L) and iopromide (11.896 µg/L). Caffeine and iopromide are the most hydrophilic substances selected ($\log K_{ow} = -0.628$ and -2.658 , respectively).

Verapamil is the only compound that is included in the selection with a final score S lower than 14 in HWW ($S = 13$) since its frequency of detection is higher in the INF ($Freq = 89\%$) compared to the HWW ($Freq = 71\%$). For this reason, it was not primarily included in the final list of key OMPs. Octinoxate is the compound with the highest score (17) among the latter group, due to its particularly high bioaccumulation potential ($\log K_{ow} = 5.921$) and high toxicity ($PNEC = 0.026 \mu\text{g/L}$). It is worth noting that these last two compounds are more frequently detected in the INF than in HWW, which implies that they are used in the households of the catchment area around the hospital. UV filters are used on a daily basis as a personal care product, and the calcium channel blocker may be prescribed for daily consumption to the inhabitants of the urban settlement.

4. Removal in the hybrid MBR

Text S6. Removal of macropollutants.

During the experimental campaigns, the removal of the macropollutants was assessed in order to evaluate whether the addition of PAC to the bioreactor may improve the overall quality of the effluent. Table S8 reports their concentration in the EFF, together with the average removal achieved during the noPAC and 0.1PAC campaigns. When adding a concentration of 0.1 g/L PAC to the MBR, the removal efficiencies of all the measured parameters increase (between 3% and 15%) except for N-NH_4^+ , the average removal efficiency of which slightly reduces from 97% to 93%. Previous studies (Alvarino et al., 2018; Cho et al., 2011; Gao et al., 2016) found that the addition of PAC has little to no effect on the removal of organic matter and nutrients, since MBRs already provide very good quality effluent, however, at times the presence of PAC may slightly improve the removal of organic matter (Johir et al., 2016; Remy et al., 2012) and nutrients, especially total nitrogen (Serrano et al., 2011). PAC has been shown to increase biological denitrification in the bioreactor since it provides anoxic zones in the microbial biofilm attached to the PAC surface (Alvarino et al., 2016, 2018). In this way, denitrification occurs not only in the denitrification tank, but also within the granules of sludge that incorporate the PAC. In our study, the average removal of total nitrogen increases from 64% to 73%, which improves the quality of the effluent (from 9.9 mg/L to 7.1 mg/L). Regarding total phosphorous (P_{tot}), its removal efficiency increases by 15% during the 0.1PAC campaign. In activated sludge systems, phosphorous is usually removed from wastewater by (co)precipitation and/or adsorption, with very poor amounts used for cell metabolism and growth (Radjenović et al., 2009). The WWTP under study possesses a tank for the removal of phosphorous, and therefore its effluent concentration was maintained at approximately around 3.2 mg/L, fulfilling the legal limit (10 mg/L, according to Italian Legislative Decree 152/2006 (Decreto Legislativo 152/06, 2006)).

Table S13. Minimum, maximum and average removal efficiencies of the 232 target OMPs analyzed during the three experimental campaigns (i.e., noPAC, 0.1PAC and 0.2PAC), classified according to their therapeutic class. *m* indicates the number of values taken into consideration to calculate the removal efficiency. The compounds in italics correspond to the transformation products. SD: Standard deviation.

Compound	noPAC				0.1PAC				0.2PAC			
	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)
Analgesics/Anti-inflammatories												
<i>4-Acetylaminoantipyrine</i>	0	--	--	--	2	3	31	17 ± 20 *	4	35	91	60 ± 25 *
<i>4-Formylaminoantipyrine</i>	1	22	22	22*	5	1	51	26 ± 19 *	3	9	61	35 ± 26 *
<i>6-Acetylmorphine</i>	2	34	38	36 ± 2	6	58	96	88 ± 15 *	3	99	99.99	99.99
Acetaminophen	2	99	99	99	8	62	99.99	95 ± 13	6	99	99.99	99.99
<i>Acetylcodeine</i>	0	n.d.	n.d.	n.d.	6	1	87	48 ± 29	0	n.d.	n.d.	n.d.
Acetylsalicylic acid	1	23	23	23*	8	36	90	56 ± 18	4	33	75	63 ± 20 *
Alfentanil	2	75	94	85 ± 13	3	20	97	70 ± 44	0	n.d.	n.d.	n.d.
Aminopyrine	1	99.99	99.99	99.99	7	99	99.99	99 ± <0.5	0	n.d.	n.d.	n.d.
Betamethasone 17,21-dipropionate	2	89	96	93 ± 5	7	87	93	90 ± 2	0	n.d.	n.d.	n.d.
Buprenorphine	2	76	84	80 ± 6	6	73	99	88 ± 9	2	99.99	99.99	99.99
<i>Buprenorphine glucuronide</i>	2	99	99	99	1	99	99	99	1	99	99	99
Carisoprodol	0	--	--	--	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Codeine	2	75	94	84 ± 13	8	92	99.99	98 ± 3	6	94	99	98 ± 2
Dextromethorphan	1	27	27	27	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Dextropropoxyphene	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Diclofenac	2	13	16	15 ± 2	5	10	98	46 ± 34 *	6	36	71	54 ± 12
Etodolac	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Fentanyl	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Hydrocodone	2	97	99	98 ± 2	8	95	99.99	97 ± 2	5	99	99.99	99 ± <0.5
Hydromorphone	2	99	99	99	8	99	99.99	99 ± <0.5	6	98	99	99 ± 1
Ibuprofen	2	92	97	95 ± 4	8	23	94	83 ± 25	6	38	99.99	76 ± 21
Ketoprofen	2	98	99	98 ± 1	8	74	99.99	85 ± 9	6	99.99	99.99	99.99
Lidocaine	0	--	--	--	5	2	88	47 ± 38 *	6	34	99	67 ± 23
Meloxicam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Morphine	2	99	99.99	99 ± 1	8	99	99.99	99 ± <0.5	6	98	99	99 ± <0.5
<i>Morphine-6-β-D-glucuronide</i>	1	39	39	39*	2	99	99.99	99 ± <0.5	0	n.d.	n.d.	n.d.
Naproxen	2	96	97	96 ± 1	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
<i>Norfentanyl</i>	1	11	11	11*	4	23	98	53 ± 33 *	4	36	99	67 ± 35 *
<i>Norpethidine</i>	2	14	37	26 ± 16	7	47	96	66 ± 17	3	90	96	93 ± 3
<i>Norpropoxyphene</i>	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
<i>O-Desmethytramadol</i>	2	9	95	52 ± 61	7	56	91	77 ± 14 *	5	41	83	68 ± 20 *
Oxycodone	2	35	45	40 ± 7	7	42	96	72 ± 20	5	71	97	87 ± 11
Oxymorphone	2	75	87	81 ± 8	7	47	98	81 ± 17	6	93	98	95 ± 2
Pentazocine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Pethidine	0	--	--	--	2	27	91	59 ± 46 *	0	n.d.	n.d.	n.d.
Phenylbutazone	0	--	--	--	0	--	--	--	0	n.d.	n.d.	n.d.
Procaine	0	--	--	--	6	21	99.99	82 ± 30 *	6	5	95	63 ± 36
Tolfenamic acid	0	n.d.	n.d.	n.d.	1	91	91	91	0	n.d.	n.d.	n.d.
Tramadol	2	3	5	4 ± 1	5	11	88	41 ± 32 *	6	13	64	43 ± 18
Antiarrhythmic agents												
Amiodarone	0	n.d.	n.d.	n.d.	0	--	--	--	0	n.d.	n.d.	n.d.
Digitoxin	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.

Table S13. (continued)

Compound	noPAC				0.1PAC				0.2PAC			
	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)
Propafenone	2	67	67	67 ± 1	8	71	99	94 ± 10	5	1	99	79 ± 43
Strophanthidin	0	n.d.	n.d.	n.d.	1	97	97	97	0	n.d.	n.d.	n.d.
Strophanthin	0	n.d.	n.d.	n.d.	0	--	--	--	1	99	99	99
Antibiotics												
2-NP-AOZ	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Amoxicillin	2	99	99.99	99 ± 1	7	35	76	60 ± 13	5	97	98	98 ± <0.5
Azithromycin	2	93	97	95 ± 3	8	89	99	97 ± 3	6	96	98	97 ± 1
Cinoxacin	0	--	--	--	0	--	--	--	0	n.d.	n.d.	n.d.
Ciprofloxacin	2	60	72	66 ± 8	8	65	90	76 ± 9	6	66	93	82 ± 11
Clarithromycin	2	94	99	97 ± 3	8	84	97	92 ± 4	6	79	95	88 ± 6
Doxycycline	1	73	73	73*	7	38	99.99	72 ± 21 *	1	99	99	99
Enoxacin	1	96	96	96	1	94	94	94	1	99.99	99.99	99.99
Erythromycin	2	51	99.99	75 ± 35	8	64	99.99	88 ± 15	5	73	99.99	94 ± 12 *
Flumequine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Furazolidon	0	n.d.	n.d.	n.d.	1	91	91	91	0	n.d.	n.d.	n.d.
Lomefloxacin	0	--	--	--	7	18	99	55 ± 29	2	98	99	98 ± 1 *
Metronidazole	2	64	85	75 ± 15	6	23	78	55 ± 19 *	6	3	90	66 ± 31
Minocycline	2	99	99	99 ± 1	7	88	99.99	96 ± 5	0	n.d.	n.d.	n.d.
Nalidixic acid	0	--	--	--	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Norfloxacin	2	99	99	99	7	56	99	83 ± 16	2	99	99.99	99 ± <0.5
Ofloxacin	0	--	--	--	8	3	57	34 ± 18	5	28	93	56 ± 25 *
Oleandomycin	2	83	87	85 ± 3	7	89	99.99	94 ± 4	3	96	99.99	98 ± 2
Oxolinic acid	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Oxytetracycline	2	42	71	57 ± 21	5	13	74	41 ± 29	1	94	94	94
Penicillin G	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Pipemidic acid	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Roxithromycin	2	65	79	72 ± 10	8	82	99.99	92 ± 6	4	56	99.99	83 ± 21
Silvadene	1	79	79	79	4	30	99.99	81 ± 34 *	1	91	91	91
Spiramycin	2	78	99.99	89 ± 16	4	86	99.99	95 ± 7	0	n.d.	n.d.	n.d.
Sulfabenzamide	0	n.d.	n.d.	n.d.	3	12	99	48 ± 45 *	0	n.d.	n.d.	n.d.
Sulfadimethoxine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfadimidine	0	n.d.	n.d.	n.d.	2	39	64	52 ± 17 *	0	n.d.	n.d.	n.d.
Sulfafurazole	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfaguandine	1	99	99	99	3	91	99	97 ± 5	0	n.d.	n.d.	n.d.
Sulfamerazine	0	n.d.	n.d.	n.d.	4	87	96	90 ± 4	0	n.d.	n.d.	n.d.
Sulfamethizole	0	--	--	--	1	98	98	98	0	n.d.	n.d.	n.d.
Sulfamethoxazole	1	56	56	56*	6	26	94	53 ± 25 *	6	24	78	63 ± 21
Sulfamethoxydiazine	0	n.d.	n.d.	n.d.	0	--	--	--	0	n.d.	n.d.	n.d.
Sulfamethoxypyridazine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	1	91	91	91
Sulfanilamide	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfaphenazole	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfapyridine	0	--	--	--	8	71	98	89 ± 11	5	49	92	74 ± 16
Sulfathiazole	0	--	--	--	3	9	20	14 ± 6 *	2	25	41	33 ± 11 *
Tinidazole	0	n.d.	n.d.	n.d.	1	95	95	95	0	n.d.	n.d.	n.d.
Trimethoprim	2	86	91	88 ± 4	8	63	97	81 ± 13	6	53	94	84 ± 15
Antifungals												
Sulfacetamide	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.

Table S13. (continued)

Compound	noPAC				0.1PAC				0.2PAC			
	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)
Terbinafine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Tiabendazole	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Antihistamines												
Diphenhydramine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Promethazine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Antihypertensive												
Clonidine	0	n.d.	n.d.	n.d.	3	89	93	91 ± 2	0	n.d.	n.d.	n.d.
Antiparasitics												
Albendazole	0	n.d.	n.d.	n.d.	3	83	95	89 ± 6	0	n.d.	n.d.	n.d.
Flubendazole	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Levamisole	1	98	98	98	2	87	98	93 ± 8	0	n.d.	n.d.	n.d.
Mebendazole	0	n.d.	n.d.	n.d.	1	79	79	79	0	n.d.	n.d.	n.d.
Praziquantel	2	56	77	66 ± 15	4	78	99	90 ± 11	3	99	99	99
Triclabendazole	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Antiseptic												
Nitrofurantoin	0	n.d.	n.d.	n.d.	0	--	--	--	0	n.d.	n.d.	n.d.
Beta-blockers												
Atenolol	2	98	98	98	8	96	98	97 ± 1	6	96	99.99	97 ± 2
Bisoprolol	2	98	99	99	8	73	99	91 ± 9	6	67	98	93 ± 13
Metoprolol	2	0	40	20 ± 28	2	24	38	31 ± 10 *	2	1	66	33 ± 46 *
Calcium channel blocker												
Verapamil	2	97	98	98 ± 1	7	98	99	99 ± <0.5	5	94	98	97 ± 2
Diuretic												
Torsemide	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Hormones												
Fludrocortisone-acetate	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Flumethasone	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Hydrocortisone	2	32	56	44 ± 17	5	27	99.99	72 ± 30 *	0	n.d.	n.d.	n.d.
Methylprednisolone	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Mometasone furoate	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Prednicarbate	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Prednisolone	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Triamcinolone	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Triamcinolone acetonide	0	n.d.	n.d.	n.d.	0	--	--	--	0	n.d.	n.d.	n.d.
Illicit drugs												
Amphetamine	2	47	87	67 ± 28	8	51	99	87 ± 17	6	80	99	95 ± 7
<i>Benzoylcegonine</i>	2	99.99	99.99	99.99	8	97	99.99	99 ± 1	6	99	99.99	99.99
Cannabinol	2	71	91	81 ± 14	2	67	86	76 ± 13	0	n.d.	n.d.	n.d.
<i>Cocaeethylene</i>	1	99	99	99	5	99	99.99	99 ± <0.5	2	99.99	99.99	99.99
Cocaine	1	78	78	78	5	54	97	85 ± 19	0	n.d.	n.d.	n.d.
<i>Ecgonine methyl ester</i>	1	79	79	79	7	30	99	84 ± 24	2	98	99	99 ± 1
Ketamine	0	n.d.	n.d.	n.d.	3	16	89	51 ± 36	0	n.d.	n.d.	n.d.
MDA	2	41	74	57 ± 23	7	66	99	81 ± 12 *	2	64	93	79 ± 20 *
MDEA	1	75	75	75*	3	66	97	87 ± 18 *	0	n.d.	n.d.	n.d.
MDMA	2	74	88	81 ± 10	5	78	94	88 ± 6	0	n.d.	n.d.	n.d.
Methamphetamine	0	n.d.	n.d.	n.d.	1	96	96	96	1	96	96	96
Phencyclidine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.

Table S13. (continued)

Compound	noPAC				0.1PAC				0.2PAC			
	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)
THC	2	96	99	98 ± 2	5	94	99	96 ± 2	0	n.d.	n.d.	n.d.
Plastic additives												
Benzotriazole	2	79	92	86 ± 9	8	45	71	59 ± 9	6	27	69	44 ± 18
p-Toluenesulfonamide	1	64	64	64*	3	81	99	92 ± 10 *	0	n.d.	n.d.	n.d.
Psychiatric drugs												
<i>10-Hydroxycarbazepine</i>	2	87	89	88 ± 1	8	41	99.99	78 ± 18	3	99.99	99.99	99.99
<i>7-Aminoclonazepam</i>	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
<i>7-Aminoflunitrazepam</i>	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Alprazolam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Amisulpride	0	--	--	--	6	30	93	71 ± 23	4	57	94	82 ± 17 *
Amitriptyline	2	40	93	66 ± 38	4	87	96	90 ± 4	0	n.d.	n.d.	n.d.
Amoxapine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Bromazepam	0	n.d.	n.d.	n.d.	1	99.99	99.99	99.99	1	85	85	85
Carbamazepine	0	--	--	--	4	5	76	40 ± 34 *	6	15	67	48 ± 20
Chlordiazepoxide	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Chlorprothixene	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Citalopram	1	48	48	48*	8	43	98	68 ± 24	4	91	97	94 ± 2
Clobazam	0	n.d.	n.d.	n.d.	0	--	--	--	0	n.d.	n.d.	n.d.
Clomipramine	1	99	99	99	0	n.d.	n.d.	n.d.	1	96	96	96
Clonazepam	0	n.d.	n.d.	n.d.	1	94	94	94	0	n.d.	n.d.	n.d.
Clorazepate	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Clozapine	1	32	32	32	4	89	98	95 ± 4	0	n.d.	n.d.	n.d.
<i>Desalkylflurazepam</i>	0	n.d.	n.d.	n.d.	1	92	92	92	0	n.d.	n.d.	n.d.
Desipramine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Desvenlafaxine	0	--	--	--	5	0	48	25 ± 18 *	6	13	99	47 ± 32
Dexametasone	0	n.d.	n.d.	n.d.	1	99	99	99	0	n.d.	n.d.	n.d.
Diazepam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Dothiepin	0	n.d.	n.d.	n.d.	2	68	74	71 ± 4	0	n.d.	n.d.	n.d.
Doxepin	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
<i>EDDP</i>	2	35	61	48 ± 19	8	28	98	72 ± 23	4	92	98	96 ± 3
Felbamate	0	--	--	--	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Fluoxetine	2	90	95	92 ± 4	7	87	97	95 ± 4	5	89	95	93 ± 2
Flupentixol	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Flurazepam	0	n.d.	n.d.	n.d.	1	94	94	94	0	n.d.	n.d.	n.d.
Fluvoxamine	2	99	99	99	7	56	99	88 ± 15	0	n.d.	n.d.	n.d.
Gabapentin	2	74	87	81 ± 10	8	85	96	90 ± 4	6	82	98	92 ± 6
Haloperidol	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Imipramine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Lamotrigine	0	--	--	--	6	9	79	29 ± 26 *	4	25	46	36 ± 9 *
Lorazepam	1	1	1	1*	7	10	99	49 ± 37	3	99	99	99 ± <0.5
Maprotiline	2	44	51	48 ± 5	8	13	98	66 ± 25	4	90	98	94 ± 3
Medazepam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Memantine	0	--	--	--	3	9	83	42 ± 38 *	5	29	92	66 ± 30
Methadone	0	n.d.	n.d.	n.d.	5	70	95	90 ± 11	0	n.d.	n.d.	n.d.
Methylphenidate	1	36	36	36	6	83	88	87 ± 2	0	n.d.	n.d.	n.d.
Mianserin	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Mirtazapine	1	37	37	37*	5	56	93	84 ± 16	1	91	91	91

Table S13. (continued)

Compound	noPAC				0.1PAC				0.2PAC			
	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)
Naltrexone	0	n.d.	n.d.	n.d.	3	30	57	40 ± 15	0	n.d.	n.d.	n.d.
<i>N-Desmethylozapine</i>	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Nitrazepam	1	56	56	56	3	21	47	37 ± 14 *	0	n.d.	n.d.	n.d.
<i>Norbuprenorphine</i>	2	93	96	95 ± 2	6	89	99.99	94 ± 4	0	n.d.	n.d.	n.d.
Nordiazepam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Nortriptyline	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Olanzapine	2	95	97	96 ± 1	3	96	98	96 ± 1	1	97	97	97
Opipramol	0	n.d.	n.d.	n.d.	2	22	28	25 ± 4	0	n.d.	n.d.	n.d.
Oxazepam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Oxcarbapazine	0	--	--	--	5	10	95	42 ± 40 *	0	n.d.	n.d.	n.d.
Paliperidone	1	96	96	96	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Paroxetine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Phenazepam	0	n.d.	n.d.	n.d.	1	75	75	75*	0	n.d.	n.d.	n.d.
Phenytoin	1	2	2	2*	2	0	15	8 ± 10 *	1	93	93	93
Pipamperone	1	89	89	89	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Prazepam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Promazine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Protriptyline	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Quetiapine	2	93	98	95 ± 4	8	96	98	97 ± 1	6	90	96	92 ± 2
Risperidone	0	n.d.	n.d.	n.d.	5	87	99	95 ± 6	0	n.d.	n.d.	n.d.
<i>Ritalinic acid</i>	0	--	--	--	4	7	88	56 ± 35 *	0	n.d.	n.d.	n.d.
Secobarbital	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sertraline	0	n.d.	n.d.	n.d.	0	--	--	--	0	n.d.	n.d.	n.d.
Temazepam	1	24	24	24*	5	6	96	31 ± 37 *	0	n.d.	n.d.	n.d.
Topiramate	0	n.d.	n.d.	n.d.	1	88	88	88	0	n.d.	n.d.	n.d.
Trazodone	2	96	98	97 ± 1	8	95	99	97 ± 1	5	77	96	91 ± 8
Triazolam	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Trimipramine	1	39	39	39	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Venlafaxine	0	--	--	--	6	6	80	33 ± 28 *	6	6	64	39 ± 24
Zolpidem	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Zopiclone	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
<i>α-Hydroxyalprazolam</i>	0	n.d.	n.d.	n.d.	1	94	94	94	0	n.d.	n.d.	n.d.
<i>α-Hydroxymidazolam</i>	2	38	46	42 ± 5	8	11	84	48 ± 24	5	49	97	80 ± 21 *
<i>α-Hydroxytriazolam</i>	0	--	--	--	1	4	4	4	0	n.d.	n.d.	n.d.
Receptor antagonists												
Atropine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Flumazenil	0	n.d.	n.d.	n.d.	1	87	87	87	0	n.d.	n.d.	n.d.
Stimulants												
Caffeine	2	54	66	60 ± 8	8	34	96	75 ± 20	6	97	98	97 ± 1
<i>Cotinine</i>	2	98	98	98	8	94	99	97 ± 2	6	98	99.99	99 ± 1
Phentermine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
UV filter												
Octinoxate	2	93	99	96 ± 4	8	94	99	99 ± 2	5	58	99	85 ± 19
Veterinary drugs												
Carprofen	0	n.d.	n.d.	n.d.	2	99	99	99 ± <0.5 *	0	n.d.	n.d.	n.d.
Diaveridine	2	88	91	90 ± 2	8	79	99.99	93 ± 6	5	86	99.99	91 ± 6
Difloxacin	1	86	86	86	1	86	86	86	0	n.d.	n.d.	n.d.

Table S13. (continued)

Compound	noPAC				0.1PAC				0.2PAC			
	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)	<i>m</i>	Min. (%)	Max. (%)	Average ± SD (%)
Dimetridazole	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Enrofloxacin	1	69	69	69	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Flunixin	0	--	--	--	0	--	--	--	0	n.d.	n.d.	n.d.
Furaltadone	2	96	99	98 ± 2	8	97	99	98 ± <0.5	0	n.d.	n.d.	n.d.
Iprnidazole	1	67	67	67	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Marbofloxacin	1	98	98	98*	6	40	85	56 ± 15	0	n.d.	n.d.	n.d.
Monensin	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Orbifloxacin	0	n.d.	n.d.	n.d.	1	86	86	86	0	n.d.	n.d.	n.d.
Oxibendazole	1	90	90	90	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Ronidazole	0	n.d.	n.d.	n.d.	1	95	95	95*	0	n.d.	n.d.	n.d.
Salinomycin	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sarafloxacin	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfachlorpyridazine	0	n.d.	n.d.	n.d.	4	5	98	65 ± 44	0	n.d.	n.d.	n.d.
Sulfaclozine	1	99	99	99	1	48	48	48	0	n.d.	n.d.	n.d.
Sulfadoxine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfamonomethoxine	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfantran	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
Sulfaquinoxaline	0	n.d.	n.d.	n.d.	1	99.99	99.99	99.99	0	n.d.	n.d.	n.d.
Tilmicosin	1	99	99	99	0	n.d.	n.d.	n.d.	0	n.d.	n.d.	n.d.
X-ray contrast medium												
Iopromide	2	98	99.99	99	8	51	99.99	87 ± 18	6	93	99.99	98 ± 3

Legend

“n.d.” indicates that the OMP was not detected in both INF and MBRperm, hence the removal efficiency was not calculated.

“--” indicates that negative removal efficiencies were obtained on all sampling days of that experimental campaign.

“*” indicates that negative removal efficiencies were obtained on certain sampling days of the corresponding experimental campaign which were then discarded for the calculation of the minimum, maximum and average removal efficiencies. To check the negative values discarded, refer to **Table S14**.

Notes

The term “removal” refers to the change in the load of a given OMP in the MBRperm compared to the load in the INF, as described in **Section 2.5** of the manuscript, regardless of whether it is mineralized, transformed or adsorbed in the system. Samples in which the OMP was not detected (n.d.) in both INF and MBRperm were not taken into consideration for removal efficiency calculation. Instead, the term “negative removal” refers to a higher load in the MBRperm with respect to the INF.

The term “transformation product” refers to compounds that are formed by sub-sequential reactions of the parent compound. These reactions include biodegradation/metabolization in living organisms (i.e., formation of metabolites), and chemical transformations that take place during the transport in the sewage or during the wastewater treatment. Transformation products can be the result of any reaction which does not completely mineralize the parent compound to water and dioxide.

Table S14. Values of negative removal efficiencies of target OMPs obtained during the three experimental campaigns (i.e., noPAC, 0.1PAC and 0.2PAC), classified according to their therapeutic class. Negative values were discarded for the calculation of the minimum, maximum and average removal efficiencies of the corresponding OMPs during each campaign (see **Table S13**). The compounds in italics correspond to the transformation products.

Compound	noPAC		0.1PAC		0.2PAC	
	num. of values	negative values	num. of values	negative values	num. of values	negative values
Analgesics/anti-inflammatories						
<i>4-Acetylaminoantipyrine</i>	2	-114; -60	6	-86; -1; -38; -25; -97; -6	1	-14
<i>4-Formylaminoantipyrine</i>	1	-38	3	-12; -42; -6	2	-1; -8
<i>6-Acetylmorphine</i>			1	-3		
Acetylsalicylic acid	1	-61			2	-125; -1
Carisoprodol	1	-46				
Diclofenac			3	-53; -20; -54		
Lidocaine	2	-20; -32	3	-8; -58; -4		
<i>Morphine-6-β-D-glucuronide</i>	1	-89753				
<i>Norfentanyl</i>	1	-23	4	-81; -142; -63; -45	1	-1090
<i>O-Desmethytramadol</i>			1	-16	1	-55
Pethidine	1	-1233	1	-55		
Phenylbutazone	1	-2	1	-5		
Procaine	1	-136	2	-23; -800		
Tramadol			3	-1; -22; -1		
Antiarrhythmic agents						
Amiodarone			1	-297		
Strophanthin			1	-1615		
Antibiotics						
Cinoxacin	1	-22	2	-866; -7		
Doxycycline	1	-35	1	-30		
Erythromycin					1	-3040
Lomefloxacin	2	-56; -42			1	-17
Metronidazole			2	-342; -58		
Nalidixic acid	1	-48				
Ofloxacin	2	-3; -13			1	-29
Silvadene			1	-918		
Sulfabenzamide			3	-73; -20; -3		
Sulfadimidine			1	-953		
Sulfamethizole	1	-61				
Sulfamethoxazole	1	-11	2	-7; -22		
Sulfamethoxydiazine			1	-1345		
Sulfapyridine	1	-17				
Sulfathiazole	1	-116	1	-30	1	-11899
Antiseptic						
Nitrofurantoin			1	-33		
Beta-blocker						
Metoprolol			6	-12; -324; -67; -99; -17; -71	4	-7; -181; -1; -3
Hormones						
Hydrocortisone			1	-103		
Triamcinolone acetonide			4	-35; -100; -54; -104		
Illicit drugs						
MDA			1	-36	1	-10875
MDEA	1	-50	3	-189; -3786; -36		
Plastic additives						
p-Toluenesulfonamide	1	-1912	2	-234; -16		
Psychiatric drugs						
Amisulpride	2	-43; -21			1	-9
Carbamazepine	2	-111; -24	4	-4; -24; -13; -35		
Citalopram	1	-63				
Clobazam			1	-1662		
Desvenlafaxine	2	-25; -2	3	-20; -5; -21		
Felbamate	1	-5378				

Compound	noPAC		0.1PAC		0.2PAC	
	num. of values	negative values	num. of values	negative values	num. of values	negative values
Lamotrigine	2	-116; -35	2	-11; -30	2	-30; -29
Lorazepam	1	-7				
Memantine	2	-19; -35	5	-244; -21; -9; -123; -44		
Mirtazapine	1	-33				
Nitrazepam			2	-10; -2		
Oxcarbazepine	2	-203; -48	2	-18; -26		
Phenazepam			1	-7		
Phenytoin	1	-84	5	-67; -52; -20; -12; -64		
<i>Ritalinic acid</i>	2	-206; -919	1	-2593		
Sertraline			1	-888		
Temazepam	1	-1697	1	-779		
Venlafaxine	2	-79; -34	2	-54; -3		
<i>α-Hydroxymidazolam</i>					1	-41
<i>α-Hydroxytriazolam</i>	1	-76				
Veterinary drugs						
Carprofen			1	-10688		
Flunixin	1	-32	7	-49; -51; -107; -28; -52; -53; -37		
Marbofloxacin	1	-1				
Ronidazole			1	-8124		

Table S15. Range of variability and average occurrence of the 232 target OMPs analyzed in HWW, INF, MBRperm and EFF during the noPAC experimental campaign (only MBR) (March – August 2021). For MBRperm, the frequency of detection (*Freq*) is displayed and the hydraulic retention time was considered for the sampling. The transformation products are written in italics. SD: Standard deviation.

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n= 3)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Analgesics/Anti-inflammatories							
<i>4-Acetylaminoantipyrine</i>	<LOD - 0.083	0.045 ± 0.041	<LOD - 0.113	0.058 ± 0.048	100	0.046 - 0.065	0.055 ± 0.013
<i>4-Formylaminoantipyrine</i>	0.007 - 0.099	0.057 ± 0.046	0.007 - 0.134	0.082 ± 0.049	100	0.05 - 0.059	0.054 ± 0.006
<i>6-Acetylmorphine</i>	0.008 - 0.009	0.009 ± 0.001	0.008 - 0.013	0.012 ± 0.001	100	0.007 - 0.009	0.008 ± 0.001
Acetaminophen	0.952 - 6.02	4.163 ± 2.792	0.952 - 7.256	4.177 ± 3.413	100	0.043 - 0.055	0.049 ± 0.008
<i>Acetylcodeine</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Acetylsalicylic acid	0.427 - 0.631	0.544 ± 0.105	0.427 - 0.776	0.631 ± 0.138	100	0.474 - 0.807	0.641 ± 0.235
Alfentanil	<LOD - 0.035	0.015 ± 0.018	<LOD - 0.007	0.004 ± 0.004	50	<LOD - 0.002	0.001 ± 0.001
Aminopyrine	0.373 - 0.725	0.502 ± 0.194	0.373 - 1.299	0.6 ± 0.654	0	<LOD	<LOD
Betamethasone 17,21-dipropionate	<LOD - 0.026	0.012 ± 0.013	<LOD - 0.033	0.023 ± 0.011	0	<LOD	<LOD
Buprenorphine	0.079 - 0.185	0.132 ± 0.053	0.079 - 0.143	0.103 ± 0.04	100	0.015 - 0.016	0.016 ± 0.001
<i>Buprenorphine glucuronide</i>	0.094 - 0.414	0.244 ± 0.161	0.094 - 0.5	0.268 ± 0.203	0	<LOD	<LOD
Carisoprodol	<LOD - 0.195	0.066 ± 0.111	<LOD - 0.091	0.031 ± 0.051	50	<LOD - 0.133	0.067 ± 0.093
Codeine	0.166 - 0.417	0.313 ± 0.131	0.166 - 0.393	0.295 ± 0.139	100	0.024 - 0.034	0.029 ± 0.007
Dextromethorphan	<LOD	<LOD	<LOD - 0.008	0.003 ± 0.004	50	<LOD - 0.006	0.003 ± 0.004
Dextropropoxyphene	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Diclofenac	0.055 - 0.102	0.075 ± 0.024	0.055 - 0.326	0.264 ± 0.071	100	0.157 - 0.241	0.199 ± 0.059
Etodolac	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fentanyl	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hydrocodone	0.146 - 0.39	0.285 ± 0.125	0.146 - 0.365	0.27 ± 0.133	50	<LOD - 0.012	0.006 ± 0.008
Hydromorphone	0.105 - 0.371	0.259 ± 0.138	0.105 - 0.277	0.198 ± 0.114	50	<LOD - 0.002	<LOD
Ibuprofen	0.747 - 1.004	0.836 ± 0.145	0.747 - 1.449	1.062 ± 0.409	100	0.032 - 0.051	0.042 ± 0.014
Ketoprofen	1.264 - 2.179	1.766 ± 0.464	1.264 - 3.828	2.504 ± 1.305	100	0.027 - 0.033	0.03 ± 0.005
Lidocaine	0.151 - 0.394	0.272 ± 0.121	0.151 - 0.376	0.268 ± 0.125	100	0.173 - 0.353	0.263 ± 0.127
Meloxicam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Morphine	0.105 - 0.371	0.259 ± 0.138	0.105 - 0.277	0.198 ± 0.114	0	<LOD	<LOD
<i>Morphine-6-β-D-glucuronide</i>	<LOD - 0.07	0.039 ± 0.035	<LOD - 0.156	0.062 ± 0.083	100	0.095 - 0.537	0.316 ± 0.313
Naproxen	<LOD - 23.256	10.926 ± 11.691	<LOD - 19.621	12.543 ± 10.892	100	0.593 - 0.726	0.66 ± 0.094
<i>Norfentanyl</i>	0.027 - 0.071	0.043 ± 0.025	0.027 - 0.085	0.048 ± 0.032	100	0.035 - 0.076	0.055 ± 0.029
<i>Norpethidine</i>	0.04 - 0.076	0.058 ± 0.018	0.04 - 0.074	0.05 ± 0.022	100	0.021 - 0.036	0.028 ± 0.011
<i>Norpropoxyphene</i>	<LOD - 0.024	0.009 ± 0.013	<LOD	<LOD	0	<LOD	<LOD
<i>O-Desmethyltramadol</i>	0.083 - 0.425	0.295 ± 0.185	0.083 - 0.479	0.413 ± 0.099	100	0.015 - 0.436	0.225 ± 0.298
Oxycodone	0.021 - 0.058	0.035 ± 0.019	0.021 - 0.035	0.025 ± 0.009	100	0.01 - 0.014	0.012 ± 0.003
Oxymorphone	0.041 - 0.041	0.041 ± 0	0.041 - 0.081	0.061 ± 0.02	100	0.01 - 0.01	0.01 ± 0
Pentazocine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Pethidine	<LOD - 0.006	0.002 ± 0.003	<LOD - 0.008	0.003 ± 0.004	50	<LOD - 0.008	0.004 ± 0.005
Phenylbutazone	<LOD - 0.017	0.006 ± 0.009	<LOD - 0.029	0.01 ± 0.016	50	<LOD - 0.03	0.015 ± 0.02
Procaine	<LOD - 0.005	0.004 ± 0.003	<LOD - 0.009	0.005 ± 0.004	50	<LOD - 0.013	0.007 ± 0.009
Tolfenamic acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Tramadol	0.31 - 0.367	0.341 ± 0.029	0.31 - 0.482	0.354 ± 0.111	100	0.275 - 0.459	0.367 ± 0.13

Table S15. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n= 3)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Antiarrhythmic agents							
Amiodarone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Digitoxin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Propafenone	0.048 - 0.111	0.071 ± 0.035	0.048 - 0.201	0.088 ± 0.099	100	0.006 - 0.015	0.011 ± 0.007
Strophanthidin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Strophanthin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antibiotics							
2-NP-AOZ	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amoxicillin	0.106 - 0.447	0.228 ± 0.19	0.106 - 0.204	0.146 ± 0.062	0	<LOD	<LOD
Azithromycin	2.998 - 10.483	5.703 ± 4.152	2.998 - 9.873	4.623 ± 4.576	100	0.075 - 0.11	0.092 ± 0.025
Cinoxacin	<LOD - 0.006	0.004 ± 0.003	<LOD - 0.008	0.005 ± 0.004	50	<LOD - 0.01	0.005 ± 0.006
Ciprofloxacin	1.466 - 2.01	1.652 ± 0.31	1.466 - 1.715	1.253 ± 0.496	100	0.288 - 0.488	0.388 ± 0.142
Clarithromycin	0.065 - 0.504	0.238 ± 0.233	0.065 - 0.33	0.185 ± 0.131	50	<LOD - 0.004	0.003 ± 0.002
Doxycycline	<LOD - 0.341	0.13 ± 0.184	<LOD - 0.416	0.174 ± 0.216	100	0.111 - 0.142	0.126 ± 0.022
Enoxacin	<LOD - 0.191	0.065 ± 0.11	<LOD - 0.388	0.13 ± 0.223	50	<LOD - 0.016	0.009 ± 0.011
Erythromycin	0.068 - 1.897	0.767 ± 0.988	0.068 - 0.362	0.241 ± 0.124	50	<LOD - 0.121	0.061 ± 0.085
Flumequine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Furazolidon	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Lomefloxacin	0.087 - 0.16	0.123 ± 0.037	0.087 - 0.169	0.13 ± 0.037	100	0.137 - 0.194	0.165 ± 0.04
Metronidazole	0.375 - 0.843	0.563 ± 0.247	0.375 - 0.556	0.31 ± 0.213	100	0.073 - 0.082	0.078 ± 0.006
Minocycline	0.141 - 0.379	0.23 ± 0.13	0.141 - 0.787	0.421 ± 0.334	0	<LOD	<LOD
Nalidixic Acid	<LOD - 0.026	0.01 ± 0.014	<LOD - 0.036	0.013 ± 0.02	50	<LOD - 0.053	0.027 ± 0.036
Norfloxacin	<LOD - 0.142	0.087 ± 0.075	<LOD - 0.15	0.091 ± 0.079	0	<LOD	<LOD
Ofloxacin	1.38 - 1.897	1.687 ± 0.272	1.38 - 1.635	1.516 ± 0.163	100	1.689 - 1.783	1.736 ± 0.067
Oleandomycin	0.602 - 1.481	0.982 ± 0.451	0.602 - 1.176	0.671 ± 0.453	100	0.052 - 0.069	0.06 ± 0.012
Oxolinic Acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxytetracycline	0.138 - 0.216	0.179 ± 0.039	0.138 - 0.277	0.206 ± 0.074	100	0.062 - 0.075	0.068 ± 0.009
Penicillin G	<LOD - 0.102	0.037 ± 0.056	<LOD - 0.163	0.057 ± 0.092	0	<LOD	<LOD
Pipemidic acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Roxithromycin	0.69 - 0.991	0.85 ± 0.151	0.69 - 1.236	0.606 ± 0.571	100	0.043 - 0.096	0.07 ± 0.037
Silvadene	<LOD - 0.052	0.018 ± 0.029	<LOD - 0.047	0.031 ± 0.026	50	<LOD - 0.01	0.005 ± 0.006
Spiramycin	1.653 - 4.439	2.735 ± 1.493	1.653 - 2.513	1.722 ± 0.701	50	<LOD - 0.262	0.133 ± 0.182
Sulfabenzamide	<LOD - 0.467	0.157 ± 0.269	<LOD - 1.677	0.56 ± 0.967	0	<LOD	<LOD
Sulfadimethoxine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfadimidine	<LOD - 0.054	0.018 ± 0.03	<LOD - 0.097	0.033 ± 0.055	0	<LOD	<LOD
Sulfafurazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaguanidine	<LOD - 0.226	0.076 ± 0.13	<LOD - 0.142	0.048 ± 0.082	0	<LOD	<LOD
Sulfamerazine	<LOD - 1.663	0.555 ± 0.959	<LOD - 1.014	0.339 ± 0.585	0	<LOD	<LOD
Sulfamethizole	<LOD - 0.036	0.013 ± 0.019	<LOD - 0.059	0.029 ± 0.029	50	<LOD - 0.042	0.022 ± 0.028
Sulfamethoxazole	0.198 - 1.315	0.7 ± 0.567	0.198 - 1.23	0.614 ± 0.538	100	0.104 - 1.371	0.737 ± 0.896
Sulfamethoxydiazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfamethoxypyridazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfanilamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaphenazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfapyridine	<LOD - 0.018	0.01 ± 0.009	<LOD - 0.009	0.004 ± 0.005	50	<LOD - 0.011	0.006 ± 0.007
Sulfathiazole	<LOD - 0.209	0.124 ± 0.109	<LOD - 0.404	0.211 ± 0.202	50	<LOD - 0.492	0.247 ± 0.347
Tinidazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD

Table S15. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n= 3)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Trimethoprim	0.087 - 0.541	0.32 ± 0.227	0.087 - 0.388	0.231 ± 0.149	100	0.008 - 0.056	0.032 ± 0.033
Antifungals							
Sulfacetamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Terbinafine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Tiabendazole	<LOD - 0.003	0.001 ± 0.001	<LOD	<LOD	100	<LOD	<LOD
Antihistamines							
Diphenhydramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Promethazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antihypertensive							
Clonidine	<LOD - 0.002	0.001 ± 0.001	<LOD - 0.002	0.001 ± 0.001	0	<LOD	<LOD
Antiparasitics							
Albendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flubendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Levamisole	<LOD - 0.02	0.008 ± 0.011	<LOD - 0.079	0.027 ± 0.045	0	<LOD	<LOD
Mebendazole	<LOD - 0.012	0.004 ± 0.007	<LOD - 0.006	0.003 ± 0.003	0	<LOD	<LOD
Praziquantel	0.028 - 0.12	0.073 ± 0.046	0.028 - 0.157	0.098 ± 0.051	100	0.017 - 0.03	0.023 ± 0.009
Triclabendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antiseptic							
Nitrofurazone	<LOD - 0.165	0.056 ± 0.095	<LOD - 0.181	0.061 ± 0.104	0	<LOD	<LOD
Beta-blockers							
Atenolol	0.33 - 0.6	0.444 ± 0.14	0.33 - 0.841	0.653 ± 0.19	100	0.009 - 0.011	0.01 ± 0.001
Bisoprolol	0.091 - 0.152	0.12 ± 0.031	0.091 - 0.165	0.122 ± 0.042	0	<LOD	<LOD
Metoprolol	0.007 - 0.074	0.039 ± 0.033	0.007 - 0.064	0.038 ± 0.027	100	0.006 - 0.063	0.035 ± 0.04
Calcium channel blocker							
Verapamil	0.043 - 0.113	0.078 ± 0.035	0.043 - 0.039	0.033 ± 0.009	0	<LOD	<LOD
Diuretic							
Torsemide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hormones							
Fludrocortisone-Acetate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flumethasone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hydrocortisone	0.263 - 0.357	0.304 ± 0.048	0.263 - 0.263	0.206 ± 0.05	100	0.074 - 0.127	0.101 ± 0.038
Methylprednisolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mometasone furoate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prednicarbate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prednisolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone Acetonide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Illicit drugs							
Amphetamine	0.246 - 11.258	6.641 ± 5.717	0.246 - 1.634	0.991 ± 0.667	100	0.206 - 0.547	0.377 ± 0.241
<i>Benzoylcegonine</i>	0.082 - 0.338	0.181 ± 0.138	0.082 - 0.348	0.303 ± 0.041	0	<LOD	<LOD
Cannabinol	<LOD	<LOD	<LOD - 0.024	0.015 ± 0.008	0	<LOD	<LOD
<i>Cocaethylene</i>	<LOD - 0.084	0.029 ± 0.048	<LOD - 0.04	0.014 ± 0.023	0	<LOD	<LOD
Cocaine	<LOD - 0.017	0.007 ± 0.009	<LOD - 0.04	0.018 ± 0.02	50	<LOD - 0.009	0.005 ± 0.005
<i>Ecgonine methyl ester</i>	<LOD - 0.258	0.087 ± 0.148	<LOD - 0.029	0.011 ± 0.016	100	<LOD - 0.006	0.004 ± 0.003
Ketamine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
MDA	1.21 - 1.656	1.43 ± 0.223	1.21 - 2.293	1.772 ± 0.641	100	0.514 - 0.624	0.569 ± 0.078
MDEA	0.007 - 0.117	0.051 ± 0.059	0.007 - 0.022	0.012 ± 0.009	50	<LOD - 0.033	0.017 ± 0.023

Table S15. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 3)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
MDMA	0.01 - 0.198	0.075 ± 0.106	0.01 - 0.289	0.115 ± 0.151	100	0.002 - 0.01	0.006 ± 0.005
Methamphetamine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Phencyclidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
THC	0.017 - 0.11	0.052 ± 0.051	0.017 - 0.247	0.118 ± 0.113	0	<LOD	<LOD
Plastic additives							
Benzotriazole	5.254 - 9.191	7.336 ± 1.978	5.254 - 10.5	7.632 ± 2.705	100	0.825 - 1.528	1.177 ± 0.497
p-Toluenesulfonamide	0.054 - 0.138	0.089 ± 0.044	0.054 - 0.133	0.056 ± 0.069	100	0.012 - 0.025	0.018 ± 0.009
Psychiatric drugs							
10-Hydroxycarbazepine	0.329 - 0.5	0.417 ± 0.085	0.329 - 0.845	0.708 ± 0.121	100	0.075 - 0.078	0.077 ± 0.002
7-Aminoclonazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
7-Aminoflunitrazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Alprazolam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amisulpride	<LOD - 0.017	0.006 ± 0.009	<LOD - 0.037	0.027 ± 0.011	100	0.018 - 0.04	0.029 ± 0.015
Amitriptyline	0.012 - 0.19	0.072 ± 0.102	0.012 - 0.149	0.054 ± 0.082	50	<LOD - 0.002	0.002 ± 0.001
Amoxapine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Bromazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Carbamazepine	0.091 - 0.143	0.121 ± 0.027	0.091 - 0.29	0.258 ± 0.038	100	0.333 - 0.456	0.395 ± 0.087
Chlordiazepoxide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Chlorprothixene	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Citalopram	0.027 - 0.098	0.056 ± 0.038	0.027 - 0.03	0.024 ± 0.009	100	0.015 - 0.023	0.019 ± 0.005
Clobazam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clomipramine	<LOD - 0.036	0.012 ± 0.02	<LOD - 0.136	0.046 ± 0.078	0	<LOD	<LOD
Clonazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clorazepate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clozapine	<LOD - 0.059	0.036 ± 0.031	<LOD - 0.019	0.01 ± 0.009	50	<LOD - 0.007	0.004 ± 0.004
Desalkylflurazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Desipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Desvenlafaxine	0.019 - 0.07	0.038 ± 0.028	0.019 - 0.103	0.07 ± 0.029	100	0.05 - 0.073	0.061 ± 0.016
Dexametasone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Diazepam	<LOD - 0.006	0.002 ± 0.003	<LOD	<LOD	0	<LOD	<LOD
Dothiepin	<LOD - 0.13	0.044 ± 0.074	<LOD - 0.104	0.035 ± 0.059	0	<LOD	<LOD
Doxepin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
EDDP	0.038 - 0.085	0.054 ± 0.027	0.038 - 0.067	0.04 ± 0.024	100	0.009 - 0.018	0.014 ± 0.006
Felbamate	<LOD - 0.173	0.058 ± 0.099	<LOD - 0.204	0.069 ± 0.118	50	<LOD - 0.049	0.025 ± 0.034
Fluoxetine	<LOD - 0.017	0.006 ± 0.01	<LOD - 0.025	0.014 ± 0.012	50	<LOD - 0.003	<LOD
Flupentixol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flurazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fluvoxamine	0.02 - 0.081	0.055 ± 0.031	0.02 - 0.102	0.067 ± 0.041	0	<LOD	<LOD
Gabapentin	1.033 - 4.981	2.491 ± 2.167	1.033 - 5.332	3.163 ± 1.88	100	0.249 - 0.563	0.406 ± 0.222
Haloperidol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Imipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Lamotrigine	0.145 - 0.188	0.171 ± 0.023	0.145 - 0.362	0.276 ± 0.08	100	0.355 - 0.44	0.397 ± 0.06
Lorazepam	0.054 - 0.12	0.086 ± 0.033	0.054 - 0.112	0.096 ± 0.014	100	0.089 - 0.091	0.09 ± 0.001
Maprotiline	0.034 - 0.082	0.051 ± 0.027	0.034 - 0.062	0.037 ± 0.023	100	0.011 - 0.013	0.012 ± 0.002
Medazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Memantine	0.01 - 0.018	0.012 ± 0.004	0.01 - 0.043	0.024 ± 0.017	100	0.024 - 0.052	0.038 ± 0.02
Methadone	<LOD - 0.085	0.03 ± 0.048	<LOD - 0.056	0.02 ± 0.032	0	<LOD	<LOD

Table S15. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 3)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Methylphenidate	0.016 - 0.018	0.017 ± 0.001	0.016 - 0.023	0.013 ± 0.011	50	<LOD - 0.015	0.009 ± 0.009
Mianserin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mirtazapine	0.011 - 0.018	0.014 ± 0.004	0.011 - 0.019	0.014 ± 0.004	100	0.008 - 0.013	0.011 ± 0.003
Naltrexone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>N-Desmethylozapine</i>	<LOD - 0.013	0.008 ± 0.006	<LOD - 0.01	0.004 ± 0.005	0	<LOD	<LOD
Nitrazepam	<LOD - 0.048	0.031 ± 0.025	<LOD - 0.06	0.035 ± 0.03	50	<LOD - 0.026	0.014 ± 0.018
<i>Norbuprenorphine</i>	<LOD - 0.063	0.032 ± 0.031	<LOD - 0.059	0.044 ± 0.013	0	<LOD	<LOD
Nordiazepam	<LOD	<LOD	<LOD - 0.004	0.002 ± 0.002	0	<LOD	<LOD
Nortriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Olanzapine	<LOD - 0.072	0.037 ± 0.035	<LOD - 0.054	0.029 ± 0.026	0	<LOD	<LOD
Opipramol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxcarbazepine	<LOD - 0.019	0.01 ± 0.009	<LOD - 0.028	0.019 ± 0.015	100	0.04 - 0.085	0.063 ± 0.032
Paliperidone	<LOD - 0.158	0.053 ± 0.091	<LOD - 0.114	0.039 ± 0.066	50	<LOD - 0.005	0.003 ± 0.003
Paroxetine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Phenazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Phenytoin	0.034 - 0.062	0.045 ± 0.015	0.034 - 0.107	0.081 ± 0.041	100	0.062 - 0.105	0.083 ± 0.03
Pipamperone	<LOD - 0.009	0.004 ± 0.004	<LOD - 0.009	0.004 ± 0.005	0	<LOD	<LOD
Prazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Promazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Protriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Quetiapine	0.02 - 0.048	0.029 ± 0.016	0.02 - 0.04	0.022 ± 0.016	0	<LOD	<LOD
Risperidone	<LOD - 0.098	0.035 ± 0.055	<LOD - 0.127	0.043 ± 0.073	0	<LOD	<LOD
<i>Ritalinic acid</i>	0.016 - 0.228	0.139 ± 0.11	0.016 - 0.102	0.051 ± 0.044	100	0.194 - 0.312	0.253 ± 0.084
Secobarbital	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sertraline	<LOD - 0.006	0.003 ± 0.003	<LOD	<LOD	0	<LOD	<LOD
Temazepam	<LOD - 0.032	0.011 ± 0.018	<LOD - 0.048	0.022 ± 0.024	100	0.012 - 0.017	0.014 ± 0.004
Topiramate	<LOD - 0.054	0.019 ± 0.03	<LOD - 0.032	0.011 ± 0.018	0	<LOD	<LOD
Trazodone	0.022 - 0.041	0.033 ± 0.01	0.022 - 0.039	0.03 ± 0.008	0	<LOD	<LOD
Triazolam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Trimipramine	<LOD - 0.249	0.084 ± 0.143	<LOD - 0.058	0.02 ± 0.033	50	<LOD - 0.035	0.018 ± 0.024
Venlafaxine	0.018 - 0.08	0.042 ± 0.033	0.018 - 0.119	0.069 ± 0.046	100	0.041 - 0.099	0.07 ± 0.041
Zolpidem	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Zopiclone	<LOD - 0.032	0.012 ± 0.017	<LOD	<LOD	0	<LOD	<LOD
<i>α-Hydroxyalprazolam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>α-Hydroxymidazolam</i>	0.012 - 0.013	0.013 ± 0.001	0.012 - 0.017	0.017 ± 0	100	0.009 - 0.01	0.01 ± 0.001
<i>α-Hydroxytriazolam</i>	<LOD - 0.109	0.048 ± 0.056	<LOD - 0.042	0.015 ± 0.024	50	<LOD - 0.073	0.037 ± 0.051
Receptor antagonists							
Atropine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flumazenil	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Stimulants							
Caffeine	2.037 - 2.619	2.291 ± 0.298	2.037 - 3.125	2.641 ± 0.428	100	0.793 - 1.133	0.963 ± 0.24
<i>Cotinine</i>	0.445 - 0.631	0.538 ± 0.093	0.445 - 0.838	0.684 ± 0.138	100	0.013 - 0.015	0.014 ± 0.002
Phentermine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
UV filter							
Octinoxate	0.058 - 0.109	0.079 ± 0.027	0.058 - 0.22	0.154 ± 0.059	50	<LOD - 0.009	0.005 ± 0.006

Table S15. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n= 3)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Veterinary drugs							
Carprofen	<LOD - 0.135	0.046 ± 0.078	<LOD	<LOD	0	<LOD	<LOD
Diaveridine	0.357 - 0.526	0.415 ± 0.096	0.357 - 0.582	0.449 ± 0.14	100	0.036 - 0.04	0.038 ± 0.003
Difloxacin	<LOD - 0.006	<LOD	<LOD - 0.014	0.008 ± 0.006	0	<LOD	<LOD
Dimetridazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Enrofloxacin	<LOD - 0.01	0.006 ± 0.005	<LOD - 0.003	<LOD	0	<LOD	<LOD
Flunixin	<LOD - 0.017	0.01 ± 0.008	<LOD - 0.022	0.013 ± 0.011	50	<LOD - 0.029	0.015 ± 0.02
Furaltadone	0.038 - 0.105	0.075 ± 0.034	0.038 - 0.111	0.085 ± 0.04	0	<LOD	<LOD
Iprnidazole	<LOD - 0.006	0.002 ± 0.003	<LOD - 0.002	<LOD	0	<LOD	<LOD
Marbofloxacin	0.39 - 0.861	0.549 ± 0.27	0.39 - 0.531	0.442 ± 0.105	100	0.011 - 0.536	0.273 ± 0.371
Monensin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Orbifloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxibendazole	<LOD - 0.004	0.002 ± 0.002	<LOD - 0.005	0.002 ± 0.002	0	<LOD	<LOD
Ronidazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Salinomycin	<LOD - 0.552	0.187 ± 0.317	<LOD - 0.5	0.169 ± 0.286	0	<LOD	<LOD
Sarafloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfachlorpyridazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaclozine	<LOD	<LOD	<LOD - 0.076	0.026 ± 0.043	0	<LOD	<LOD
Sulfadoxine	<LOD	<LOD	<LOD	<LOD	100	<LOD	<LOD
Sulfamonomethoxine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfanitran	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaquinoxaline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Tilmicosin	<LOD - 0.335	0.113 ± 0.192	<LOD - 0.178	0.061 ± 0.102	0	<LOD	<LOD
X-ray contrast medium							
Iopromide	0.294 - 3.3	1.632 ± 1.53	0.294 - 3.644	2.418 ± 1.907	50	<LOD - 0.079	0.04 ± 0.056

Table S16. Range of variability and average occurrence of the 232 target OMPs analyzed in HWW, INF, MBRperm and EFF during the 0.1PAC experimental campaign (September – November 2021). For MBRperm, the frequency of detection (*Freq*) is displayed and the hydraulic retention time was considered for the sampling. The transformation products are written in italics. SD: standard deviation.

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Analgesics/Anti-inflammatories							
4-Acetylaminoantipyrine	<LOD - 0.143	0.054 ± 0.051	0.014 - 0.176	0.057 ± 0.053	100	0.022 - 0.187	0.061 ± 0.053
4-FormylAminoAntipyrine	<LOD - 0.147	0.052 ± 0.046	0.019 - 0.127	0.058 ± 0.041	100	0.022 - 0.135	0.047 ± 0.038
6-Acetylmorphine	0.007 - 0.019	0.011 ± 0.004	<LOD - 0.015	0.009 ± 0.006	22	<LOD - 0.006	0.002 ± 0.002
Acetaminophen	0.134 - 6.261	5.122 ± 2.031	0.095 - 6.759	5.442 ± 2.035	100	0.021 - 0.06	0.038 ± 0.014
Acetylcodeine	<LOD - 0.017	0.01 ± 0.005	<LOD - 0.019	0.009 ± 0.007	56	<LOD - 0.01	0.005 ± 0.004
Acetylsalicylic acid	0.476 - 1.212	0.703 ± 0.23	0.431 - 0.772	0.662 ± 0.107	100	0.061 - 0.443	0.287 ± 0.128
Alfentanil	<LOD - 0.04	0.009 ± 0.014	<LOD - 0.065	0.01 ± 0.021	22	<LOD - 0.052	0.006 ± 0.017
Aminopyrine	<LOD - 0.65	0.326 ± 0.233	<LOD - 1.139	0.422 ± 0.317	0	<LOD	<LOD
Betamethasone 17,21-dipropionate	0.01 - 0.019	0.014 ± 0.003	<LOD - 0.018	0.011 ± 0.006	0	<LOD	<LOD
Buprenorphine	<LOD - 0.114	0.064 ± 0.044	<LOD - 0.18	0.097 ± 0.066	67	<LOD - 0.019	0.01 ± 0.008
<i>Buprenorphine glucuronide</i>	<LOD - 0.216	0.029 ± 0.076	<LOD - 0.528	0.093 ± 0.19	0	<LOD	<LOD
Carisoprodol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Codeine	0.186 - 0.382	0.285 ± 0.066	0.211 - 0.407	0.304 ± 0.067	44	<LOD - 0.023	0.006 ± 0.007
Dextromethorphan	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Dextropropoxyphene	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Diclofenac	0.054 - 0.207	0.11 ± 0.054	0.05 - 15.491	1.89 ± 5.101	100	0.058 - 0.258	0.17 ± 0.071
Etodolac	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fentanyl	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hydrocodone	0.165 - 0.356	0.261 ± 0.063	0.19 - 0.38	0.278 ± 0.063	67	<LOD - 0.013	0.007 ± 0.005
Hydromorphone	0.088 - 0.35	0.157 ± 0.081	0.087 - 0.327	0.163 ± 0.078	0	<LOD	<LOD
Ibuprofen	0.621 - 1.092	0.769 ± 0.163	0.102 - 0.928	0.678 ± 0.331	100	0.052 - 0.081	0.067 ± 0.011
Ketoprofen	1.136 - 2.34	1.74 ± 0.4	1.226 - 2.296	1.781 ± 0.335	89	<LOD - 0.414	0.235 ± 0.129
Lidocaine	0.133 - 0.403	0.24 ± 0.094	0.144 - 0.384	0.253 ± 0.087	100	0.029 - 0.273	0.159 ± 0.085
Meloxicam	<LOD - 0.002	<LOD	<LOD	<LOD	0	<LOD	<LOD
Morphine	0.088 - 0.35	0.157 ± 0.081	0.087 - 0.327	0.163 ± 0.078	0	<LOD	<LOD
<i>Morphine-6-β-D-glucuronide</i>	<LOD - 0.153	0.053 ± 0.066	<LOD - 0.143	0.023 ± 0.049	11	<LOD - 0.073	0.009 ± 0.024
Naproxen	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>Norfentanyl</i>	0.014 - 0.105	0.033 ± 0.03	0.009 - 0.036	0.027 ± 0.01	89	<LOD - 0.049	0.022 ± 0.013
<i>Norpethidine</i>	0.016 - 0.041	0.029 ± 0.01	<LOD - 0.04	0.025 ± 0.012	78	<LOD - 0.014	0.008 ± 0.005
<i>Norpropoxyphene</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>O-Desmethyltramadol</i>	0.075 - 0.355	0.145 ± 0.095	0.108 - 0.414	0.259 ± 0.101	100	0.017 - 0.393	0.094 ± 0.123
Oxycodone	0.01 - 0.05	0.032 ± 0.012	<LOD - 0.044	0.023 ± 0.016	56	<LOD - 0.019	0.007 ± 0.007
Oxymorphone	0.025 - 0.066	0.042 ± 0.012	<LOD - 0.078	0.04 ± 0.024	67	<LOD - 0.028	0.01 ± 0.009
Pentazocine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Pethidine	<LOD - 0.008	0.002 ± 0.003	<LOD - 0.01	0.003 ± 0.004	22	<LOD - 0.009	0.002 ± 0.003
Phenylbutazone	<LOD - 0.019	0.005 ± 0.008	<LOD - 0.015	0.002 ± 0.005	22	<LOD - 0.016	0.003 ± 0.005
Procaine	0.005 - 0.235	0.063 ± 0.079	<LOD - 0.135	0.049 ± 0.053	67	<LOD - 0.009	0.005 ± 0.004
Tolfenamic acid	<LOD - 0.007	0.001 ± 0.002	<LOD - 0.007	0.001 ± 0.002	0	<LOD	<LOD
Tramadol	0.242 - 0.421	0.303 ± 0.061	0.23 - 0.478	0.314 ± 0.075	100	0.043 - 0.353	0.208 ± 0.098

Table S16. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Antiarrhythmic agents							
Amiodarone	<LOD	<LOD	<LOD	<LOD	11	<LOD - 0.005	<LOD
Digitoxin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Propafenone	0.018 - 0.096	0.046 ± 0.03	0.019 - 0.069	0.037 ± 0.016	22	<LOD - 0.009	0.002 ± 0.003
Strophanthidin	<LOD	<LOD	<LOD - 0.069	0.009 ± 0.022	0	<LOD	<LOD
Strophanthin	<LOD	<LOD	<LOD	<LOD	11	<LOD - 0.038	0.006 ± 0.012
Antibiotics							
2-NP-AOZ	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amoxicillin	0.067 - 0.166	0.1 ± 0.032	<LOD - 0.219	0.089 ± 0.056	89	<LOD - 0.057	0.036 ± 0.017
Azithromycin	1.379 - 6.82	4.31 ± 1.653	2.061 - 4.961	3.424 ± 0.971	100	0.026 - 0.235	0.093 ± 0.067
Cinoxacin	<LOD - 0.002	<LOD	<LOD - 0.007	0.001 ± 0.002	22	<LOD - 0.008	0.002 ± 0.003
Ciprofloxacin	1.04 - 2.884	2.237 ± 0.606	1.186 - 2.834	1.79 ± 0.54	100	0.14 - 0.699	0.423 ± 0.202
Clarithromycin	0.013 - 0.562	0.248 ± 0.162	0.026 - 0.498	0.185 ± 0.141	89	<LOD - 0.022	0.012 ± 0.006
Doxycycline	0.353 - 2.533	1.308 ± 0.753	<LOD - 1.947	0.899 ± 0.531	89	<LOD - 0.568	0.316 ± 0.204
Enoxacin	<LOD - 0.179	0.024 ± 0.063	<LOD - 0.224	0.026 ± 0.074	11	<LOD - 0.013	<LOD
Erythromycin	0.106 - 0.849	0.39 ± 0.246	<LOD - 1.441	0.366 ± 0.423	56	<LOD - 0.108	0.035 ± 0.042
Flumequine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Furazolidon	<LOD	<LOD	<LOD - 0.01	0.002 ± 0.003	0	<LOD	<LOD
Lomefloxacin	<LOD - 0.185	0.114 ± 0.06	<LOD - 0.156	0.105 ± 0.061	78	<LOD - 0.103	0.052 ± 0.038
Metronidazole	<LOD - 0.883	0.255 ± 0.304	0.022 - 0.387	0.15 ± 0.111	100	0.041 - 0.098	0.079 ± 0.016
Minocycline	0.174 - 0.473	0.283 ± 0.101	<LOD - 0.458	0.26 ± 0.163	33	<LOD - 0.057	0.018 ± 0.025
Nalidixic Acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Norfloxacin	0.023 - 0.122	0.065 ± 0.034	<LOD - 0.141	0.048 ± 0.044	44	<LOD - 0.021	0.007 ± 0.008
Ofloxacin	0.7 - 2.485	1.527 ± 0.53	0.745 - 1.922	1.479 ± 0.381	100	0.347 - 1.425	0.962 ± 0.406
Oleandomycin	0.031 - 1.057	0.716 ± 0.329	<LOD - 0.962	0.659 ± 0.375	67	<LOD - 0.101	0.039 ± 0.035
Oxolinic Acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxytetracycline	<LOD - 0.6	0.155 ± 0.189	<LOD - 0.315	0.105 ± 0.114	67	<LOD - 0.225	0.068 ± 0.076
Penicillin G	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Pipemidic acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Roxithromycin	0.108 - 0.836	0.527 ± 0.287	0.43 - 0.715	0.576 ± 0.094	78	<LOD - 0.127	0.041 ± 0.041
Silvadene	<LOD - 1.167	0.309 ± 0.496	<LOD - 1.075	0.18 ± 0.368	44	<LOD - 0.243	0.032 ± 0.079
Spiramycin	<LOD - 3.275	1.607 ± 1.456	<LOD - 2.668	0.927 ± 1.161	33	<LOD - 0.249	0.048 ± 0.083
Sulfabenzamide	<LOD - 1.524	0.926 ± 0.461	<LOD - 1.569	0.814 ± 0.662	78	<LOD - 1.338	0.773 ± 0.585
Sulfadimethoxine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfadimidine	<LOD - 0.06	0.013 ± 0.023	<LOD - 0.073	0.015 ± 0.029	33	<LOD - 0.044	0.009 ± 0.015
Sulfafurazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaguanidine	<LOD - 0.116	0.042 ± 0.057	<LOD - 0.132	0.037 ± 0.055	11	<LOD - 0.009	0.002 ± 0.003
Sulfamerazine	<LOD - 1.766	0.228 ± 0.621	<LOD - 1.37	0.156 ± 0.455	11	<LOD - 0.051	0.007 ± 0.017
Sulfamethizole	<LOD - 0.132	0.018 ± 0.046	<LOD - 0.087	0.011 ± 0.028	0	<LOD	<LOD
Sulfamethoxazole	0.151 - 0.92	0.459 ± 0.24	0.108 - 0.725	0.412 ± 0.187	100	0.047 - 0.564	0.25 ± 0.185
Sulfamethoxydiazine	<LOD	<LOD	<LOD	<LOD	22	<LOD - 0.028	0.007 ± 0.011
Sulfamethoxypyridazine	<LOD - 0.055	0.007 ± 0.019	<LOD	<LOD	0	<LOD	<LOD
Sulfanilamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaphenazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfapyridine	0.007 - 0.119	0.057 ± 0.043	0.017 - 0.127	0.057 ± 0.034	44	<LOD - 0.013	0.005 ± 0.006
Sulfathiazole	<LOD - 0.361	0.194 ± 0.169	<LOD - 0.441	0.207 ± 0.202	56	<LOD - 0.571	0.195 ± 0.211

Table S16. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Tinidazole	<LOD - 1.208	0.152 ± 0.427	<LOD - 1.567	0.175 ± 0.522	11	<LOD - 0.081	0.01 ± 0.027
Trimethoprim	0.08 - 0.305	0.188 ± 0.075	0.081 - 0.324	0.19 ± 0.071	100	0.007 - 0.069	0.033 ± 0.023
Antifungals							
Sulfacetamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Terbinafine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Tiabendazole	<LOD	<LOD	<LOD - 0.003	<LOD	100	<LOD	<LOD
Antihistamines							
Diphenhydramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Promethazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antihypertensive							
Clonidine	<LOD - 0.002	0.001 ± 0.001	<LOD - 0.002	0.001 ± 0.001	0	<LOD	<LOD
Antiparasitics							
Albendazole	<LOD - 1.972	0.28 ± 0.687	<LOD - 0.031	0.006 ± 0.01	11	<LOD - 0.005	<LOD
Flubendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Levamisole	<LOD - 0.146	0.037 ± 0.062	<LOD - 0.101	0.022 ± 0.041	11	<LOD - 0.011	<LOD
Mebendazole	<LOD - 1.489	0.192 ± 0.524	<LOD - 0.031	0.004 ± 0.01	11	<LOD - 0.006	0.001 ± 0.002
Praziquantel	<LOD - 0.152	0.034 ± 0.054	<LOD - 0.172	0.06 ± 0.063	22	<LOD - 0.017	0.005 ± 0.006
Triclabendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antiseptic							
Nitrofurazone	<LOD - 1.453	0.183 ± 0.513	<LOD - 1.686	0.188 ± 0.562	11	<LOD - 2.235	0.249 ± 0.745
Beta-blockers							
Atenolol	0.397 - 0.595	0.525 ± 0.07	0.414 - 0.721	0.61 ± 0.102	100	0.01 - 0.023	0.016 ± 0.004
Bisoprolol	0.071 - 0.132	0.107 ± 0.019	0.089 - 0.15	0.119 ± 0.021	56	<LOD - 0.024	0.009 ± 0.008
Metoprolol	0.034 - 0.066	0.045 ± 0.011	<LOD - 0.077	0.036 ± 0.022	100	0.022 - 0.089	0.053 ± 0.02
Calcium channel blocker							
Verapamil	<LOD - 0.107	0.055 ± 0.048	<LOD - 0.112	0.07 ± 0.036	0	<LOD	<LOD
Diuretic							
Torsemide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hormones							
Fludrocortisone-Acetate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flumethasone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hydrocortisone	<LOD - 0.295	0.135 ± 0.11	<LOD - 0.438	0.133 ± 0.165	56	<LOD - 0.104	0.036 ± 0.041
Methylprednisolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mometasone furoate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prednicarbate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prednisolone	<LOD - 0.09	0.014 ± 0.031	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone Acetonide	<LOD - 0.155	0.06 ± 0.07	<LOD - 0.215	0.062 ± 0.08	44	<LOD - 0.331	0.103 ± 0.128
Illicit drugs							
Amphetamine	<LOD - 0.181	0.12 ± 0.054	0.075 - 0.275	0.181 ± 0.054	56	<LOD - 0.037	0.019 ± 0.017
Benzoylcegonine	0.071 - 0.375	0.236 ± 0.12	0.104 - 0.379	0.257 ± 0.095	44	<LOD - 0.01	0.004 ± 0.004
Cannabinol	<LOD - 0.057	0.018 ± 0.018	<LOD - 0.016	<LOD	0	<LOD	<LOD
Cocacethylene	<LOD - 0.083	0.035 ± 0.038	<LOD - 0.111	0.035 ± 0.04	11	<LOD - 0.006	0.001 ± 0.002
Cocaine	<LOD - 0.053	0.021 ± 0.024	<LOD - 0.073	0.027 ± 0.028	11	<LOD - 0.006	<LOD
Ecgonine methyl ester	<LOD - 0.365	0.065 ± 0.122	<LOD - 0.17	0.049 ± 0.063	100	<LOD - 0.025	0.006 ± 0.009
Ketamine	<LOD - 0.021	0.006 ± 0.008	<LOD - 0.018	0.005 ± 0.007	22	<LOD - 0.014	0.003 ± 0.005

Table S16. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
MDA	0.054 - 2.234	1.013 ± 0.872	0.075 - 1.725	1.171 ± 0.581	89	<LOD - 0.557	0.235 ± 0.194
MDEA	<LOD - 0.026	0.016 ± 0.009	<LOD - 0.033	0.012 ± 0.014	56	<LOD - 0.033	0.009 ± 0.011
MDMA	<LOD - 0.031	0.007 ± 0.01	<LOD - 0.134	0.035 ± 0.051	33	<LOD - 0.023	0.005 ± 0.008
Methamphetamine	<LOD - 0.014	0.002 ± 0.005	<LOD - 0.013	0.002 ± 0.004	0	<LOD	<LOD
Phencyclidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
THC	<LOD - 0.047	0.026 ± 0.018	<LOD - 0.109	0.034 ± 0.035	0	<LOD	<LOD
Plastic additives							
Benzotriazole	2.581 - 8.235	4.103 ± 1.839	1.678 - 9.794	3.844 ± 2.479	100	0.543 - 2.797	1.623 ± 0.738
p-Toluenesulfonamide	<LOD - 0.386	0.094 ± 0.126	<LOD - 0.233	0.053 ± 0.075	44	<LOD - 0.295	0.071 ± 0.124
Psychiatric drugs							
<i>10-Hydroxycarbazepine</i>	0.329 - 1.663	1.024 ± 0.482	<LOD - 1.503	0.825 ± 0.504	89	<LOD - 0.345	0.166 ± 0.091
<i>7-Aminoclonazepam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>7-Aminoflunitrazepam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Alprazolam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amisulpride	<LOD - 0.08	0.022 ± 0.028	<LOD - 0.937	0.219 ± 0.407	56	<LOD - 0.106	0.015 ± 0.034
Amitriptyline	<LOD - 0.106	0.018 ± 0.036	<LOD - 0.016	0.004 ± 0.005	11	<LOD - 0.018	0.003 ± 0.006
Amoxapine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Bromazepam	<LOD	<LOD	<LOD - 0.49	0.055 ± 0.163	0	<LOD	<LOD
Carbamazepine	0.12 - 0.264	0.166 ± 0.054	0.116 - 0.273	0.205 ± 0.054	100	0.028 - 0.299	0.185 ± 0.101
Chlordiazepoxide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Chlorprothixene	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Citalopram	0.02 - 0.032	0.026 ± 0.005	0.016 - 0.054	0.028 ± 0.012	56	<LOD - 0.014	0.006 ± 0.005
Clobazam	<LOD - 0.005	0.001 ± 0.001	<LOD	<LOD	11	<LOD - 0.012	0.002 ± 0.004
Clomipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clonazepam	<LOD	<LOD	<LOD - 0.02	0.003 ± 0.006	0	<LOD	<LOD
Clorazepate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clozapine	<LOD - 0.019	0.009 ± 0.008	<LOD - 0.036	0.008 ± 0.012	0	<LOD	<LOD
<i>Desalkylflurazepam</i>	<LOD - 0.006	0.001 ± 0.002	<LOD - 0.006	0.001 ± 0.002	0	<LOD	<LOD
Desipramine	<LOD - 0.17	0.023 ± 0.059	<LOD	<LOD	0	<LOD	<LOD
Desvenlafaxine	0.027 - 0.062	0.04 ± 0.014	0.032 - 0.086	0.06 ± 0.015	100	0.017 - 0.081	0.053 ± 0.02
Dexametasone	<LOD - 0.405	0.11 ± 0.172	<LOD - 0.304	0.035 ± 0.101	0	<LOD	<LOD
Diazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Dothiepin	<LOD - 0.101	0.032 ± 0.044	<LOD - 0.093	0.02 ± 0.038	33	<LOD - 0.025	0.007 ± 0.01
Doxepin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>EDDP</i>	0.013 - 0.047	0.03 ± 0.011	0.013 - 0.037	0.026 ± 0.008	89	<LOD - 0.01	0.007 ± 0.004
Felbamate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fluoxetine	<LOD - 0.038	0.02 ± 0.01	<LOD - 0.029	0.019 ± 0.011	11	<LOD - 0.004	<LOD
Flupentixol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flurazepam	<LOD	<LOD	<LOD - 0.009	0.001 ± 0.003	0	<LOD	<LOD
Fluvoxamine	0.014 - 0.103	0.049 ± 0.032	<LOD - 0.086	0.039 ± 0.031	44	<LOD - 0.009	0.004 ± 0.004
Gabapentin	0.501 - 3.608	2.511 ± 0.969	2.905 - 4.908	3.819 ± 0.658	100	0.175 - 0.67	0.361 ± 0.148
Haloperidol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Imipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Lamotrigine	0.176 - 0.324	0.267 ± 0.058	0.131 - 0.435	0.317 ± 0.092	100	0.06 - 0.513	0.273 ± 0.157
Lorazepam	<LOD - 0.119	0.067 ± 0.044	<LOD - 0.132	0.083 ± 0.05	56	<LOD - 0.087	0.041 ± 0.039
Maprotiline	0.018 - 0.043	0.028 ± 0.009	0.01 - 0.03	0.021 ± 0.007	89	<LOD - 0.009	0.006 ± 0.003
Medazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD

Table S16. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Memantine	0.003 - 0.068	0.02 ± 0.021	0.01 - 0.057	0.028 ± 0.016	100	0.006 - 0.062	0.027 ± 0.02
Methadone	<LOD - 0.041	0.019 ± 0.013	<LOD - 0.035	0.016 ± 0.016	0	<LOD	<LOD
Methylphenidate	<LOD - 0.02	0.011 ± 0.008	<LOD - 0.018	0.011 ± 0.007	0	<LOD	<LOD
Mianserin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mirtazapine	<LOD - 0.014	0.007 ± 0.005	<LOD - 0.019	0.008 ± 0.007	11	<LOD - 0.008	<LOD
Naltrexone	<LOD - 0.024	0.008 ± 0.01	<LOD - 0.026	0.008 ± 0.011	33	<LOD - 0.016	0.005 ± 0.006
<i>N-Desmethylclozapine</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Nitrazepam	<LOD - 0.097	0.049 ± 0.033	<LOD - 0.097	0.042 ± 0.04	67	<LOD - 0.077	0.039 ± 0.03
<i>Norbuprenorphine</i>	<LOD - 0.576	0.102 ± 0.194	<LOD - 1.139	0.162 ± 0.371	0	<LOD	<LOD
Nordiazepam	<LOD - 0.004	<LOD	<LOD - 0.002	<LOD	0	<LOD	<LOD
Nortriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Olanzapine	<LOD - 0.148	0.031 ± 0.052	<LOD - 0.069	0.018 ± 0.026	0	<LOD	<LOD
Opi Pramol	<LOD - 0.022	0.005 ± 0.009	<LOD - 0.017	0.004 ± 0.007	22	<LOD - 0.014	0.003 ± 0.005
Oxazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxcarbazepine	0.007 - 0.055	0.028 ± 0.019	<LOD - 0.055	0.024 ± 0.02	67	<LOD - 0.063	0.017 ± 0.022
Paliperidone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Paroxetine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Phenazepam	<LOD - 0.426	0.102 ± 0.158	<LOD - 0.441	0.061 ± 0.146	33	<LOD - 0.12	0.038 ± 0.056
Phenytoin	0.073 - 0.21	0.11 ± 0.047	<LOD - 0.165	0.113 ± 0.049	89	<LOD - 0.271	0.15 ± 0.079
Pipamperone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Promazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Protriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Quetiapine	0.019 - 0.035	0.026 ± 0.005	0.017 - 0.034	0.026 ± 0.005	0	<LOD	<LOD
Risperidone	<LOD - 0.107	0.027 ± 0.042	<LOD - 0.115	0.035 ± 0.049	0	<LOD	<LOD
<i>Ritalinic acid</i>	<LOD - 0.123	0.018 ± 0.043	<LOD - 0.108	0.021 ± 0.036	56	<LOD - 0.297	0.042 ± 0.096
Secobarbital	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sertraline	<LOD	<LOD	<LOD	<LOD	11	<LOD - 0.014	<LOD
Temazepam	<LOD - 0.014	0.008 ± 0.006	<LOD - 0.026	0.008 ± 0.009	56	<LOD - 0.012	0.006 ± 0.004
Topiramate	<LOD	<LOD	<LOD - 0.009	<LOD	0	<LOD	<LOD
Trazodone	0.02 - 0.076	0.037 ± 0.02	0.018 - 0.084	0.036 ± 0.02	0	<LOD	<LOD
Triazolam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Trimipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Venlafaxine	0.034 - 0.086	0.059 ± 0.02	0.048 - 0.102	0.064 ± 0.019	100	0.01 - 0.089	0.051 ± 0.028
Zolpidem	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Zopiclone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>α-Hydroxyalprazolam</i>	<LOD - 0.018	0.003 ± 0.006	<LOD - 0.024	0.004 ± 0.007	0	<LOD	<LOD
<i>α-Hydroxymidazolam</i>	0.008 - 0.052	0.02 ± 0.016	0.008 - 0.043	0.017 ± 0.011	100	0.003 - 0.018	0.008 ± 0.005
<i>α-Hydroxytriazolam</i>	<LOD	<LOD	<LOD - 0.013	0.002 ± 0.004	11	<LOD - 0.013	0.002 ± 0.004
Receptor antagonists							
Atropine	<LOD - 0.009	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flumazenil	<LOD - 0.016	<LOD	<LOD - 0.014	<LOD	0	<LOD	<LOD
Stimulants							
Caffeine	2.185 - 3.976	2.655 ± 0.661	2.177 - 5.971	3.221 ± 1.468	100	0.077 - 1.709	0.797 ± 0.496
<i>Cotinine</i>	0.538 - 0.701	0.63 ± 0.045	0.576 - 0.75	0.691 ± 0.055	100	0.007 - 0.043	0.018 ± 0.011
Phentermine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
UV filters							

Table S16. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Av. ± SD (µg/L)	Range (µg/L)	Av. ± SD (µg/L)	Freq. (%)	Range (µg/L)	Av. ± SD (µg/L)
Octinoxate	0.051 - 0.11	0.076 ± 0.018	0.079 - 0.141	0.118 ± 0.022	11	<LOD - 0.008	<LOD
Veterinary drugs							
Carprofen	<LOD - 0.042	0.01 ± 0.018	<LOD - 0.132	0.03 ± 0.048	11	<LOD - 0.1	0.012 ± 0.033
Diaveridine	0.344 - 0.557	0.407 ± 0.07	0.342 - 0.621	0.463 ± 0.092	89	<LOD - 0.072	0.031 ± 0.021
Difloxacin	<LOD - 0.022	0.005 ± 0.007	<LOD - 0.014	<LOD	0	<LOD	<LOD
Dimetridazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Enrofloxacin	<LOD - 0.013	0.003 ± 0.004	<LOD	<LOD	0	<LOD	<LOD
Flunixin	0.011 - 0.017	0.015 ± 0.002	<LOD - 0.021	0.014 ± 0.008	89	<LOD - 0.028	0.024 ± 0.009
Furaltadone	0.063 - 0.115	0.082 ± 0.017	<LOD - 0.097	0.064 ± 0.026	0	<LOD	<LOD
Iprnidazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Marbofloxacin	<LOD - 1.462	0.424 ± 0.518	<LOD - 0.777	0.234 ± 0.28	56	<LOD - 0.377	0.12 ± 0.147
Monensin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Orbifloxacin	<LOD	<LOD	<LOD - 0.008	<LOD	0	<LOD	<LOD
Oxibendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Ronidazole	<LOD - 0.034	0.005 ± 0.012	<LOD - 0.029	0.004 ± 0.009	11	<LOD - 0.109	0.013 ± 0.036
Salinomycin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sarafloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfachlorpyridazine	<LOD - 0.065	0.02 ± 0.027	<LOD - 0.049	0.016 ± 0.019	22	<LOD - 0.029	0.006 ± 0.011
Sulfaclozine	<LOD - 0.046	0.006 ± 0.016	<LOD - 0.045	0.006 ± 0.015	11	<LOD - 0.023	0.003 ± 0.008
Sulfadoxine	<LOD	<LOD	<LOD	<LOD	100	<LOD	<LOD
Sulfamonomethoxine	<LOD	<LOD	<LOD	<LOD	11	<LOD - 0.006	<LOD
Sulfanitran	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaquinoxaline	<LOD - 0.06	0.008 ± 0.021	<LOD - 0.152	0.018 ± 0.05	0	<LOD	<LOD
Tilmicosin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
X-ray contrast medium							
Iopromide	1.104 - 50.728	15.862 ± 19.349	0.41 - 44.481	8.855 ± 14.184	89	<LOD - 0.778	0.282 ± 0.246

Table S17. Range of variability and average occurrence of the 232 target OMPs analyzed in HWW, INF and MBRperm during the 0.2PAC experimental campaign (April – May 2022). For MBRperm, the frequency of detection (*Freq*) is displayed and the hydraulic retention time was considered for the sampling. The transformation products are written in italics. SD: standard deviation.

Compound	HWW (n = 8)		INF (n = 9)		Freq (%)	MBRperm (n = 9)	
	Range (µg/L)	Average ± SD (µg/L)	Range (µg/L)	Average ± SD (µg/L)		Range (µg/L)	Average ± SD (µg/L)
Analgesics/anti-inflammatories							
<i>4-Acetylaminoantipyrine</i>	<LOD - 0.193	0.052 ± 0.072	<LOD - 0.133	0.048 ± 0.049	67	<LOD - 0.086	0.027 ± 0.031
<i>4-Formylaminoantipyrine</i>	<LOD - 0.073	0.027 ± 0.025	<LOD - 0.042	0.021 ± 0.015	83	<LOD - 0.042	0.017 ± 0.015
<i>6-Acetylmorphine</i>	<LOD - 0.686	0.262 ± 0.314	<LOD - 0.665	0.186 ± 0.274	0	<LOD	<LOD
Acetaminophen	4.585 - 6.504	5.696 ± 0.772	3.895 - 5.258	4.704 ± 0.509	67	<LOD - 0.054	0.021 ± 0.019
<i>Acetylcodeine</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Acetylsalicylic acid	0.136 - 0.476	0.252 ± 0.135	0.053 - 0.369	0.21 ± 0.103	100	0.044 - 0.202	0.116 ± 0.058
Alfentanil	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Aminopyrine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Betamethasone 17,21-dipropionate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Buprenorphine	<LOD - 0.141	0.099 ± 0.053	<LOD - 0.112	0.037 ± 0.056	0	<LOD	<LOD
<i>Buprenorphine glucuronide</i>	<LOD - 0.362	0.185 ± 0.152	<LOD - 0.277	0.048 ± 0.112	0	<LOD	<LOD
Carisoprodol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Codeine	0.059 - 0.263	0.195 ± 0.085	0.076 - 0.191	0.141 ± 0.04	50	<LOD - 0.009	0.003 ± 0.004
Dextromethorphan	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Dextropropoxyphene	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Diclofenac	0.026 - 0.082	0.048 ± 0.022	0.104 - 0.22	0.154 ± 0.041	100	0.048 - 0.114	0.07 ± 0.024
Etodolac	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fentanyl	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hydrocodone	<LOD - 0.241	0.111 ± 0.106	<LOD - 0.177	0.107 ± 0.065	0	<LOD	<LOD
Hydromorphone	0.045 - 0.16	0.096 ± 0.045	0.041 - 0.143	0.071 ± 0.037	0	<LOD	<LOD
Ibuprofen	<LOD - 0.83	0.197 ± 0.313	0.067 - 0.518	0.242 ± 0.158	83	<LOD - 0.05	0.034 ± 0.017
Ketoprofen	0.52 - 1.895	1.187 ± 0.554	0.659 - 1.74	1.125 ± 0.387	0	<LOD	<LOD
Lidocaine	0.105 - 0.251	0.177 ± 0.058	0.084 - 0.149	0.121 ± 0.03	83	<LOD - 0.099	0.045 ± 0.036
Meloxicam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Morphine	0.045 - 0.16	0.102 ± 0.043	0.041 - 0.143	0.074 ± 0.035	0	<LOD	<LOD
<i>Morphine-6-β-D-glucuronide</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Naproxen	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>Norfentanyl</i>	<LOD - 0.055	0.018 ± 0.019	<LOD - 0.041	0.013 ± 0.015	50	<LOD - 0.007	0.003 ± 0.003
<i>Norpethidine</i>	<LOD - 0.037	0.017 ± 0.014	<LOD - 0.022	0.007 ± 0.008	0	<LOD	<LOD
<i>Norpropoxyphene</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>O-Desmethyltramadol</i>	0.058 - 0.436	0.22 ± 0.172	0.108 - 0.347	0.199 ± 0.102	100	0.018 - 0.206	0.099 ± 0.082
Oxycodone	<LOD - 0.049	0.016 ± 0.021	<LOD - 0.029	0.017 ± 0.011	33	<LOD - 0.006	0.003 ± 0.003
Oxymorphone	<LOD - 0.041	0.02 ± 0.015	0.014 - 0.044	0.022 ± 0.011	0	<LOD	<LOD
Pentazocine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Pethidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Phenylbutazone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Procaine	0.006 - 0.044	0.024 ± 0.018	0.007 - 0.108	0.038 ± 0.038	83	<LOD - 0.011	0.007 ± 0.004
Tolfenamic acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Tramadol	0.047 - 0.452	0.253 ± 0.161	0.21 - 0.336	0.249 ± 0.048	100	0.09 - 0.194	0.139 ± 0.042
Antiarrhythmic agents							
Amiodarone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD

Table S17. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Average ± SD (µg/L)	Range (µg/L)	Average ± SD (µg/L)	Freq (%)	Range (µg/L)	Average ± SD (µg/L)
Digitoxin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Propafenone	0.019 - 0.108	0.062 ± 0.04	<LOD - 0.062	0.029 ± 0.025	17	<LOD - 0.01	0.002 ± 0.004
Strophanthidin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Strophanthin	<LOD	<LOD	<LOD - 0.203	0.036 ± 0.082	0	<LOD	<LOD
Antibiotics							
2-NP-AOZ	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amoxicillin	<LOD - 0.1	0.04 ± 0.035	<LOD - 0.057	0.039 ± 0.02	0	<LOD	<LOD
Azithromycin	1.526 - 4.235	2.749 ± 1.088	1.064 - 3.172	1.799 ± 0.837	100	0.025 - 0.096	0.056 ± 0.024
Cinoxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Ciprofloxacin	0.345 - 1.394	0.836 ± 0.397	0.236 - 0.775	0.487 ± 0.193	100	0.029 - 0.176	0.079 ± 0.052
Clarithromycin	0.101 - 0.377	0.244 ± 0.108	0.114 - 0.291	0.165 ± 0.064	100	0.01 - 0.03	0.019 ± 0.008
Doxycycline	<LOD	<LOD	<LOD - 0.09	0.016 ± 0.037	0	<LOD	<LOD
Enoxacin	<LOD - 0.653	0.117 ± 0.263	<LOD - 0.529	0.089 ± 0.216	0	<LOD	<LOD
Erythromycin	0.59 - 0.855	0.698 ± 0.103	<LOD - 0.791	0.52 ± 0.31	33	<LOD - 0.152	0.033 ± 0.06
Flumequine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Furazolidon	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Lomefloxacin	<LOD - 0.077	0.031 ± 0.035	<LOD - 0.083	0.032 ± 0.035	17	<LOD - 0.063	0.012 ± 0.025
Metronidazole	0.059 - 0.508	0.239 ± 0.17	0.008 - 0.288	0.075 ± 0.105	100	0.007 - 0.03	0.012 ± 0.009
Minocycline	<LOD - 0.261	0.085 ± 0.13	<LOD	<LOD	0	<LOD	<LOD
Nalidixic Acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Norfloxacin	<LOD - 0.317	0.081 ± 0.124	<LOD - 0.284	0.066 ± 0.115	0	<LOD	<LOD
Ofloxacin	0.494 - 1.39	0.816 ± 0.362	0.504 - 0.849	0.662 ± 0.162	100	0.037 - 0.694	0.374 ± 0.225
Oleandomycin	<LOD - 0.338	0.08 ± 0.138	<LOD - 0.424	0.091 ± 0.167	0	<LOD	<LOD
Oxolinic Acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxytetracycline	<LOD - 0.117	0.021 ± 0.047	<LOD - 0.033	0.007 ± 0.013	0	<LOD	<LOD
Penicillin G	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Pipemidic acid	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Roxithromycin	<LOD - 0.462	0.225 ± 0.155	<LOD - 0.427	0.239 ± 0.194	33	<LOD - 0.145	0.036 ± 0.059
Silvadene	<LOD	<LOD	<LOD - 0.012	0.003 ± 0.005	0	<LOD	<LOD
Spiramycin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfabenzamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfadimethoxine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfadimidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfafurazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaguanidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfamerazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfamethizole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfamethoxazole	0.267 - 0.902	0.469 ± 0.233	0.159 - 0.609	0.326 ± 0.151	100	0.056 - 0.241	0.114 ± 0.068
Sulfamethoxydiazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfamethoxyipyridazine	<LOD	<LOD	<LOD - 0.006	0.002 ± 0.002	0	<LOD	<LOD
Sulfanilamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaphenazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfapyridine	0.035 - 0.32	0.117 ± 0.111	<LOD - 0.211	0.083 ± 0.083	67	<LOD - 0.107	0.03 ± 0.041
Sulfathiazole	<LOD - 0.167	0.078 ± 0.066	<LOD - 0.244	0.068 ± 0.107	50	<LOD - 0.184	0.064 ± 0.076
Tinidazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Trimethoprim	0.07 - 0.388	0.188 ± 0.114	0.065 - 0.192	0.117 ± 0.049	100	0.008 - 0.034	0.016 ± 0.011

Table S17. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Average ± SD (µg/L)	Range (µg/L)	Average ± SD (µg/L)	Freq (%)	Range (µg/L)	Average ± SD (µg/L)
Antifungals							
Sulfacetamide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Terbinafine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Tiabendazole	<LOD	<LOD	<LOD	<LOD	100	<LOD	<LOD
Antihistamines							
Diphenhydramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Promethazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antihypertensive							
Clonidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antiparasitics							
Albendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flubendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Levamisole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mebendazole	<LOD - 0.006	0.001 ± 0.002	<LOD	<LOD	0	<LOD	<LOD
Praziquantel	<LOD - 0.206	0.076 ± 0.078	<LOD - 0.12	0.057 ± 0.061	0	<LOD	<LOD
Triclabendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Antiseptic							
Nitrofurantoin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Beta-blockers							
Atenolol	0.196 - 0.433	0.318 ± 0.098	0.155 - 0.496	0.331 ± 0.126	83	<LOD - 0.012	0.008 ± 0.004
Bisoprolol	0.057 - 0.092	0.071 ± 0.014	0.051 - 0.079	0.064 ± 0.012	17	<LOD - 0.026	0.005 ± 0.01
Metoprolol	0.095 - 0.214	0.164 ± 0.042	0.163 - 0.221	0.179 ± 0.021	100	0.056 - 0.621	0.231 ± 0.197
Calcium channel blocker							
Verapamil	<LOD - 0.03	0.019 ± 0.014	<LOD - 0.033	0.02 ± 0.012	0	<LOD	<LOD
Diuretic							
Torsemide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hormones							
Fludrocortisone-Acetate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flumethasone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Hydrocortisone	<LOD - 0.146	0.025 ± 0.059	<LOD	<LOD	0	<LOD	<LOD
Methylprednisolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mometasone furoate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prednicarbate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prednisolone	<LOD - 0.187	0.034 ± 0.075	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Triamcinolone Acetonide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Illicit drugs							
Amphetamine	0.04 - 0.229	0.118 ± 0.069	0.025 - 0.202	0.093 ± 0.067	17	<LOD - 0.027	0.005 ± 0.01
<i>Benzoyllecgonine</i>	0.12 - 0.421	0.281 ± 0.098	0.137 - 0.403	0.265 ± 0.086	0	<LOD	<LOD
Cannabinol	<LOD - 0.056	0.011 ± 0.022	<LOD	<LOD	0	<LOD	<LOD
<i>Cocaeethylene</i>	<LOD - 0.099	0.038 ± 0.045	<LOD - 0.091	0.028 ± 0.043	0	<LOD	<LOD
Cocaine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>Ecgonine methyl ester</i>	<LOD - 0.485	0.143 ± 0.19	<LOD - 0.253	0.064 ± 0.105	100	<LOD	<LOD
Ketamine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
MDA	0.022 - 0.872	0.173 ± 0.343	<LOD - 0.514	0.091 ± 0.207	33	<LOD - 0.195	0.064 ± 0.097
MDEA	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
MDMA	0.008 - 0.079	0.031 ± 0.029	<LOD	<LOD	0	<LOD	<LOD

Table S17. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Average ± SD (µg/L)	Range (µg/L)	Average ± SD (µg/L)	Freq (%)	Range (µg/L)	Average ± SD (µg/L)
Methamphetamine	<LOD	<LOD	<LOD - 0.011	0.002 ± 0.004	0	<LOD	<LOD
Phencyclidine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
THC	<LOD - 0.041	0.023 ± 0.018	<LOD	<LOD	0	<LOD	<LOD
Plastic additives							
Benzotriazole	1.212 - 6.654	4.594 ± 2.06	0.891 - 7.585	4.346 ± 2.417	100	0.277 - 4.506	2.486 ± 1.435
p-Toluenesulfonamide	<LOD - 0.126	0.022 ± 0.051	<LOD	<LOD	0	<LOD	<LOD
Psychiatric drugs							
<i>10-Hydroxycarbazepine</i>	<LOD - 0.374	0.179 ± 0.196	<LOD - 0.55	0.213 ± 0.244	0	<LOD	<LOD
<i>7-Aminoclonazepam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>7-Aminoflunitrazepam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Alprazolam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amisulpride	<LOD - 0.012	0.005 ± 0.005	<LOD - 0.014	0.009 ± 0.005	33	<LOD - 0.013	0.004 ± 0.005
Amitriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Amoxapine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Bromazepam	<LOD	<LOD	<LOD - 0.006	<LOD	0	<LOD	<LOD
Carbamazepine	0.043 - 0.133	0.083 ± 0.039	0.106 - 0.21	0.139 ± 0.04	100	0.043 - 0.142	0.077 ± 0.048
Chlordiazepoxide	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Chlorprothixene	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Citalopram	0.023 - 0.036	0.027 ± 0.005	<LOD - 0.036	0.016 ± 0.014	0	<LOD	<LOD
Clobazam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clomipramine	<LOD - 0.023	0.007 ± 0.009	<LOD - 0.024	0.005 ± 0.009	0	<LOD	<LOD
Clonazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clorazepate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Clozapine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>Desalkylflurazepam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Desipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Desvenlafaxine	0.014 - 0.043	0.025 ± 0.01	0.029 - 0.057	0.038 ± 0.011	83	<LOD - 0.035	0.019 ± 0.012
Dexametasone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Diazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Dothiepin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Doxepin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>EDDP</i>	<LOD - 0.041	0.018 ± 0.015	<LOD - 0.022	0.009 ± 0.009	0	<LOD	<LOD
Felbamate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fluoxetine	<LOD - 0.026	0.016 ± 0.008	<LOD - 0.018	0.011 ± 0.006	0	<LOD	<LOD
Flupentixol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flurazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Fluvoxamine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Gabapentin	0.69 - 5.065	2.803 ± 1.67	1.259 - 4.793	2.817 ± 1.5	100	0.075 - 0.439	0.181 ± 0.137
Haloperidol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Imipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Lamotrigine	0.051 - 0.147	0.087 ± 0.036	0.136 - 0.217	0.173 ± 0.032	100	0.084 - 0.262	0.149 ± 0.066
Lorazepam	<LOD - 0.166	0.117 ± 0.063	<LOD - 0.108	0.045 ± 0.049	0	<LOD	<LOD
Maprotiline	<LOD - 0.039	0.014 ± 0.015	<LOD - 0.02	0.007 ± 0.007	0	<LOD	<LOD
Medazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Memantine	<LOD - 0.025	0.013 ± 0.01	<LOD - 0.022	0.011 ± 0.007	33	<LOD - 0.014	0.005 ± 0.006
Methadone	<LOD - 0.012	0.003 ± 0.004	<LOD	<LOD	0	<LOD	<LOD
Methylphenidate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD

Table S17. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		
	Range (µg/L)	Average ± SD (µg/L)	Range (µg/L)	Average ± SD (µg/L)	Freq (%)	Range (µg/L)	Average ± SD (µg/L)
Mianserin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Mirtazapine	<LOD - 0.014	0.005 ± 0.006	<LOD - 0.012	0.003 ± 0.004	0	<LOD	<LOD
Naltrexone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>N-Desmethylozapine</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Nitrazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>Norbuprenorphine</i>	<LOD - 0.071	0.014 ± 0.028	<LOD	<LOD	0	<LOD	<LOD
Nordiazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Nortriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Olanzapine	<LOD - 0.089	0.016 ± 0.036	<LOD - 0.064	0.012 ± 0.025	0	<LOD	<LOD
Opipramol	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxcarbazepine	<LOD - 0.141	0.027 ± 0.056	<LOD	<LOD	0	<LOD	<LOD
Paliperidone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Paroxetine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Phenazepam	<LOD - 0.072	0.013 ± 0.029	<LOD	<LOD	0	<LOD	<LOD
Phenytoin	<LOD	<LOD	<LOD - 0.036	0.008 ± 0.014	0	<LOD	<LOD
Pipamperone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Prazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Promazine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Protriptyline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Quetiapine	<LOD - 0.023	0.015 ± 0.008	0.007 - 0.017	0.01 ± 0.004	0	<LOD	<LOD
Risperidone	<LOD - 0.103	0.018 ± 0.042	<LOD	<LOD	0	<LOD	<LOD
<i>Ritalinic acid</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Secobarbital	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sertraline	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Temazepam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Topiramate	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Trazodone	<LOD - 0.064	0.027 ± 0.021	<LOD - 0.053	0.021 ± 0.018	17	<LOD - 0.012	0.003 ± 0.005
Triazolam	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Trimipramine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Venlafaxine	0.015 - 0.07	0.031 ± 0.021	0.026 - 0.07	0.039 ± 0.017	100	0.014 - 0.039	0.022 ± 0.01
Zolpidem	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Zopiclone	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>α-Hydroxyalprazolam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
<i>α-Hydroxymidazolam</i>	0.005 - 0.011	0.007 ± 0.002	0.004 - 0.011	0.007 ± 0.002	50	<LOD - 0.006	0.002 ± 0.002
<i>α-Hydroxytriazolam</i>	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Receptor antagonists							
Atropine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flumazenil	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Stimulants							
Caffeine	1.652 - 1.998	1.835 ± 0.139	1.648 - 1.892	1.759 ± 0.087	100	0.032 - 0.056	0.047 ± 0.009
<i>Cotinine</i>	0.424 - 0.514	0.457 ± 0.041	0.434 - 0.583	0.501 ± 0.057	67	<LOD - 0.011	0.007 ± 0.004
Phentermine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
UV filter							
Octinoxate	<LOD - 0.064	0.031 ± 0.025	<LOD - 0.091	0.039 ± 0.029	33	<LOD - 0.016	0.005 ± 0.006
Veterinary drugs							
Carprofen	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD

Table S17. (continued)

Compound	HWW (n = 8)		INF (n = 9)		Freq (%)	MBRperm (n = 9)	
	Range (µg/L)	Average ± SD (µg/L)	Range (µg/L)	Average ± SD (µg/L)		Range (µg/L)	Average ± SD (µg/L)
Diaveridine	<LOD - 0.773	0.32 ± 0.262	<LOD - 0.657	0.294 ± 0.211	67	<LOD - 0.042	0.025 ± 0.019
Difloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Dimetridazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Enrofloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Flunixin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Furaltadone	<LOD - 0.053	0.01 ± 0.021	<LOD	<LOD	0	<LOD	<LOD
Ipronidazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Marbofloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Monensin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Orbifloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Oxibendazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Ronidazole	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Salinomycin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sarafloxacin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfachlorpyridazine	<LOD - 0.022	0.004 ± 0.009	<LOD	<LOD	0	<LOD	<LOD
Sulfaclozine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfadoxine	<LOD	<LOD	<LOD	<LOD	100	<LOD	<LOD
Sulfamonomethoxine	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfanitran	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
Sulfaquinoxaline	<LOD - 0.051	0.016 ± 0.023	<LOD	<LOD	0	<LOD	<LOD
Tilmicosin	<LOD	<LOD	<LOD	<LOD	0	<LOD	<LOD
X-ray contrast medium							
lopromide	0.937 - 35.468	11.742 ± 12.173	0.556 - 11.893	6.938 ± 3.983	50	<LOD - 0.64	0.17 ± 0.25

Table S18. Range of variability and average load of target OMPs in HWW, INF, MBRperm and EFF during the noPAC experimental campaign (only MBR), classified by OMP class. For MBRperm, the hydraulic retention time was taken into consideration when sampling. The transformation products are written in italics. SD: Standard deviation.

Table S18. Range of variability and average load of target OMPs in HWW, INF, MBRperm and EFF during the noPAC experimental campaign (only MBR), classified by OMP class. For MBRperm, the hydraulic retention time was taken into consideration when sampling. The transformation products are written in italics. SD: Standard deviation.

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 2)		EFF (n = 3)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Analgesics/anti-inflammatory								
<i>4-Acetylaminoantipyrine</i>	0.58 - 57	35 ± 30	15 - 72	47 ± 29	32 - 88	60 ± 40	5.8 - 46	32 ± 23
<i>4-Formylaminoantipyrine</i>	4.3 - 72	44 ± 35	25 - 102	71 ± 41	35 - 80	57 ± 32	8.2 - 51	30 ± 22
<i>6-Acetylmorphine</i>	5.2 - 8.9	6.5 ± 2.1	6.8 - 16	10 ± 2.1	5.9 - 9.7	7.8 ± 2.7	5.4 - 10	8.2 ± 2.4
Acetaminophen	538 - 6,810	3,556 ± 3,143	323 - 6,472	3,945 ± 3,217	38 - 59	48 ± 15	21 - 50	32 ± 16
<i>Acetylcodeine</i>	0.54 - 1.1	0.73 ± 0.3	0.61 - 1.3	0.85 ± 0.38	0.66 - 1.3	0.98 ± 0.45	0.66 - 1.3	0.88 ± 0.35
Acetylsalicylic acid	324 - 483	396 ± 81	347 - 837	560 ± 251	561 - 644	602 ± 59	39 - 923	472 ± 443
Alfentanil	0.23 - 21	11 ± 11	0.26 - 8.7	4.5 ± 10.5	0.55 - 1.1	0.83 ± 0.4	0.29 - 3.4	1.4 ± 1.7
Aminopyrine	225 - 820	425 ± 342	2.6 - 902	408 ± 456	1.3 - 2.6	2 ± 0.89	1.3 - 2.6	1.8 ± 0.71
Betamethasone 17,21-dipropionate	0.76 - 15	8.8 ± 7.2	15 - 23	18 ± 4	0.87 - 1.7	1.3 ± 0.59	0.87 - 1.7	1.2 ± 0.47
Buprenorphine	75 - 111	92 ± 18	72 - 91	83 ± 10	11 - 20	16 ± 6	0.36 - 16	6.9 ± 8.4
<i>Buprenorphine glucuronide</i>	57 - 254	182 ± 108	87 - 319	216 ± 118	1.3 - 2.5	1.9 ± 0.87	1.3 - 110	38 ± 62
Carisoprodol	0.88 - 220	74 ± 127	0.99 - 123	42 ± 70	1.1 - 180	91 ± 127	1.1 - 349	151 ± 179
Codeine	188 - 251	213 ± 33	184 - 273	228 ± 45	17 - 46	31 ± 21	0.59 - 50	23 ± 25
Dextromethorphan	0.45 - 0.9	0.61 ± 0.25	0.51 - 11	4.1 ± 0.3	0.55 - 8.2	4.4 ± 5.4	0.55 - 1.1	0.73 ± 0.29
Dextropropoxyphene	1.5 - 2.9	2 ± 0.82	1.6 - 3.5	2.3 ± 0.8	1.8 - 3.5	2.6 ± 1.2	1.8 - 3.5	2.4 ± 0.96
Diclofenac	33 - 78	56 ± 22	193 - 254	218 ± 32	167 - 213	190 ± 32	36 - 147	84 ± 57
Etodolac	0.48 - 0.96	0.65 ± 0.27	0.54 - 1.2	0.76 ± 0.34	0.59 - 1.2	0.87 ± 0.4	0.59 - 1.2	0.79 ± 0.32
Fentanyl	0.31 - 0.62	0.42 ± 0.17	0.35 - 0.75	0.49 ± 0.22	0.38 - 0.75	0.56 ± 0.26	0.38 - 0.75	0.51 ± 0.2
Hydrocodone	166 - 234	193 ± 36	160 - 253	208 ± 47	1.1 - 8.3	4.7 ± 5.1	0.58 - 22	10 ± 11
Hydromorphone	119 - 209	170 ± 46	91 - 193	147 ± 52	1.2 - 1.3	1.2 ± 0.09	1.2 - 2.8	1.9 ± 0.81
Ibuprofen	449 - 856	624 ± 209	765 - 925	851 ± 80	22 - 70	46 ± 34	28 - 124	71 ± 49
Ketoprofen	1,115 - 1,430	1,259 ± 159	1,573 - 2,659	1,962 ± 605	23 - 37	30 ± 9	1.4 - 14	6.1 ± 7
Lidocaine	162 - 222	185 ± 33	178 - 240	208 ± 31	235 - 245	240 ± 7	52 - 321	190 ± 135
Meloxicam	0.58 - 1.2	0.78 ± 0.32	0.65 - 1.4	0.91 ± 0.41	0.71 - 1.4	1 ± 0.48	0.71 - 1.4	0.95 ± 0.38
Morphine	119 - 209	170 ± 46	91 - 193	147 ± 52	0.6 - 1.2	0.88 ± 0.4	0.6 - 1.2	0.8 ± 0.32
<i>Morphine-6-β-D-glucuronide</i>	0.36 - 79	36 ± 40	0.42 - 212	77 ± 117	129 - 373	251 ± 173	0.44 - 143	68 ± 72
Naproxen	0.34 - 26,311	10,679 ± 13,837	0.38 - 26,625	13,044 ± 13,320	504 - 805	655 ± 213	0.43 - 316	145 ± 159
<i>Norfentanyl</i>	17 - 43	30 ± 13	19 - 59	39 ± 20	47 - 53	50 ± 4	34 - 80	53 ± 24
<i>Norpethidine</i>	34 - 46	41 ± 6	29 - 47	40 ± 10	25 - 28	27 ± 2	11 - 19	16 ± 4
<i>Norpropoxyphene</i>	0.49 - 14	5.3 ± 7.9	0.55 - 1.2	0.77 ± 0.35	0.6 - 1.2	0.89 ± 0.4	0.6 - 1.2	0.8 ± 0.32
<i>O-Desmethyltramadol</i>	94 - 240	187 ± 81	295 - 406	344 ± 56	20 - 303	161 ± 200	27 - 330	129 ± 174
Oxycodone	13 - 33	26 ± 11	15 - 24	21 ± 5	9.7 - 13	12 ± 3	0.55 - 13	5.2 ± 6.9
Oxymorphone	23 - 46	31 ± 13	38 - 56	50 ± 11	7.2 - 14	11 ± 5	0.68 - 1.3	0.91 ± 0.36
Pentazocine	0.36 - 0.71	0.48 ± 0.2	0.4 - 0.86	0.57 ± 0.25	0.44 - 0.86	0.65 ± 0.3	0.44 - 0.86	0.58 ± 0.23
Pethidine	0.35 - 3.3	1.4 ± 1.6	0.41 - 4.9	2 ± 1.6	0.8 - 5.4	3.1 ± 3.3	0.41 - 8.9	3.4 ± 4.8
Phenylbutazone	0.49 - 20	6.8 ± 11	0.55 - 39	13 ± 22	0.6 - 40	20 ± 28	0.6 - 39	20 ± 19
Procaine	0.73 - 3.2	2.3 ± 1.4	0.87 - 5.9	3.5 ± 1.4	0.87 - 9	4.9 ± 5.8	0.87 - 9.7	6.2 ± 4.7
Tolfenamic acid	0.37 - 0.73	0.49 ± 0.2	0.41 - 0.88	0.58 ± 0.26	0.45 - 0.88	0.66 ± 0.3	0.45 - 0.88	0.6 ± 0.24
Tramadol	196 - 351	256 ± 83	190 - 385	303 ± 102	319 - 373	346 ± 38	98 - 489	315 ± 199

Table S18. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 2)		EFF (n = 3)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Antiarrhythmic agents								
Amiodarone	0.77 - 1.5	1 ± 0.43	0.87 - 1.8	1.2 ± 0.54	0.94 - 1.8	1.4 ± 0.64	0.94 - 1.8	1.3 ± 0.51
Digitoxin	1.7 - 3.5	2.4 ± 0.98	2 - 4.2	2.8 ± 1	2.1 - 4.2	3.2 ± 1.4	2.1 - 4.2	2.9 ± 1.1
Propafenone	33 - 63	50 ± 16	24 - 128	61 ± 58	7.9 - 11	9.2 ± 1.9	0.65 - 19	11 ± 9
Strophanthidin	1.1 - 2.2	1.5 ± 0.63	1.3 - 2.7	1.8 ± 0.79	1.4 - 2.7	2 ± 0.93	1.4 - 2.7	1.8 ± 0.74
Strophanthin	1.3 - 2.5	1.7 ± 0.7	1.4 - 3	2 ± 0.89	1.5 - 3	2.3 ± 1	1.5 - 3	2.1 ± 0.83
Antibiotics								
2-NP-AOZ	0.56 - 1.1	0.76 ± 0.32	0.64 - 1.4	0.89 ± 0.4	0.69 - 1.4	1 ± 0.47	0.69 - 1.4	0.92 ± 0.37
Amoxicillin	79 - 253	150 ± 91	99 - 141	117 ± 22	0.71 - 1.4	1 ± 0.48	0.71 - 1.4	0.94 ± 0.38
Azithromycin	2,182 - 5,923	3,832 ± 1,909	1,744 - 6,303	3,354 ± 2,558	52 - 149	100 ± 68	8.9 - 47	33 ± 21
Cinoxacin	0.34 - 5.8	3.2 ± 2.7	0.39 - 11	5.3 ± 2.7	0.39 - 13	6.7 ± 9	0.39 - 12	7.1 ± 6.1
Ciprofloxacin	837 - 1,659	1,235 ± 412	839 - 1,191	1,006 ± 177	339 - 391	365 ± 36	64 - 787	388 ± 367
Clarithromycin	39 - 285	163 ± 123	98 - 210	139 ± 62	0.79 - 5.5	3.1 ± 3.3	5.9 - 49	24 ± 22
Doxycycline	0.41 - 205	87 ± 106	0.47 - 289	144 ± 144	77 - 193	135 ± 82	15 - 312	121 ± 166
Enoxacin	0.76 - 115	39 ± 66	0.86 - 269	91 ± 155	1.8 - 11	6.6 ± 6.8	1.8 - 51	31 ± 26
Erythromycin	39 - 1,141	520 ± 564	73 - 334	219 ± 134	0.95 - 165	83 ± 116	1.9 - 121	51 ± 63
Flumequine	0.52 - 1	0.7 ± 0.29	0.58 - 1.2	0.82 ± 0.37	0.63 - 1.2	0.94 ± 0.43	0.63 - 1.2	0.85 ± 0.34
Furazolidon	0.47 - 0.95	0.64 ± 0.27	0.54 - 1.1	0.75 ± 0.34	0.58 - 1.1	0.86 ± 0.39	0.58 - 1.1	0.78 ± 0.31
Lomefloxacin	70 - 98	88 ± 16	86 - 130	108 ± 22	135 - 186	160 ± 36	34 - 243	142 ± 104
Metronidazole	266 - 507	399 ± 122	109 - 386	258 ± 140	57 - 100	78 ± 30	11 - 69	39 ± 29
Minocycline	85 - 214	163 ± 69	178 - 502	307 ± 172	1.2 - 2.4	1.8 ± 0.81	1.2 - 2.4	1.6 ± 0.65
Nalidixic acid	1 - 16	6.2 ± 8.2	1.1 - 25	9.4 ± 13	2.4 - 37	20 ± 24	1.3 - 30	11 ± 16
Norfloxacin	0.69 - 135	73 ± 68	0.78 - 204	96 ± 102	0.84 - 1.6	1.2 ± 0.57	0.84 - 1.6	1.1 ± 0.45
Ofloxacin	780 - 2,020	1,313 ± 638	849 - 2,148	1,378 ± 682	1,173 - 2,420	1,797 ± 882	363 - 3,528	1,692 ± 1,642
Oleandomycin	488 - 890	687 ± 201	373 - 750	510 ± 209	48 - 71	59 ± 16	0.77 - 233	90 ± 126
Oxolinic acid	0.42 - 0.85	0.57 ± 0.24	0.48 - 1	0.67 ± 0.3	0.52 - 1	0.77 ± 0.35	0.52 - 1	0.7 ± 0.28
Oxytetracycline	83 - 207	137 ± 63	90 - 288	185 ± 100	52 - 84	68 ± 22	1.5 - 62	22 ± 34
Penicillin G	2.7 - 58	22 ± 31	3.1 - 104	38 ± 58	3.1 - 6.1	4.6 ± 2.1	3.1 - 6.1	4.2 ± 1.7
Pipemidic acid	0.91 - 1.8	1.2 ± 0.51	1 - 2.2	1.4 ± 0.64	1.1 - 2.2	1.7 ± 0.75	1.1 - 2.2	1.5 ± 0.6
Roxithromycin	523 - 781	621 ± 139	166 - 789	425 ± 325	59 - 67	63 ± 6	1.5 - 172	60 ± 97
Silvadene	0.65 - 59	20 ± 34	0.8 - 62	31 ± 31	0.8 - 13	6.9 ± 8.7	0.8 - 1.6	1.1 ± 0.43
Spiramycin	934 - 2,670	1,998 ± 932	818 - 2,003	1,475 ± 603	5.3 - 182	94 ± 125	2.9 - 69	26 ± 38
Sulfabenzamide	0.97 - 264	89 ± 152	1.1 - 1,070	358 ± 617	1.1 - 2.2	1.7 ± 0.75	1.1 - 713	239 ± 411
Sulfadimethoxine	0.59 - 1.2	0.81 ± 0.33	0.67 - 1.4	0.94 ± 0.42	0.73 - 1.4	1.1 ± 0.49	0.73 - 1.4	0.98 ± 0.39
Sulfadimidine	0.59 - 30	11 ± 17	0.68 - 62	21 ± 35	0.68 - 1.3	1 ± 0.46	0.68 - 1.3	0.91 ± 0.37
Sulfafurazole	1.1 - 2.2	1.5 ± 0.6	1.2 - 2.6	1.7 ± 0.76	1.3 - 2.6	2 ± 0.89	1.3 - 2.6	1.8 ± 0.71
Sulfaguandine	0.4 - 256	86 ± 148	0.45 - 193	65 ± 111	0.49 - 0.97	0.73 ± 0.33	0.49 - 0.97	0.66 ± 0.26
Sulfamerazine	0.62 - 939	314 ± 542	0.71 - 647	217 ± 373	0.71 - 1.4	1 ± 0.48	0.71 - 1.4	0.95 ± 0.38
Sulfamethizole	1.1 - 20	7.8 ± 11	1.3 - 38	25 ± 20	1.3 - 57	29 ± 39	1.3 - 2.5	1.7 ± 0.7
Sulfamethoxazole	119 - 1,488	646 ± 736	163 - 1,669	691 ± 848	72 - 1,860	966 ± 1,264	16 - 1,131	504 ± 571
Sulfamethoxydiazine	1.1 - 2.2	1.5 ± 0.6	1.2 - 2.6	1.7 ± 0.76	1.3 - 2.6	2 ± 0.89	1.3 - 2.6	1.8 ± 0.71
Sulfamethoxypyridazine	0.32 - 0.63	0.43 ± 0.18	0.36 - 0.76	0.5 ± 0.22	0.39 - 0.76	0.57 ± 0.26	0.39 - 0.76	0.52 ± 0.21
Sulfanilamide	0.94 - 1.9	1.3 ± 0.52	1.1 - 2.2	1.5 ± 0.66	1.1 - 2.2	1.7 ± 0.78	1.1 - 2.2	1.5 ± 0.62
Sulfaphenazole	0.75 - 1.5	1 ± 0.42	0.84 - 1.8	1.2 ± 0.53	0.92 - 1.8	1.4 ± 0.62	0.92 - 1.8	1.2 ± 0.49
Sulfapyridine	0.5 - 13	7.8 ± 6.4	0.54 - 12	4.5 ± 6.4	0.58 - 15	7.5 ± 9.8	0.58 - 18	9.3 ± 8.7
Sulfathiazole	0.97 - 118	72 ± 62	1.2 - 258	139 ± 129	1.2 - 342	172 ± 241	0.63 - 150	51 ± 86
Tinidazole	0.6 - 1.2	0.81 ± 0.34	0.68 - 1.4	0.95 ± 0.42	0.74 - 1.4	1.1 ± 0.5	0.74 - 1.4	0.99 ± 0.4

Table S18. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 2)		EFF (n = 3)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Trimethoprim	52 - 612	284 ± 292	65 - 527	242 ± 249	5.8 - 76	41 ± 49	9.6 - 101	43 ± 50
Antifungals								
Sulfacetamide	0.49 - 0.99	0.67 ± 0.28	0.56 - 1.2	0.78 ± 0.35	0.61 - 1.2	0.89 ± 0.41	0.61 - 1.2	0.81 ± 0.32
Terbinafine	0.42 - 0.85	0.58 ± 0.24	0.48 - 1	0.67 ± 0.3	0.52 - 1	0.77 ± 0.35	0.52 - 1	0.7 ± 0.28
Tiabendazole	0.2 - 1.6	0.72 ± 0.74	0.22 - 0.46	0.3 ± 0.14	0.24 - 0.46	0.35 ± 0.16	0.24 - 0.46	0.31 ± 0.13
Antihistamines								
Diphenhydramine	0.5 - 1	0.68 ± 0.28	0.57 - 1.2	0.8 ± 0.36	0.62 - 1.2	0.91 ± 0.42	0.62 - 1.4	5.2 ± 7.4
Promethazine	0.84 - 1.7	1.1 ± 0.47	0.95 - 2	1.3 ± 0.59	1 - 2	1.5 ± 0.7	1 - 2	1.4 ± 0.55
Antihypertensives								
Clonidine	0.08 - 1.1	0.45 ± 0.58	0.09 - 1.3	0.53 ± 0.69	0.09 - 0.18	0.13 ± 0.06	0.09 - 0.18	0.12 ± 0.05
Antiparasitics								
Albendazole	0.4 - 0.8	0.54 ± 0.22	0.45 - 0.96	0.64 ± 0.28	0.49 - 0.96	0.73 ± 0.33	0.49 - 0.96	0.66 ± 0.26
Flubendazole	0.92 - 1.8	1.2 ± 0.52	1 - 2.2	1.5 ± 0.65	1.1 - 2.2	1.7 ± 0.76	1.1 - 2.2	1.5 ± 0.61
Levamisole	0.89 - 22	8.1 ± 12	1 - 107	37 ± 61	1.1 - 2.1	1.6 ± 0.74	1.1 - 7.7	3.6 ± 3.5
Mebendazole	0.38 - 6.8	2.6 ± 3.6	0.44 - 4.1	1.8 ± 3.6	0.44 - 0.85	0.65 ± 0.29	0.44 - 0.85	0.58 ± 0.23
Praziquantel	17 - 81	55 ± 34	47 - 100	81 ± 30	21 - 23	22 ± 1	1.8 - 32	19 ± 16
Triclabendazole	0.28 - 0.56	0.38 ± 0.16	0.32 - 0.68	0.45 ± 0.2	0.35 - 0.68	0.51 ± 0.23	0.35 - 0.68	0.46 ± 0.19
Antiseptic								
Nitrofurantoin	0.65 - 93	32 ± 53	0.75 - 115	39 ± 66	0.75 - 1.5	1.1 ± 0.5	0.75 - 1.5	1 ± 0.4
Beta-blockers								
Atenolol	241 - 373	318 ± 69	457 - 625	540 ± 84	7.9 - 13	10 ± 3.5	3.2 - 29	17 ± 13
Bisoprolol	71 - 103	87 ± 16	83 - 111	100 ± 15	0.9 - 1.7	1.3 ± 0.6	0.9 - 19	8.6 ± 9.1
Metoprolol	4.5 - 42	29 ± 21	7.4 - 86	40 ± 41	4.4 - 86	45 ± 58	28 - 58	45 ± 15
Calcium channel blocker								
Verapamil	26 - 89	60 ± 32	16 - 53	31 ± 19	0.41 - 0.79	0.6 ± 0.27	0.41 - 0.79	0.54 ± 0.22
Diuretic								
Torsemide	0.68 - 1.4	0.92 ± 0.38	0.77 - 1.6	1.1 ± 0.48	0.84 - 1.6	1.2 ± 0.56	0.84 - 1.6	1.1 ± 0.45
Hormones								
Fludrocortisone acetate	1.1 - 2.2	1.5 ± 0.6	1.2 - 2.6	1.7 ± 0.76	1.3 - 2.6	2 ± 0.89	1.3 - 2.6	1.8 ± 0.71
Flumethasone	0.84 - 1.7	1.1 ± 0.47	0.95 - 2	1.3 ± 0.59	1 - 2	1.5 ± 0.7	1 - 2	1.4 ± 0.55
Hydrocortisone	176 - 297	225 ± 64	131 - 229	176 ± 50	88 - 100	94 ± 9	0.57 - 85	32 ± 46
Methylprednisolone	1.4 - 2.9	1.9 ± 0.8	1.6 - 3.4	2.3 ± 0.8	1.8 - 3.4	2.6 ± 1.2	1.8 - 3.4	2.4 ± 0.94
Mometasone furoate	0.57 - 1.1	0.77 ± 0.32	0.64 - 1.4	0.91 ± 0.4	0.7 - 1.4	1 ± 0.47	0.7 - 1.4	0.94 ± 0.38
Prednicarbate	1.1 - 2.1	1.4 ± 0.6	1.2 - 2.6	1.7 ± 0.76	1.3 - 2.6	1.9 ± 0.89	1.3 - 2.6	1.8 ± 0.7
Prednisolone	1.8 - 3.7	2.5 ± 1	2.1 - 4.4	2.9 ± 1	2.3 - 4.4	3.3 ± 1.5	2.3 - 4.4	3 ± 1.2
Triamcinolone	0.28 - 0.56	0.38 ± 0.16	0.32 - 0.67	0.44 ± 0.2	0.34 - 0.67	0.51 ± 0.23	0.34 - 0.67	0.46 ± 0.18
Triamcinolone acetonide	0.54 - 1.1	0.74 ± 0.31	0.61 - 1.3	0.86 ± 0.38	0.67 - 1.3	0.99 ± 0.45	1.3 - 588	250 ± 304
Illicit drugs								
Amphetamine	139 - 9,524	5,478 ± 4,824	192 - 2,217	1,043 ± 1,050	280 - 380	330 ± 71	33 - 361	216 ± 167
Benzoylcegonine	49 - 383	167 ± 187	171 - 472	282 ± 165	0.67 - 1.3	0.99 ± 0.45	0.67 - 1.3	0.89 ± 0.36
Cannabinol	1.3 - 2.6	1.7 ± 0.72	5.4 - 33	16 ± 15	1.6 - 3.1	2.3 ± 1.1	1.6 - 3.1	2.1 ± 0.85
Cocaethylene	0.16 - 95	32 ± 54	0.17 - 54	18 ± 31	0.18 - 0.36	0.27 ± 0.12	0.18 - 1.6	0.72 ± 0.79
Cocaine	0.91 - 9.7	4.1 ± 4.9	2 - 28	13 ± 13	2 - 6.2	4.1 ± 3	1.1 - 6	3.1 ± 2.6
Ecgonine methyl ester	1.1 - 292	98 ± 168	1.2 - 20	8.1 ± 11	2.6 - 4.3	3.4 ± 1.2	1.3 - 18	7.3 ± 9.3
Ketamine	0.55 - 1.1	0.75 ± 0.31	0.63 - 1.3	0.88 ± 0.39	0.68 - 1.3	1 ± 0.46	0.68 - 1.3	0.91 ± 0.36
MDA	728 - 1,609	1,091 ± 461	1,366 - 1,464	1,421 ± 50	357 - 847	602 ± 347	239 - 614	430 ± 187

Table S18. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 2)		EFF (n = 3)	
	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)
MDEA	8.1 - 66	30 \pm 31	4.6 - 15	8.8 \pm 31.4	1.1 - 23	12 \pm 15	1.1 - 21	9.3 \pm 11
MDMA	5.9 - 112	46 \pm 58	12 - 185	83 \pm 90	1.4 - 13	7.3 \pm 8.3	0.49 - 2.6	1.4 \pm 1.1
Methamphetamine	0.27 - 0.54	0.37 \pm 0.15	0.3 - 0.65	0.43 \pm 0.19	0.33 - 0.65	0.49 \pm 0.22	0.33 - 0.65	0.44 \pm 0.18
Phencyclidine	1.1 - 2.2	1.5 \pm 0.6	1.2 - 2.6	1.7 \pm 0.76	1.3 - 2.6	1.9 \pm 0.89	1.3 - 2.6	1.8 \pm 0.71
THC	9.6 - 66	36 \pm 29	45 - 171	89 \pm 71	1 - 2	1.5 \pm 0.68	1 - 30	17 \pm 14
Plastic additives								
Benzotriazole	2,968 - 8,555	5,684 \pm 2,797	3,272 - 9,867	6,811 \pm 3,323	573 - 2,073	1,323 \pm 1,061	471 - 2,611	1,285 \pm 1,158
p-Toluenesulfonamide	45 - 78	61 \pm 16	0.86 - 85	43 \pm 42	16 - 17	17 \pm 1	0.91 - 58	26 \pm 29
Psychiatric drugs								
10-Hydroxycarbazepine	253 - 373	303 \pm 62	458 - 839	612 \pm 201	52 - 106	79 \pm 38	0.47 - 0.91	0.62 \pm 0.25
7-Aminoclonazepam	0.23 - 0.46	0.31 \pm 0.13	0.26 - 0.55	0.36 \pm 0.16	0.28 - 0.55	0.42 \pm 0.19	0.28 - 0.55	0.38 \pm 0.15
7-Aminoflunitrazepam	0.23 - 0.46	0.31 \pm 0.13	0.26 - 0.55	0.36 \pm 0.16	0.28 - 0.55	0.42 \pm 0.19	0.28 - 0.55	0.38 \pm 0.15
Alprazolam	0.44 - 0.88	0.6 \pm 0.25	0.5 - 1.1	0.7 \pm 0.31	0.54 - 1.1	0.8 \pm 0.37	0.54 - 1.1	0.73 \pm 0.29
Amisulpride	0.42 - 19	6.7 \pm 11	19 - 24	21 \pm 2	25 - 27	26 \pm 2	0.52 - 36	22 \pm 19
Amitriptyline	9.5 - 107	43 \pm 55	5.3 - 95	36 \pm 52	0.46 - 3.2	1.8 \pm 2	0.46 - 24	8.6 \pm 14
Amoxapine	0.52 - 1	0.71 \pm 0.29	0.59 - 1.3	0.83 \pm 0.37	0.64 - 1.3	0.95 \pm 0.43	0.64 - 1.3	0.86 \pm 0.35
Bromazepam	0.53 - 1.1	0.72 \pm 0.3	0.6 - 1.3	0.85 \pm 0.38	0.66 - 1.3	0.97 \pm 0.44	0.66 - 1.3	0.88 \pm 0.35
Carbamazepine	55 - 161	96 \pm 57	150 - 365	233 \pm 115	317 - 452	384 \pm 96	295 - 416	348 \pm 62
Chlordiazepoxide	0.61 - 1.2	0.83 \pm 0.34	0.69 - 1.5	0.97 \pm 0.43	0.75 - 1.5	1.1 \pm 0.51	0.75 - 1.5	1 \pm 0.4
Chlorprothixene	0.94 - 1.9	1.3 \pm 0.53	1.1 - 2.2	1.5 \pm 0.66	1.2 - 2.2	1.7 \pm 0.78	1.2 - 2.2	1.5 \pm 0.62
Citalopram	24 - 59	38 \pm 19	18 - 21	19 \pm 1	11 - 31	21 \pm 14	0.82 - 22	10 \pm 11
Clobazam	0.38 - 0.77	0.52 \pm 0.21	0.43 - 0.92	0.61 \pm 0.27	0.47 - 0.92	0.69 \pm 0.32	0.47 - 0.92	0.63 \pm 0.25
Clomipramine	0.47 - 22	7.6 \pm 12	0.53 - 95	32 \pm 54	0.58 - 1.1	0.86 \pm 0.39	0.58 - 1.1	0.78 \pm 0.31
Clonazepam	0.68 - 1.4	0.92 \pm 0.38	0.77 - 1.6	1.1 \pm 0.48	0.84 - 1.6	1.2 \pm 0.56	0.84 - 1.6	1.1 \pm 0.45
Clorazepate	0.89 - 1.8	1.2 \pm 0.5	1 - 2.1	1.4 \pm 0.63	1.1 - 2.1	1.6 \pm 0.74	1.1 - 2.1	1.5 \pm 0.59
Clozapine	0.66 - 35	21 \pm 18	0.79 - 12	6.6 \pm 18.3	0.79 - 4.8	2.8 \pm 2.8	2.4 - 11	6.5 \pm 4.1
Desalkylflurazepam	0.24 - 0.49	0.33 \pm 0.14	0.27 - 0.58	0.39 \pm 0.17	0.3 - 0.58	0.44 \pm 0.2	0.3 - 0.58	0.4 \pm 0.16
Desipramine	1.1 - 2.3	1.5 \pm 0.64	1.3 - 2.7	1.8 \pm 0.8	1.4 - 2.7	2.1 \pm 0.94	1.4 - 2.7	1.9 \pm 0.75
Desvenlafaxine	15 - 39	25 \pm 13	41 - 66	57 \pm 15	51 - 68	59 \pm 12	7.4 - 82	49 \pm 38
Dexametasone	0.91 - 1.8	1.2 \pm 0.51	1 - 2.2	1.4 \pm 0.64	1.1 - 2.2	1.6 \pm 0.75	1.1 - 244	82 \pm 140
Diazepam	0.45 - 3.4	1.6 \pm 1.6	0.47 - 1	0.66 \pm 0.3	0.51 - 1	0.76 \pm 0.35	0.51 - 1	0.69 \pm 0.28
Dothiepin	0.72 - 73	25 \pm 42	0.84 - 66	23 \pm 38	0.84 - 1.6	1.2 \pm 0.56	0.84 - 1.6	1.1 \pm 0.45
Doxepin	0.47 - 0.94	0.63 \pm 0.26	0.53 - 1.1	0.74 \pm 0.33	0.58 - 1.1	0.85 \pm 0.39	0.58 - 1.1	0.77 \pm 0.31
EDDP	23 - 48	38 \pm 13	19 - 43	32 \pm 12	12 - 13	13 \pm 0	0.28 - 13	8.4 \pm 7.1
Felbamate	0.54 - 98	33 \pm 56	0.62 - 131	44 \pm 75	1.2 - 34	18 \pm 23	13 - 44	26 \pm 16
Fluoxetine	0.5 - 20	6.9 \pm 11	0.57 - 23	14 \pm 11	1.2 - 1.8	1.5 \pm 0.43	0.62 - 9.5	6.4 \pm 5
Flupentixol	0.45 - 0.9	0.61 \pm 0.25	0.51 - 1.1	0.71 \pm 0.32	0.55 - 1.1	0.81 \pm 0.37	0.55 - 1.1	0.74 \pm 0.3
Flurazepam	0.29 - 0.58	0.39 \pm 0.16	0.33 - 0.7	0.46 \pm 0.2	0.36 - 0.7	0.53 \pm 0.24	0.36 - 10	3.7 \pm 5.6
Fluvoxamine	11 - 70	44 \pm 30	14 - 103	63 \pm 45	0.5 - 0.98	0.74 \pm 0.34	0.5 - 0.98	0.67 \pm 0.27
Gabapentin	621 - 2,814	1,696 \pm 1,097	1,383 - 3,404	2,576 \pm 1,059	173 - 763	468 \pm 418	38 - 355	192 \pm 159
Haloperidol	0.35 - 0.69	0.47 \pm 0.19	0.39 - 0.83	0.55 \pm 0.24	0.43 - 0.83	0.63 \pm 0.29	0.43 - 0.83	0.57 \pm 0.23
Imipramine	0.14 - 0.28	0.19 \pm 0.08	0.16 - 0.33	0.22 \pm 0.1	0.17 - 0.33	0.25 \pm 0.12	0.17 - 0.33	0.23 \pm 0.09
Lamotrigine	87 - 204	132 \pm 63	142 - 356	243 \pm 108	305 - 482	394 \pm 125	135 - 489	316 \pm 177
Lorazepam	33 - 95	65 \pm 31	63 - 116	83 \pm 28	62 - 123	93 \pm 44	44 - 218	119 \pm 90
Maprotiline	21 - 46	36 \pm 14	19 - 40	29 \pm 10	9.3 - 15	12 \pm 4	0.34 - 0.67	0.46 \pm 0.18
Medazepam	0.83 - 1.7	1.1 \pm 0.47	0.94 - 2	1.3 \pm 0.59	1 - 2	1.5 \pm 0.69	1 - 2	1.4 \pm 0.55
Memantine	5.8 - 11	9.1 \pm 2.9	6.5 - 30	20 \pm 12	32 - 36	34 \pm 3	28 - 125	65 \pm 53

Table S18. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 2)		EFF (n = 3)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Methadone	0.96 - 48	17 ± 27	1.1 - 36	13 ± 20	1.1 - 2.2	1.6 ± 0.75	1.1 - 2.2	1.5 ± 0.59
Methylphenidate	10 - 18	13 ± 4	2.8 - 16	9.5 ± 4.4	2.8 - 10	6.7 ± 5.4	2.8 - 37	19 ± 17
Mianserin	0.42 - 0.85	0.58 ± 0.24	0.48 - 1	0.67 ± 0.3	0.52 - 1	0.77 ± 0.35	0.52 - 1	0.7 ± 0.28
Mirtazapine	7.9 - 12	10 ± 2.1	6.8 - 18	12 ± 6	9.1 - 11	10 ± 1.5	0.71 - 1.4	0.95 ± 0.38
Naltrexone	0.68 - 1.4	0.92 ± 0.38	0.76 - 1.6	1.1 ± 0.48	0.83 - 1.6	1.2 ± 0.56	0.83 - 1.6	1.1 ± 0.45
<i>N-Desmethylozapine</i>	1.4 - 7.5	4.7 ± 3.1	0.86 - 6.5	3 ± 3.1	0.86 - 1.7	1.3 ± 0.58	0.86 - 1.7	1.1 ± 0.46
Nitrazepam	1.7 - 27	18 ± 14	2 - 42	24 ± 20	2 - 18	10 ± 12	1.1 - 9.5	4.2 ± 4.6
<i>Norbuprenorphine</i>	1.5 - 36	24 ± 19	23 - 50	38 ± 14	1.7 - 3.3	2.5 ± 1.1	1.7 - 3.3	2.3 ± 0.91
Nordiazepam	0.31 - 0.62	0.42 ± 0.17	0.38 - 2.6	1.2 ± 0.2	0.38 - 0.75	0.56 ± 0.26	0.38 - 0.75	0.51 ± 0.2
Nortriptyline	0.41 - 0.83	0.56 ± 0.23	0.47 - 1	0.66 ± 0.29	0.51 - 1	0.75 ± 0.34	0.51 - 1	0.68 ± 0.27
Olanzapine	0.96 - 81	35 ± 42	1.1 - 73	32 ± 37	1.2 - 2.3	1.7 ± 0.79	1.2 - 2.3	1.6 ± 0.63
Opipramol	0.36 - 0.73	0.49 ± 0.2	0.41 - 0.87	0.58 ± 0.26	0.45 - 0.87	0.66 ± 0.3	0.45 - 0.87	0.6 ± 0.24
Oxazepam	0.3 - 0.6	0.41 ± 0.17	0.34 - 0.72	0.48 ± 0.21	0.37 - 0.72	0.55 ± 0.25	0.37 - 0.72	0.49 ± 0.2
Oxcarbazepine	0.52 - 12	7.7 ± 6.2	0.58 - 37	19 ± 18	55 - 59	57 ± 3	44 - 70	59 ± 14
Paliperidone	0.4 - 95	32 ± 55	0.45 - 79	27 ± 45	0.95 - 3.4	2.2 ± 1.7	0.49 - 0.95	0.65 ± 0.26
Paroxetine	0.85 - 1.7	1.2 ± 0.48	0.96 - 2.1	1.4 ± 0.6	1 - 2.1	1.5 ± 0.71	1 - 2.1	1.4 ± 0.56
Phenazepam	0.71 - 1.4	0.96 ± 0.4	0.8 - 1.7	1.1 ± 0.5	0.87 - 1.7	1.3 ± 0.59	0.87 - 1.7	1.2 ± 0.47
Phenytoin	22 - 38	32 ± 9	23 - 145	78 ± 62	43 - 142	92 ± 70	13 - 298	149 ± 143
Pipamperone	0.59 - 9.9	3.7 ± 5.4	0.67 - 13	4.7 ± 5.4	0.72 - 1.4	1.1 ± 0.49	0.72 - 1.4	0.97 ± 0.39
Prazepam	0.34 - 0.67	0.46 ± 0.19	0.38 - 0.81	0.53 ± 0.24	0.41 - 0.81	0.61 ± 0.28	0.41 - 0.81	0.55 ± 0.22
Promazine	1.1 - 2.2	1.5 ± 0.62	1.3 - 2.7	1.8 ± 0.78	1.4 - 2.7	2 ± 0.92	1.4 - 2.7	1.8 ± 0.73
Protriptyline	0.35 - 0.7	0.47 ± 0.2	0.39 - 0.84	0.55 ± 0.25	0.43 - 0.84	0.63 ± 0.29	0.43 - 0.84	0.57 ± 0.23
Quetiapine	11 - 29	21 ± 9	10 - 28	17 ± 9	0.5 - 0.99	0.75 ± 0.34	0.5 - 0.99	0.67 ± 0.27
Risperidone	0.44 - 55	21 ± 30	0.51 - 81	28 ± 46	0.51 - 1	0.76 ± 0.35	0.51 - 1	0.69 ± 0.27
<i>Ritalinic acid</i>	18 - 129	84 ± 58	21 - 71	39 ± 27	217 - 263	240 ± 33	0.79 - 84	29 ± 48
Secobarbital	0.49 - 0.98	0.66 ± 0.27	0.55 - 1.2	0.77 ± 0.34	0.6 - 1.2	0.89 ± 0.4	0.6 - 1.2	0.8 ± 0.32
Sertraline	0.79 - 7	2.9 ± 3.5	0.89 - 1.9	1.3 ± 0.56	0.97 - 1.9	1.4 ± 0.65	0.97 - 1.9	1.3 ± 0.52
Temazepam	0.57 - 18	6.5 ± 9.9	0.66 - 31	18 ± 15	12 - 16	14 ± 3	14 - 23	17 ± 5
Topiramate	0.69 - 30	11 ± 17	0.8 - 20	7.6 ± 11	0.8 - 1.6	1.2 ± 0.54	0.8 - 1.6	1.1 ± 0.43
Trazodone	13 - 40	26 ± 14	16 - 34	26 ± 9	0.65 - 1.3	0.96 ± 0.44	0.65 - 1.3	0.87 ± 0.35
Triazolam	0.35 - 0.7	0.47 ± 0.2	0.39 - 0.84	0.55 ± 0.25	0.43 - 0.84	0.63 ± 0.29	0.43 - 0.84	0.57 ± 0.23
Trimipramine	0.83 - 150	51 ± 86	0.94 - 40	14 ± 22	2 - 24	13 ± 16	1.1 - 38	14 ± 21
Venlafaxine	17 - 45	28 ± 16	38 - 76	52 ± 21	56 - 69	63 ± 9	22 - 83	61 ± 34
Zolpidem	0.32 - 0.65	0.44 ± 0.18	0.37 - 0.78	0.51 ± 0.23	0.4 - 0.78	0.59 ± 0.27	0.4 - 0.78	0.53 ± 0.21
Zopiclone	1.1 - 19	7.5 ± 10	1.2 - 2.6	1.7 ± 0.75	1.3 - 2.6	1.9 ± 0.88	1.3 - 2.6	1.8 ± 0.7
<i>α-Hydroxyalprazolam</i>	0.74 - 1.5	1 ± 0.41	0.83 - 1.8	1.2 ± 0.52	0.91 - 1.8	1.3 ± 0.61	0.91 - 1.8	1.2 ± 0.49
<i>α-Hydroxyimidazolam</i>	6.7 - 15	9.9 ± 4.6	11 - 22	15 ± 7	7.1 - 12	9.6 ± 3.6	5.1 - 11	7.6 ± 3.2
<i>α-Hydroxytriazolam</i>	1 - 62	28 ± 31	0.57 - 29	10 ± 16	1.2 - 51	26 ± 35	0.66 - 73	25 ± 41
Receptor antagonists								
Atropine	0.58 - 1.2	0.78 ± 0.32	0.65 - 1.4	0.92 ± 0.41	0.71 - 1.4	1 ± 0.48	0.71 - 1.4	0.95 ± 0.38
Flumazenil	1.1 - 2.2	1.5 ± 0.61	1.2 - 2.6	1.7 ± 0.77	1.3 - 2.6	2 ± 0.91	1.3 - 2.6	1.8 ± 0.72
Stimulants								
Caffeine	1,225 - 2,506	1,737 ± 678	1,727 - 3,138	2,287 ± 749	787 - 1,076	931 ± 205	364 - 1,434	777 ± 575
<i>Cotinine</i>	268 - 609	411 ± 177	445 - 778	586 ± 172	11 - 17	14 ± 5	0.76 - 16	11 ± 9
Phentermine	0.72 - 1.4	0.98 ± 0.4	0.81 - 1.7	1.1 ± 0.51	0.89 - 1.7	1.3 ± 0.6	0.89 - 1.7	1.2 ± 0.47
UV filter								
Octinoxate	35 - 79	59 ± 22	94 - 146	127 ± 29	1.2 - 6.3	3.7 ± 3.6	0.61 - 29	10 ± 16

Table S18. (continued)

Compound	HWW (n = 3)		INF (n = 3)		MBRperm (n = 2)		EFF (n = 3)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Veterinary drugs								
Carprofen	0.56 - 76	26 ± 44	0.59 - 1.3	0.83 ± 0.37	0.65 - 1.3	0.95 ± 0.44	0.65 - 1.3	0.86 ± 0.35
Diaveridine	214 - 411	307 ± 99	321 - 411	368 ± 45	28 - 49	39 ± 15	30 - 56	43 ± 13
Difloxacin	1.2 - 3.4	2.3 ± 1.1	1.4 - 19	8.4 ± 1.1	1.4 - 2.7	2.1 ± 0.94	1.4 - 187	64 ± 107
Dimetridazole	0.31 - 0.62	0.42 ± 0.17	0.35 - 0.74	0.49 ± 0.22	0.38 - 0.74	0.56 ± 0.26	0.38 - 0.74	0.51 ± 0.2
Enrofloxacin	0.64 - 11	5.5 ± 5.2	0.68 - 4.6	2 ± 5.2	0.74 - 1.4	1.1 ± 0.5	0.74 - 1.4	0.99 ± 0.4
Flunixin	0.53 - 15	8.4 ± 7.3	0.61 - 30	13 ± 15	0.61 - 40	20 ± 28	0.61 - 89	42 ± 44
Furaltadone	23 - 93	58 ± 35	53 - 73	66 ± 11	0.98 - 1.9	1.4 ± 0.66	0.98 - 1.9	1.3 ± 0.53
Iprnidazole	0.31 - 7.1	2.6 ± 3.9	0.36 - 2.3	1 ± 3.9	0.39 - 0.76	0.57 ± 0.26	0.39 - 0.76	0.52 ± 0.21
Marbofloxacin	223 - 518	394 ± 153	209 - 635	404 ± 215	16 - 372	194 ± 252	2.4 - 306	127 ± 159
Monensin	0.69 - 1.4	0.94 ± 0.39	0.78 - 1.7	1.1 ± 0.49	0.85 - 1.7	1.3 ± 0.57	0.85 - 1.7	1.1 ± 0.45
Orbifloxacin	0.65 - 1.3	0.89 ± 0.37	0.74 - 1.6	1 ± 0.46	0.8 - 1.6	1.2 ± 0.54	0.8 - 1.6	1.1 ± 0.43
Oxibendazole	0.27 - 2.4	1.1 ± 1.1	0.31 - 3.3	1.4 ± 1.1	0.33 - 0.65	0.49 ± 0.23	0.33 - 0.65	0.45 ± 0.18
Ronidazole	0.75 - 1.5	1 ± 0.42	0.85 - 1.8	1.2 ± 0.53	0.92 - 1.8	1.4 ± 0.62	0.92 - 1.8	1.2 ± 0.49
Salinomycin	2.4 - 312	106 ± 178	2.8 - 319	109 ± 182	2.8 - 5.5	4.2 ± 1.9	2.8 - 5.5	3.8 ± 1.5
Sarafloxacin	1.1 - 2.2	1.5 ± 0.61	1.2 - 2.6	1.7 ± 0.77	1.3 - 2.6	2 ± 0.91	1.3 - 2.6	1.8 ± 0.72
Sulfachlorpyridazine	0.31 - 0.62	0.42 ± 0.17	0.35 - 0.74	0.49 ± 0.22	0.38 - 0.74	0.56 ± 0.26	0.38 - 0.74	0.51 ± 0.2
Sulfaclozine	0.36 - 0.71	0.48 ± 0.2	0.4 - 53	18 ± 30	0.44 - 0.85	0.65 ± 0.29	0.44 - 0.85	0.58 ± 0.23
Sulfadoxine	0.77 - 1.5	1 ± 0.43	0.87 - 1.9	1.2 ± 0.55	0.95 - 1.9	1.4 ± 0.64	0.95 - 1.9	1.3 ± 0.51
Sulfamonomethoxine	0.47 - 0.95	0.64 ± 0.26	0.53 - 1.1	0.75 ± 0.33	0.58 - 1.1	0.86 ± 0.39	0.58 - 1.1	0.78 ± 0.31
Sulfanitran	0.62 - 1.2	0.84 ± 0.35	0.7 - 1.5	0.98 ± 0.44	0.76 - 1.5	1.1 ± 0.51	0.76 - 1.5	1 ± 0.41
Sulfaquinoxaline	0.42 - 0.84	0.57 ± 0.24	0.48 - 1	0.67 ± 0.3	0.52 - 1	0.76 ± 0.35	0.52 - 1	0.69 ± 0.28
Tilmicosin	1.1 - 201	68 ± 115	1.2 - 124	42 ± 70	1.3 - 2.6	2 ± 0.9	1.3 - 2.6	1.8 ± 0.71
X-ray contrast medium								
Iopromide	166 - 1,985	1,207 ± 938	141 - 4,598	2,423 ± 2,230	0.35 - 108	54 ± 76	0.35 - 0.68	0.47 ± 0.19

Table S19. Range of variability and average load of target OMPs in HWW, INF, MBRperm and EFF during the 0.1PAC sampling campaign, classified by OMP class. For MBRperm, the hydraulic retention time was taken into consideration in the sampling. The transformation products are written in italics. SD: Standard deviation.

Table S19. Range of variability and average load of target OMPs in HWW, INF, MBRperm and EFF during the 0.1PAC sampling campaign, classified by OMP class. For MBRperm, the hydraulic retention time was taken into consideration in the sampling. The transformation products are written in italics. SD: Standard deviation.

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		EFF (n = 9)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Analgesics/anti-inflammatory								
<i>4-Acetylaminoantipyrine</i>	0.54 - 71	34 ± 28	9.6 - 117	48 ± 39	19 - 124	51 ± 38	12 - 85	38 ± 29
<i>4-Formylaminoantipyrine</i>	0.33 - 73	33 ± 26	14 - 174	56 ± 52	17 - 90	40 ± 31	0.57 - 107	33 ± 33
<i>6-Acetylmorphine</i>	3.6 - 10	6.9 ± 2.5	0.44 - 15	8 ± 5.3	0.44 - 4.4	1.4 ± 1.5	0.44 - 1.3	0.6 ± 0.28
Acetaminophen	67 - 5,753	3,386 ± 1,589	63 - 11,500	5,056 ± 2,974	18 - 58	33 ± 13	2.5 - 94	34 ± 26
<i>Acetylcodeine</i>	0.65 - 10	6.3 ± 3.3	0.62 - 14	7.4 ± 5.8	0.62 - 8	3.7 ± 3	0.62 - 8.4	2.9 ± 3.1
Acetylsalicylic acid	255 - 745	446 ± 158	282 - 1,410	612 ± 326	60 - 699	266 ± 196	89 - 1,074	266 ± 318
Alfentanil	0.2 - 25	6.2 ± 8.9	0.26 - 62	11 ± 21	0.26 - 50	6.1 ± 16	0.26 - 0.79	0.36 ± 0.17
Aminopyrine	1.1 - 366	206 ± 146	1.9 - 745	342 ± 216	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79
Betamethasone 17,21-dipropionate	6.2 - 11	8.5 ± 1.5	0.82 - 21	9.9 ± 6.5	0.82 - 2.5	1.1 ± 0.52	0.82 - 18	3.1 ± 5.8
Buprenorphine	0.24 - 117	45 ± 38	0.32 - 353	101 ± 106	0.32 - 23	9.6 ± 8.4	0.32 - 44	19 ± 17
<i>Buprenorphine glucuronide</i>	0.93 - 147	19 ± 52	1.2 - 415	80 ± 158	1.2 - 3.6	1.7 ± 0.77	1.2 - 3.6	1.7 ± 0.77
Carisoprodol	0.77 - 1.6	1 ± 0.26	1 - 3	1.4 ± 0.64	1 - 3	1.4 ± 0.65	1 - 3	1.4 ± 0.65
Codeine	127 - 309	181 ± 59	159 - 455	264 ± 86	0.59 - 16	5.3 ± 6.4	0.59 - 15	5.1 ± 5.9
Dextromethorphan	0.39 - 0.81	0.51 ± 0.13	0.52 - 1.6	0.72 ± 0.33	0.52 - 1.6	0.71 ± 0.33	0.52 - 1.6	0.71 ± 0.33
Dextropropoxyphene	1.3 - 2.6	1.7 ± 0.42	1.7 - 5.1	2.3 ± 1.1	1.7 - 5.1	2.3 ± 1.1	1.7 - 5.1	2.3 ± 1.1
Diclofenac	29 - 141	73 ± 42	33 - 14,905	1,814 ± 4,911	51 - 248	146 ± 70	35 - 209	96 ± 53
Etodolac	0.42 - 0.87	0.54 ± 0.14	0.55 - 1.7	0.77 ± 0.35	0.55 - 1.7	0.76 ± 0.35	0.55 - 1.7	0.76 ± 0.35
Fentanyl	0.27 - 0.56	0.35 ± 0.09	0.36 - 1.1	0.5 ± 0.23	0.36 - 1.1	0.49 ± 0.23	0.36 - 1.1	0.49 ± 0.23
Hydrocodone	113 - 283	166 ± 54	143 - 416	241 ± 79	0.54 - 16	6.3 ± 5.4	0.54 - 13	3.9 ± 4.2
Hydromorphone	60 - 174	96 ± 39	78 - 252	139 ± 65	0.56 - 1.7	0.77 ± 0.36	0.56 - 1.7	0.77 ± 0.36
Ibuprofen	317 - 635	486 ± 114	68 - 1,616	642 ± 458	38 - 151	61 ± 35	20 - 145	74 ± 33
Ketoprofen	608 - 1,554	1,100 ± 278	925 - 3,228	1,586 ± 675	1.3 - 812	241 ± 235	1.3 - 101	29 ± 31
Lidocaine	73 - 222	151 ± 56	121 - 292	211 ± 56	28 - 315	141 ± 93	0.63 - 182	121 ± 61
Meloxicam	0.55 - 1.1	0.73 ± 0.22	0.67 - 2	0.92 ± 0.42	0.67 - 2	0.92 ± 0.42	0.67 - 2	0.92 ± 0.42
Morphine	60 - 174	96 ± 39	78 - 252	139 ± 65	0.56 - 1.7	0.77 ± 0.36	0.56 - 1.7	0.77 ± 0.36
<i>Morphine-6-β-D-glucuronide</i>	0.3 - 82	33 ± 38	0.39 - 139	20 ± 46	0.39 - 53	6.3 ± 17	0.39 - 144	17 ± 48
Naproxen	0.3 - 0.61	0.38 ± 0.1	0.39 - 1.2	0.54 ± 0.25	0.39 - 1.2	0.53 ± 0.25	0.39 - 1.2	0.53 ± 0.25
<i>Norfentanyl</i>	9.2 - 52	20 ± 14	9 - 60	24 ± 15	0.58 - 39	19 ± 12	0.57 - 50	26 ± 18
<i>Norpethidine</i>	9.2 - 39	19 ± 10	0.57 - 46	23 ± 13	0.57 - 15	7 ± 4.5	0.57 - 46	13 ± 15
<i>Norpropoxyphene</i>	0.43 - 0.88	0.55 ± 0.14	0.57 - 1.7	0.78 ± 0.36	0.57 - 1.7	0.78 ± 0.36	0.57 - 1.7	0.78 ± 0.36
<i>O-Desmethyltramadol</i>	40 - 225	93 ± 62	105 - 495	233 ± 129	12 - 378	91 ± 125	11 - 374	89 ± 125
Oxycodone	7.1 - 28	20 ± 7	0.52 - 31	19 ± 12	0.52 - 18	5.6 ± 5.7	0.57 - 14	6.4 ± 5.5
Oxymorphone	16 - 41	27 ± 9	0.64 - 85	37 ± 25	0.64 - 27	7.9 ± 8.3	0.64 - 10	3.9 ± 3.8
Pentazocine	0.31 - 0.64	0.4 ± 0.1	0.41 - 1.2	0.57 ± 0.26	0.41 - 1.2	0.57 ± 0.26	0.41 - 1.2	0.57 ± 0.26
Pethidine	0.31 - 7.4	1.7 ± 2.6	0.41 - 19	3.4 ± 6.1	0.38 - 14	2.6 ± 4.6	0.38 - 40	5.8 ± 13
Phenylbutazone	0.43 - 18	4 ± 6.8	0.56 - 30	3.9 ± 9.7	0.56 - 31	4.5 ± 10	0.56 - 33	5.6 ± 11
Procaine	3.1 - 117	34 ± 40	0.42 - 90	38 ± 37	0.43 - 8.5	4.1 ± 2.9	0.43 - 20	4.5 ± 6.4
Tolfenamic acid	0.32 - 4	0.87 ± 1.3	0.42 - 5	1.1 ± 1.5	0.42 - 1.3	0.58 ± 0.27	0.42 - 1.3	0.58 ± 0.27
Tramadol	136 - 292	191 ± 47	174 - 502	277 ± 110	42 - 373	183 ± 109	39 - 398	214 ± 101

Table S19. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		EFF (n = 9)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Antiarrhythmic agents								
Amiodarone	0.68 - 1.4	0.87 ± 0.22	0.89 - 2.7	1.2 ± 0.56	0.89 - 3.7	1.5 ± 1	0.89 - 3.4	1.5 ± 0.91
Digitoxin	1.5 - 3.1	2 ± 0.51	2 - 6	2.8 ± 1.3	2 - 6	2.8 ± 1.3	2 - 6	2.8 ± 1.3
Propafenone	12 - 60	29 ± 19	20 - 66	32 ± 16	0.31 - 6.6	1.7 ± 2.6	0.31 - 21	4.6 ± 6.6
Strophanthidin	0.99 - 2	1.3 ± 0.33	1.3 - 67	9.1 ± 22	1.3 - 3.9	1.8 ± 0.82	1.3 - 3.9	1.8 ± 0.82
Strophanthin	1.1 - 2.3	1.4 ± 0.37	1.5 - 4.4	2 ± 0.92	1.5 - 37	5.9 ± 12	1.5 - 4.4	2 ± 0.93
Antibiotics								
2-NP-AOZ	0.5 - 1	0.64 ± 0.16	0.65 - 2	0.9 ± 0.41	0.65 - 2	0.9 ± 0.42	0.65 - 2	0.9 ± 0.42
Amoxicillin	38 - 86	62 ± 17	0.67 - 189	81 ± 56	0.67 - 76	33 ± 22	0.67 - 71	25 ± 23
Azithromycin	939 - 3,401	2,645 ± 831	2,003 - 4,146	2,855 ± 618	17 - 460	103 ± 139	19 - 309	115 ± 99
Cinoxacin	0.28 - 1.1	0.46 ± 0.27	0.36 - 7.2	1.2 ± 2.2	0.36 - 11	2.3 ± 3.9	0.36 - 11	2.7 ± 3.9
Ciprofloxacin	708 - 1,940	1,392 ± 346	895 - 2,656	1,548 ± 555	137 - 605	356 ± 169	142 - 745	353 ± 208
Clarithromycin	7.5 - 356	167 ± 123	18 - 481	173 ± 155	0.8 - 42	12 ± 12	0.8 - 56	21 ± 21
Doxycycline	183 - 1,583	844 ± 506	0.58 - 2,279	842 ± 658	0.48 - 556	279 ± 196	53 - 998	373 ± 292
Enoxacin	0.67 - 183	24 ± 65	0.89 - 440	50 ± 146	0.89 - 26	3.8 ± 8.3	0.89 - 2.7	1.2 ± 0.56
Erythromycin	67 - 588	254 ± 180	1.1 - 943	282 ± 265	0.9 - 107	34 ± 40	0.91 - 208	67 ± 68
Flumequine	0.46 - 0.94	0.59 ± 0.15	0.6 - 1.8	0.83 ± 0.38	0.6 - 1.8	0.82 ± 0.38	0.6 - 1.8	0.82 ± 0.38
Furazolidon	0.42 - 0.86	0.54 ± 0.14	0.56 - 6.3	1.4 ± 1.9	0.55 - 1.6	0.75 ± 0.35	0.55 - 1.6	0.75 ± 0.35
Lomefloxacin	0.76 - 166	76 ± 51	0.94 - 305	100 ± 91	0.78 - 128	47 ± 41	1.1 - 146	54 ± 42
Metronidazole	0.42 - 440	143 ± 150	22 - 273	127 ± 87	27 - 183	73 ± 45	39 - 163	69 ± 41
Minocycline	125 - 236	173 ± 41	1.1 - 444	232 ± 147	1.1 - 43	13 ± 18	1.1 - 30	7.9 ± 13
Nalidixic acid	0.88 - 1.8	1.1 ± 0.29	1.2 - 3.5	1.6 ± 0.73	1.2 - 3.5	1.6 ± 0.74	1.2 - 8.6	2.4 ± 2.4
Norfloxacin	12 - 63	40 ± 18	0.8 - 107	45 ± 41	0.8 - 27	7.9 ± 9.7	0.8 - 13	2.4 ± 3.9
Ofloxacin	477 - 1,245	945 ± 274	724 - 2,107	1,270 ± 423	337 - 1,307	803 ± 333	416 - 1,951	936 ± 477
Oleandomycin	21 - 899	462 ± 261	0.69 - 1,724	615 ± 496	0.69 - 73	34 ± 30	0.69 - 172	60 ± 55
Oxolinic acid	0.37 - 0.77	0.48 ± 0.12	0.49 - 1.5	0.68 ± 0.31	0.49 - 1.5	0.67 ± 0.31	0.49 - 1.5	0.67 ± 0.31
Oxytetracycline	1.1 - 299	88 ± 91	1.4 - 209	82 ± 83	1.4 - 149	53 ± 57	1.4 - 105	42 ± 40
Penicillin G	2.2 - 4.6	2.9 ± 0.74	2.9 - 8.8	4.1 ± 1.9	2.9 - 8.8	4 ± 1.9	2.9 - 8.8	4 ± 1.9
Pipemidic acid	0.8 - 1.6	1 ± 0.27	1.1 - 3.2	1.5 ± 0.67	1.1 - 3.2	1.4 ± 0.67	1.1 - 3.2	1.4 ± 0.67
Roxithromycin	74 - 807	350 ± 243	358 - 844	499 ± 145	1.4 - 88	38 ± 36	1.4 - 223	50 ± 77
Silvadene	0.61 - 669	189 ± 296	0.75 - 1,035	160 ± 343	0.75 - 168	23 ± 55	0.75 - 316	36 ± 105
Spiramycin	2 - 1,877	940 ± 845	2.6 - 2,014	716 ± 891	2.6 - 240	41 ± 78	2.6 - 89	20 ± 32
Sulfabenzamide	1.6 - 816	539 ± 256	1.1 - 1,337	634 ± 521	1.1 - 1,174	607 ± 475	1.1 - 1,223	688 ± 466
Sulfadimethoxine	0.52 - 1.1	0.68 ± 0.17	0.69 - 2.1	0.95 ± 0.44	0.69 - 2.1	0.95 ± 0.44	0.69 - 2.1	0.95 ± 0.44
Sulfadimidine	0.49 - 61	10 ± 21	0.64 - 143	21 ± 48	0.64 - 87	13 ± 28	0.64 - 14	2.3 ± 4.3
Sulfafurazole	0.95 - 1.9	1.2 ± 0.31	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79
Sulfaguanidine	0.36 - 112	31 ± 45	0.47 - 172	41 ± 65	0.47 - 8.9	1.6 ± 2.8	0.47 - 1.4	0.64 ± 0.3
Sulfamerazine	0.58 - 945	122 ± 333	0.67 - 950	108 ± 315	0.67 - 35	4.8 ± 12	0.67 - 2	0.92 ± 0.43
Sulfamethizole	1 - 66	9.3 ± 23	1.2 - 58	8 ± 19	1.2 - 3.7	1.7 ± 0.78	1.2 - 3.7	1.7 ± 0.78
Sulfamethoxazole	85 - 627	294 ± 165	77 - 484	345 ± 131	31 - 424	211 ± 150	30 - 384	112 ± 107
Sulfamethoxydiazine	0.95 - 1.9	1.2 ± 0.31	1.2 - 3.7	1.7 ± 0.79	1.2 - 21	5.7 ± 7.8	1.2 - 3.7	1.7 ± 0.79
Sulfamethoxypridazine	0.28 - 32	4.3 ± 11	0.37 - 1.1	0.51 ± 0.23	0.37 - 1.1	0.5 ± 0.23	0.37 - 1.1	0.5 ± 0.23
Sulfanilamide	0.83 - 1.7	1.1 ± 0.27	1.1 - 3.2	1.5 ± 0.68	1.1 - 3.2	1.5 ± 0.69	1.1 - 3.2	1.5 ± 0.69
Sulfaphenazole	0.66 - 1.4	0.85 ± 0.22	0.87 - 2.6	1.2 ± 0.55	0.87 - 2.6	1.2 ± 0.55	0.87 - 2.6	1.2 ± 0.55
Sulfapyridine	4.7 - 64	35 ± 24	21 - 88	46 ± 22	0.55 - 13	4.4 ± 4.5	0.55 - 9.6	2.6 ± 3.1
Sulfathiazole	0.46 - 301	128 ± 119	0.56 - 577	190 ± 203	0.56 - 461	170 ± 182	0.56 - 421	158 ± 165
Tinidazole	0.53 - 680	86 ± 240	0.69 - 1,106	124 ± 368	0.69 - 57	7.2 ± 19	0.69 - 2.1	0.95 ± 0.44

Table S19. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		EFF (n = 9)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Trimethoprim	45 - 208	121 ± 53	57 - 310	167 ± 75	6.3 - 114	34 ± 36	6 - 278	52 ± 86
Antifungals								
Sulfacetamide	0.43 - 0.89	0.56 ± 0.14	0.57 - 1.7	0.79 ± 0.36	0.57 - 1.7	0.78 ± 0.36	0.57 - 1.7	0.78 ± 0.36
Terbinafine	0.37 - 0.77	0.48 ± 0.12	0.49 - 1.5	0.68 ± 0.31	0.49 - 1.5	0.67 ± 0.31	0.49 - 1.5	0.67 ± 0.31
Tiabendazole	0.17 - 0.35	0.22 ± 0.06	0.22 - 2.1	0.51 ± 0.62	0.22 - 0.66	0.3 ± 0.14	0.22 - 0.66	0.3 ± 0.14
Antihistamines								
Diphenhydramine	0.44 - 0.91	0.57 ± 0.15	0.58 - 1.7	0.81 ± 0.37	0.58 - 1.7	0.8 ± 0.37	0.58 - 1.7	0.8 ± 0.37
Promethazine	0.74 - 1.5	0.95 ± 0.24	0.97 - 2.9	1.3 ± 0.61	0.97 - 2.9	1.3 ± 0.62	0.97 - 2.9	1.3 ± 0.62
Antihypertensives								
Clonidine	0.07 - 1.2	0.54 ± 0.51	0.09 - 1.9	0.5 ± 0.62	0.09 - 0.26	0.12 ± 0.05	0.09 - 0.26	0.12 ± 0.05
Antiparasitics								
Albendazole	0.48 - 1,110	161 ± 385	0.46 - 61	8.8 ± 20	0.46 - 11	1.7 ± 3.4	0.46 - 1.4	0.64 ± 0.3
Flubendazole	0.81 - 1.7	1 ± 0.27	1.1 - 3.2	1.5 ± 0.67	1.1 - 3.2	1.5 ± 0.68	1.1 - 3.2	1.5 ± 0.68
Levamisole	0.79 - 84	22 ± 37	1 - 98	21 ± 40	1 - 11	2.5 ± 3.3	1 - 42	6.6 ± 13
Mebendazole	0.31 - 838	110 ± 294	0.41 - 61	7.3 ± 20	0.41 - 13	1.8 ± 4.1	0.41 - 28	3.5 ± 9.1
Praziquantel	0.66 - 87	20 ± 31	0.93 - 113	43 ± 43	0.87 - 12	3.4 ± 4.3	0.87 - 16	4.5 ± 6.5
Triclabendazole	0.25 - 0.51	0.32 ± 0.08	0.33 - 0.98	0.45 ± 0.21	0.33 - 0.98	0.45 ± 0.21	0.33 - 0.98	0.45 ± 0.21
Antiseptic								
Nitrofurural	0.54 - 919	116 ± 325	0.7 - 1,272	142 ± 424	0.7 - 1,687	188 ± 562	0.7 - 1,823	203 ± 607
Beta-blockers								
Atenolol	198 - 599	342 ± 117	322 - 1,344	558 ± 305	6.9 - 45	16 ± 12	0.43 - 56	19 ± 20
Bisoprolol	48 - 91	67 ± 13	70 - 175	103 ± 30	0.84 - 47	10 ± 15	0.84 - 44	14 ± 17
Metoprolol	18 - 38	29 ± 7	0.64 - 84	35 ± 28	15 - 94	48 ± 24	17 - 98	48 ± 31
Calcium channel blocker								
Verapamil	0.29 - 68	33 ± 28	0.44 - 109	61 ± 34	0.38 - 1.1	0.53 ± 0.24	0.38 - 1.1	0.53 ± 0.24
Diuretic								
Torsemide	0.6 - 1.2	0.77 ± 0.2	0.79 - 2.4	1.1 ± 0.5	0.79 - 2.4	1.1 ± 0.5	0.79 - 2.4	1.1 ± 0.5
Hormones								
Fludrocortisone-acetate	0.95 - 1.9	1.2 ± 0.31	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79
Flumethasone	0.74 - 1.5	0.95 ± 0.24	0.97 - 2.9	1.3 ± 0.61	0.97 - 2.9	1.3 ± 0.62	0.97 - 2.9	1.3 ± 0.62
Hydrocortisone	0.39 - 187	87 ± 68	0.52 - 426	116 ± 147	0.52 - 96	28 ± 35	0.52 - 101	27 ± 39
Methylprednisolone	1.3 - 2.6	1.6 ± 0.42	1.7 - 5	2.3 ± 1	1.7 - 5	2.3 ± 1.1	1.7 - 5	2.3 ± 1.1
Mometasone furoate	0.5 - 1	0.65 ± 0.17	0.66 - 2	0.91 ± 0.42	0.66 - 2	0.91 ± 0.42	0.66 - 2	0.91 ± 0.42
Prednicarbate	0.94 - 1.9	1.2 ± 0.31	1.2 - 3.7	1.7 ± 0.78	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79
Prednisolone	1.6 - 52	8.3 ± 18	2.1 - 6.4	2.9 ± 1.3	2.1 - 6.4	2.9 ± 1.4	2.1 - 6.4	2.9 ± 1.4
Triamcinolone	0.25 - 0.51	0.32 ± 0.08	0.32 - 0.97	0.45 ± 0.21	0.32 - 0.97	0.45 ± 0.21	0.32 - 0.97	0.45 ± 0.21
Triamcinolone acetonide	0.54 - 106	35 ± 41	0.63 - 149	48 ± 61	0.63 - 229	78 ± 95	0.63 - 899	157 ± 299
Illicit drugs								
Amphetamine	0.51 - 148	80 ± 42	57 - 436	169 ± 109	0.66 - 63	18 ± 21	0.7 - 19	5.3 ± 6.9
<i>Benzoyllecgonine</i>	36 - 317	157 ± 97	76 - 543	235 ± 141	0.63 - 17	4.6 ± 5.6	0.63 - 30	6 ± 10
Cannabinol	1.1 - 36	12 ± 13	1.5 - 11	3.5 ± 3.1	1.5 - 4.5	2 ± 0.95	1.5 - 4.5	2 ± 0.95
<i>Cocaethylene</i>	0.13 - 64	25 ± 27	0.18 - 73	30 ± 31	0.17 - 4.4	0.7 ± 1.4	0.17 - 0.52	0.24 ± 0.11
Cocaine	0.75 - 34	13 ± 15	1 - 57	22 ± 22	0.99 - 5.9	1.8 ± 1.6	0.99 - 14	2.8 ± 4.2
<i>Ecgonine methyl ester</i>	1.3 - 373	57 ± 128	1.2 - 333	59 ± 107	1.2 - 24	5.4 ± 7.9	1.2 - 54	7.6 ± 18
Ketamine	0.49 - 12	3.8 ± 4.8	0.64 - 16	4.5 ± 5.9	0.64 - 13	2.9 ± 4.4	0.64 - 10	2.9 ± 3.9
MDA	29 - 1,281	618 ± 511	52 - 1,387	952 ± 405	3.5 - 393	179 ± 143	3.5 - 315	123 ± 134

Table S19. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		EFF (n = 9)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
MDEA	0.58 - 19	10 ± 6.3	0.55 - 64	13 ± 21	0.55 - 23	8.8 ± 10	0.55 - 48	14 ± 16
MDMA	0.38 - 18	3.8 ± 5.9	0.49 - 105	26 ± 37	0.49 - 15	3.2 ± 4.9	0.49 - 11	2.5 ± 3.5
Methamphetamine	0.24 - 8	1.3 ± 2.7	0.31 - 9.3	1.4 ± 3	0.31 - 0.94	0.43 ± 0.2	0.31 - 0.94	0.43 ± 0.2
Phencyclidine	0.95 - 1.9	1.2 ± 0.31	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79
THC	0.73 - 26	17 ± 10	0.95 - 75	25 ± 24	0.95 - 2.9	1.3 ± 0.61	0.95 - 13	2.6 ± 3.8
Plastic additives								
Benzotriazole	1,471 - 5,605	2,705 ± 1,516	1,124 - 9,520	3,768 ± 3,238	355 - 3,904	1,574 ± 1,181	312 - 3,885	1,613 ± 1,116
p-Toluenesulfonamide	0.7 - 207	53 ± 66	0.81 - 173	52 ± 69	0.81 - 579	92 ± 194	0.81 - 418	87 ± 151
Psychiatric drugs								
<i>10-Hydroxycarbazepine</i>	185 - 1,132	660 ± 335	0.53 - 2,040	792 ± 641	0.44 - 678	176 ± 196	0.44 - 515	138 ± 171
<i>7-Aminoclonazepam</i>	0.2 - 0.41	0.26 ± 0.07	0.26 - 0.79	0.37 ± 0.17	0.26 - 0.79	0.36 ± 0.17	0.26 - 0.79	0.36 ± 0.17
<i>7-Aminoflunitrazepam</i>	0.2 - 0.41	0.26 ± 0.07	0.26 - 0.79	0.37 ± 0.17	0.26 - 0.79	0.36 ± 0.17	0.26 - 0.79	0.36 ± 0.17
Alprazolam	0.39 - 0.8	0.5 ± 0.13	0.51 - 1.5	0.71 ± 0.32	0.51 - 1.5	0.7 ± 0.33	0.51 - 1.5	0.7 ± 0.33
Amisulpride	0.4 - 47	15 ± 19	0.53 - 737	164 ± 292	0.5 - 69	11 ± 22	0.5 - 73	11 ± 23
Amitriptyline	0.33 - 61	11 ± 20	0.43 - 12	3.8 ± 4.6	0.43 - 13	2 ± 4.1	0.43 - 58	8.5 ± 19
Amoxapine	0.46 - 0.95	0.6 ± 0.15	0.61 - 1.8	0.84 ± 0.38	0.61 - 1.8	0.83 ± 0.39	0.61 - 1.8	0.83 ± 0.39
Bromazepam	0.47 - 0.97	0.61 ± 0.16	0.62 - 472	53 ± 157	0.62 - 1.9	0.85 ± 0.39	0.62 - 1.9	0.85 ± 0.39
Carbamazepine	69 - 152	105 ± 33	94 - 311	178 ± 67	27 - 297	161 ± 98	18 - 234	155 ± 70
Chlordiazepoxide	0.54 - 1.1	0.69 ± 0.18	0.71 - 2.1	0.98 ± 0.45	0.71 - 2.1	0.97 ± 0.45	0.71 - 2.1	0.97 ± 0.45
Chlorprothixene	0.83 - 1.7	1.1 ± 0.27	1.1 - 3.3	1.5 ± 0.69	1.1 - 3.3	1.5 ± 0.69	1.1 - 3.3	1.5 ± 0.69
Citalopram	11 - 29	17 ± 6	12 - 44	24 ± 12	0.77 - 16	5.7 ± 5.3	0.77 - 19	7.7 ± 7.4
Clobazam	0.34 - 3.3	0.9 ± 1	0.44 - 1.3	0.61 ± 0.28	0.44 - 9	1.6 ± 2.8	0.44 - 8.2	1.5 ± 2.5
Clomipramine	0.42 - 0.86	0.54 ± 0.14	0.55 - 1.6	0.76 ± 0.35	0.55 - 1.6	0.75 ± 0.35	0.55 - 1.6	0.75 ± 0.35
Clonazepam	0.6 - 1.2	0.77 ± 0.2	0.79 - 14	2.6 ± 4.4	0.79 - 2.4	1.1 ± 0.5	0.79 - 2.4	1.1 ± 0.5
Clorazepate	0.79 - 1.6	1 ± 0.26	1 - 3.1	1.4 ± 0.65	1 - 3.1	1.4 ± 0.66	1 - 3.1	1.4 ± 0.66
Clozapine	0.29 - 17	6.7 ± 6.1	0.38 - 35	9.6 ± 15	0.38 - 1.1	0.52 ± 0.24	0.38 - 18	4 ± 5.9
<i>Desalkylflurazepam</i>	0.24 - 3	0.83 ± 1	0.28 - 3.9	0.8 ± 1.2	0.28 - 0.84	0.39 ± 0.18	0.28 - 0.84	0.39 ± 0.18
Desipramine	1 - 96	13 ± 33	1.3 - 3.9	1.8 ± 0.83	1.3 - 3.9	1.8 ± 0.84	1.3 - 3.9	1.8 ± 0.84
Desvenlafaxine	14 - 39	26 ± 10	31 - 106	53 ± 24	16 - 84	46 ± 23	12 - 101	50 ± 26
Dexametasone	0.9 - 364	79 ± 135	1 - 202	24 ± 67	1 - 3.1	1.4 ± 0.67	1 - 3.1	1.4 ± 0.67
Diazepam	0.37 - 0.76	0.48 ± 0.12	0.48 - 1.5	0.67 ± 0.31	0.48 - 1.5	0.67 ± 0.31	0.48 - 1.5	0.67 ± 0.31
Dothiepin	0.6 - 71	22 ± 30	0.79 - 156	25 ± 53	0.79 - 49	8.7 ± 16	0.79 - 7.5	1.8 ± 2.2
Doxepin	0.41 - 0.85	0.53 ± 0.14	0.54 - 1.6	0.75 ± 0.34	0.54 - 1.6	0.74 ± 0.35	0.54 - 1.6	0.74 ± 0.35
<i>EDDP</i>	7.6 - 38	20 ± 9	12 - 65	24 ± 16	0.39 - 17	6.3 ± 4.9	0.26 - 35	9.2 ± 11
Felbamate	0.45 - 0.92	0.58 ± 0.15	0.59 - 1.8	0.81 ± 0.37	0.59 - 1.8	0.81 ± 0.37	0.59 - 1.8	0.81 ± 0.37
Fluoxetine	0.56 - 21	13 ± 6	0.7 - 43	18 ± 13	0.58 - 2.4	1 ± 0.64	0.58 - 17	4 ± 5.8
Flupentixol	0.4 - 0.81	0.51 ± 0.13	0.52 - 1.6	0.72 ± 0.33	0.52 - 1.6	0.71 ± 0.33	0.52 - 1.6	0.71 ± 0.33
Flurazepam	0.26 - 0.52	0.33 ± 0.08	0.34 - 18	2.3 ± 5.8	0.34 - 1	0.46 ± 0.21	0.34 - 9.4	1.4 ± 3
Fluvoxamine	7.3 - 62	32 ± 22	0.47 - 121	40 ± 41	0.47 - 9.1	3 ± 3	0.47 - 28	4.1 ± 9
Gabapentin	250 - 3,370	1,673 ± 878	1,981 - 8,558	3,528 ± 1,991	124 - 1,314	368 ± 365	113 - 1,285	327 ± 371
Haloperidol	0.31 - 0.63	0.39 ± 0.1	0.4 - 1.2	0.56 ± 0.25	0.4 - 1.2	0.55 ± 0.26	0.4 - 1.2	0.55 ± 0.26
Imipramine	0.12 - 0.25	0.16 ± 0.04	0.16 - 0.48	0.22 ± 0.1	0.16 - 0.48	0.22 ± 0.1	0.16 - 0.48	0.22 ± 0.1
Lamotrigine	88 - 270	173 ± 56	86 - 517	283 ± 123	58 - 465	236 ± 146	45 - 381	231 ± 112
Lorazepam	0.57 - 60	39 ± 24	0.78 - 93	62 ± 36	0.65 - 77	31 ± 30	0.65 - 83	29 ± 35
Maprotiline	9.9 - 34	18 ± 8	8.4 - 57	20 ± 15	0.32 - 15	6 ± 4.2	0.32 - 22	6.6 ± 7
Medazepam	0.74 - 1.5	0.95 ± 0.24	0.97 - 2.9	1.3 ± 0.61	0.97 - 2.9	1.3 ± 0.61	0.97 - 2.9	1.3 ± 0.61
Memantine	1.7 - 43	13 ± 13	6.4 - 75	27 ± 23	4.6 - 60	26 ± 22	6.4 - 72	32 ± 25

Table S19. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		EFF (n = 9)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Methadone	1.1 - 26	11 ± 8	1.1 - 33	12 ± 13	1 - 3.1	1.4 ± 0.66	1 - 3.1	1.4 ± 0.66
Methylphenidate	1 - 13	7.4 ± 5.3	1.4 - 24	10 ± 7.6	1.4 - 4.1	1.9 ± 0.87	1.4 - 68	9.7 ± 22
Mianserin	0.37 - 0.77	0.48 ± 0.12	0.49 - 1.5	0.68 ± 0.31	0.49 - 1.5	0.68 ± 0.31	0.49 - 1.5	0.68 ± 0.31
Mirtazapine	0.55 - 9	4.5 ± 3.4	0.67 - 18	7.4 ± 6.9	0.67 - 6	1.5 ± 1.7	0.67 - 2	0.92 ± 0.43
Naltrexone	0.6 - 14	4.7 ± 5.5	0.78 - 18	6.5 ± 8	0.78 - 12	4.2 ± 4.7	0.78 - 13	2.4 ± 4
<i>N-Desmethyloclozapine</i>	0.62 - 1.3	0.79 ± 0.2	0.81 - 2.4	1.1 ± 0.51	0.81 - 2.4	1.1 ± 0.51	0.81 - 2.4	1.1 ± 0.51
Nitrazepam	1 - 55	28 ± 18	0.98 - 68	32 ± 30	0.98 - 69	30 ± 25	0.98 - 89	26 ± 29
<i>Norbuprenorphine</i>	1.2 - 324	61 ± 108	1.6 - 804	126 ± 261	1.6 - 4.8	2.2 ± 1	1.6 - 4.8	2.2 ± 1
Nordiazepam	0.27 - 2.2	0.59 ± 0.65	0.36 - 1.5	0.61 ± 0.39	0.36 - 1.1	0.49 ± 0.23	0.36 - 1.1	0.49 ± 0.23
Nortriptyline	0.37 - 0.75	0.47 ± 0.12	0.48 - 1.4	0.67 ± 0.3	0.48 - 1.4	0.66 ± 0.31	0.48 - 1.4	0.66 ± 0.31
Olanzapine	0.96 - 74	17 ± 27	1.1 - 67	15 ± 23	1.1 - 3.3	1.5 ± 0.71	1.1 - 3.3	1.5 ± 0.71
Opipramol	0.34 - 11	3 ± 4.8	0.42 - 16	3.5 ± 5.8	0.42 - 11	2.7 ± 4.3	0.42 - 23	4 ± 7.7
Oxazepam	0.27 - 0.54	0.34 ± 0.09	0.35 - 1	0.48 ± 0.22	0.35 - 1	0.48 ± 0.22	0.35 - 1	0.48 ± 0.22
Oxcarbazepine	3.7 - 37	18 ± 12	0.6 - 51	21 ± 16	0.6 - 60	15 ± 20	0.6 - 73	28 ± 25
Paliperidone	0.35 - 0.72	0.45 ± 0.12	0.46 - 1.4	0.63 ± 0.29	0.46 - 1.4	0.63 ± 0.29	0.46 - 1.4	0.63 ± 0.29
Paroxetine	0.75 - 1.5	0.97 ± 0.25	0.99 - 3	1.4 ± 0.62	0.99 - 3	1.4 ± 0.63	0.99 - 3	1.4 ± 0.63
Phenazepam	0.62 - 244	59 ± 90	0.82 - 428	56 ± 141	0.82 - 106	30 ± 45	0.82 - 101	28 ± 42
Phenytoin	40 - 120	70 ± 31	1.6 - 297	108 ± 80	1.6 - 296	135 ± 86	1.6 - 258	92 ± 80
Pipamperone	0.52 - 1.1	0.67 ± 0.17	0.68 - 2	0.94 ± 0.43	0.68 - 2	0.94 ± 0.43	0.68 - 2	0.94 ± 0.43
Prazepam	0.3 - 0.61	0.38 ± 0.1	0.39 - 1.2	0.54 ± 0.25	0.39 - 1.2	0.53 ± 0.25	0.39 - 1.2	0.53 ± 0.25
Promazine	0.98 - 2	1.3 ± 0.32	1.3 - 3.8	1.8 ± 0.81	1.3 - 3.8	1.8 ± 0.82	1.3 - 3.8	1.8 ± 0.82
Protriptyline	0.31 - 0.63	0.4 ± 0.1	0.4 - 1.2	0.56 ± 0.26	0.4 - 1.2	0.55 ± 0.26	0.4 - 1.2	0.55 ± 0.26
Quetiapine	12 - 29	17 ± 6	13 - 38	23 ± 7	0.48 - 1.4	0.65 ± 0.3	0.48 - 1.4	0.65 ± 0.3
Risperidone	0.42 - 85	20 ± 32	0.48 - 154	35 ± 55	0.48 - 1.5	0.66 ± 0.31	0.48 - 1.5	0.66 ± 0.31
<i>Ritalinic acid</i>	0.57 - 69	10 ± 24	0.75 - 75	16 ± 24	0.75 - 209	30 ± 68	0.75 - 108	28 ± 37
Secobarbital	0.43 - 0.88	0.55 ± 0.14	0.56 - 1.7	0.78 ± 0.36	0.56 - 1.7	0.78 ± 0.36	0.56 - 1.7	0.78 ± 0.36
Sertraline	0.7 - 1.4	0.9 ± 0.23	0.91 - 2.7	1.3 ± 0.58	0.91 - 9.6	2.2 ± 2.8	0.91 - 2.7	1.3 ± 0.58
Temazepam	0.54 - 8.9	4.8 ± 3.6	0.62 - 52	9.5 ± 16	0.62 - 8	4.3 ± 3.2	0.62 - 11	3.7 ± 4.3
Topiramate	0.58 - 1.2	0.74 ± 0.19	0.76 - 9	1.9 ± 2.7	0.76 - 2.3	1 ± 0.48	0.76 - 2.3	1 ± 0.48
Trazodone	12 - 48	23 ± 11	13 - 81	32 ± 22	0.61 - 1.8	0.84 ± 0.39	0.61 - 1.8	0.84 ± 0.39
Triazolam	0.31 - 0.63	0.4 ± 0.1	0.4 - 1.2	0.56 ± 0.26	0.4 - 1.2	0.55 ± 0.26	0.4 - 1.2	0.55 ± 0.26
Trimipramine	0.74 - 1.5	0.95 ± 0.24	0.97 - 2.9	1.3 ± 0.61	0.97 - 2.9	1.3 ± 0.62	0.97 - 2.9	1.3 ± 0.62
Venlafaxine	19 - 54	37 ± 12	33 - 95	55 ± 20	10 - 86	44 ± 27	3.6 - 91	46 ± 33
Zolpidem	0.29 - 0.59	0.37 ± 0.09	0.37 - 1.1	0.52 ± 0.24	0.37 - 1.1	0.51 ± 0.24	0.37 - 1.1	0.51 ± 0.24
Zopiclone	0.94 - 1.9	1.2 ± 0.31	1.2 - 3.7	1.7 ± 0.78	1.2 - 3.7	1.7 ± 0.79	1.2 - 3.7	1.7 ± 0.79
<i>α-Hydroxyalprazolam</i>	0.65 - 12	2.2 ± 3.8	0.85 - 18	3.1 ± 5.6	0.85 - 2.6	1.2 ± 0.54	0.85 - 2.6	1.2 ± 0.54
<i>α-Hydroxymidazolam</i>	4.9 - 33	13 ± 10	6.4 - 32	14 ± 9	2.2 - 14	6.9 ± 4.8	0.34 - 15	6.2 ± 4.6
<i>α-Hydroxytriazolam</i>	0.45 - 0.92	0.58 ± 0.15	0.59 - 26	3.5 ± 8.5	0.59 - 25	3.4 ± 8.1	0.59 - 1.8	0.81 ± 0.37
Receptor antagonists								
Atropine	0.51 - 5.4	1.3 ± 1.7	0.67 - 2	0.93 ± 0.42	0.67 - 2	0.92 ± 0.43	0.67 - 2	0.92 ± 0.43
Flumazenil	0.96 - 10	2.4 ± 3.2	1.3 - 11	2.8 ± 3.1	1.3 - 3.8	1.7 ± 0.81	1.3 - 3.8	1.7 ± 0.81
Stimulants								
Caffeine	1,183 - 2,518	1,683 ± 492	1,424 - 5,745	2,882 ± 1,617	50 - 1,705	748 ± 586	60 - 1,520	744 ± 581
<i>Cotinine</i>	268 - 655	406 ± 113	377 - 1,343	625 ± 282	4.4 - 41	16 ± 12	0.6 - 28	14 ± 10
Phentermine	0.64 - 1.3	0.82 ± 0.21	0.83 - 2.5	1.2 ± 0.53	0.83 - 2.5	1.1 ± 0.53	0.83 - 2.5	1.1 ± 0.53
UV filter								
Octinoxate	26 - 75	49 ± 16	57 - 210	105 ± 44	0.57 - 5.7	1.4 ± 1.7	0.57 - 4.3	1.2 ± 1.2

Table S19. (continued)

Compound	HWW (n = 8)		INF (n = 9)		MBRperm (n = 9)		EFF (n = 9)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Veterinary drugs								
Carprofen	0.46 - 27	6.2 ± 10	0.61 - 92	22 ± 34	0.62 - 66	8.1 ± 22	0.61 - 1.8	0.84 ± 0.39
Diaveridine	185 - 570	271 ± 128	278 - 1,184	440 ± 296	0.62 - 69	26 ± 20	0.57 - 64	29 ± 20
Difloxacin	1 - 23	3.9 ± 7.6	1.3 - 28	4.5 ± 9	1.3 - 3.9	1.8 ± 0.83	1.3 - 3.9	1.8 ± 0.83
Dimetridazole	0.27 - 0.56	0.35 ± 0.09	0.36 - 1.1	0.49 ± 0.23	0.36 - 1.1	0.49 ± 0.23	0.36 - 1.1	0.49 ± 0.23
Enrofloxacin	0.57 - 6.6	1.4 ± 2.1	0.7 - 2.1	0.97 ± 0.44	0.7 - 2.1	0.96 ± 0.45	0.7 - 2.1	0.96 ± 0.45
Flunixin	6.4 - 16	9.6 ± 3.2	0.57 - 36	14 ± 11	0.57 - 55	23 ± 14	0.57 - 127	40 ± 44
Furaltadone	37 - 84	53 ± 16	1.1 - 110	58 ± 31	0.92 - 2.8	1.3 ± 0.59	0.92 - 2.8	1.3 ± 0.59
Iprnidazole	0.28 - 0.57	0.36 ± 0.09	0.36 - 1.1	0.5 ± 0.23	0.36 - 1.1	0.5 ± 0.23	0.36 - 1.1	0.5 ± 0.23
Marbofloxacin	0.96 - 729	254 ± 268	1.2 - 548	203 ± 220	1.2 - 266	103 ± 113	1.2 - 418	120 ± 143
Monensin	0.61 - 1.2	0.78 ± 0.2	0.8 - 2.4	1.1 ± 0.51	0.8 - 2.4	1.1 ± 0.51	0.8 - 2.4	1.1 ± 0.51
Orbifloxacin	0.58 - 1.2	0.74 ± 0.19	0.76 - 7.9	1.8 ± 2.3	0.76 - 2.3	1 ± 0.48	0.76 - 7.3	1.7 ± 2.2
Oxibendazole	0.24 - 0.49	0.31 ± 0.08	0.31 - 0.94	0.44 ± 0.2	0.31 - 0.94	0.43 ± 0.2	0.31 - 0.94	0.43 ± 0.2
Ronidazole	0.66 - 22	3.5 ± 7.4	0.87 - 28	4.2 ± 9	0.87 - 76	9.5 ± 25	0.87 - 2.6	1.2 ± 0.55
Salinomycin	2 - 4.2	2.6 ± 0.67	2.7 - 8	3.7 ± 1.7	2.7 - 8	3.7 ± 1.7	2.7 - 8	3.7 ± 1.7
Sarafloxacin	0.96 - 2	1.2 ± 0.32	1.3 - 3.8	1.8 ± 0.8	1.3 - 3.8	1.7 ± 0.81	1.3 - 3.8	1.7 ± 0.81
Sulfachlorpyridazine	0.31 - 35	11 ± 15	0.39 - 34	11 ± 13	0.36 - 19	4 ± 7.1	0.36 - 8.6	1.4 ± 2.7
Sulfaclozine	0.34 - 23	3.2 ± 7.9	0.41 - 30	3.9 ± 9.8	0.41 - 16	2.2 ± 5	0.41 - 1.2	0.57 ± 0.26
Sulfadoxine	0.68 - 1.4	0.88 ± 0.23	0.89 - 2.7	1.2 ± 0.57	0.89 - 2.7	1.2 ± 0.57	0.89 - 2.7	1.2 ± 0.57
Sulfamonomethoxine	0.42 - 0.85	0.54 ± 0.14	0.55 - 1.6	0.76 ± 0.35	0.55 - 4	1.1 ± 1.1	0.55 - 1.6	0.75 ± 0.35
Sulfanitran	0.55 - 1.1	0.71 ± 0.18	0.72 - 2.2	0.99 ± 0.45	0.72 - 2.2	0.99 ± 0.46	0.72 - 2.2	0.99 ± 0.46
Sulfaquinoxaline	0.37 - 41	5.5 ± 14	0.49 - 148	17 ± 49	0.49 - 1.5	0.67 ± 0.31	0.49 - 1.5	0.67 ± 0.31
Tilmicosin	0.95 - 2	1.2 ± 0.31	1.3 - 3.8	1.7 ± 0.79	1.3 - 3.8	1.7 ± 0.8	1.3 - 3.8	1.7 ± 0.8
X-ray contrast medium								
Iopromide	751 - 28,550	10,279 ± 12,024	399 - 31,829	8,605 ± 13,098	0.33 - 1,527	317 ± 467	0.36 - 1,621	308 ± 506

Table S20. Range of variability and average load of target OMPs in HWW, INF and MBRperm during the 0.2PAC sampling campaign, classified by OMP class. For MBRperm, the hydraulic retention time was taken into consideration in the sampling. The transformation products are written in italics. SD: Standard deviation.

Table S20. Range of variability and average load of target OMPs in HWW, INF and MBRperm during the 0.2PAC sampling campaign, classified by OMP class. For MBRperm, the hydraulic retention time was taken into consideration in the sampling. The transformation products are written in italics. SD: Standard deviation.

Compound	HWW (n = 6)		INF (n = 6)		MBRperm (n = 6)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Analgesics/anti-inflammatories						
<i>4-Acetylaminoantipyrine</i>	0.5 - 76	23 ± 27	0.64 - 71	32 ± 27	0.64 - 46	18 ± 17
<i>4-Formylaminoantipyrine</i>	0.31 - 29	13 ± 9	0.39 - 28	16 ± 10	0.39 - 23	12 ± 8
<i>6-Acetylmorphine</i>	0.35 - 450	162 ± 203	0.44 - 593	151 ± 240	0.36 - 0.71	0.51 ± 0
Acetaminophen	2,556 - 4,769	3,132 ± 830	2,626 - 5,208	3,640 ± 1,084	1.7 - 39	17 ± 15
<i>Acetylcodeine</i>	0.37 - 0.72	0.52 ± 0.11	0.51 - 1	0.73 ± 0.18	0.51 - 1	0.73 ± 0.18
Acetylsalicylic acid	74 - 238	135 ± 66	35 - 329	165 ± 96	44 - 147	84 ± 38
Alfentanil	0.16 - 0.3	0.22 ± 0.05	0.22 - 0.43	0.31 ± 0.07	0.22 - 0.43	0.31 ± 0.07
Aminopyrine	0.75 - 1.4	1.1 ± 0.23	1 - 2	1.5 ± 0.35	1 - 2	1.5 ± 0.35
Betamethasone 17,21-dipropionate	0.49 - 0.95	0.69 ± 0.15	0.68 - 1.3	0.97 ± 0.23	0.68 - 1.3	0.97 ± 0.23
Buprenorphine	0.29 - 74	54 ± 30	0.26 - 112	36 ± 55	0.26 - 0.52	0.37 ± 0
<i>Buprenorphine glucuronide</i>	0.93 - 274	108 ± 105	1 - 247	42 ± 100	1 - 2	1.4 ± 0
Carisoprodol	0.61 - 1.2	0.86 ± 0.19	0.84 - 1.7	1.2 ± 0.29	0.84 - 1.7	1.2 ± 0.29
Codeine	31 - 156	106 ± 47	50 - 156	111 ± 45	0.56 - 6.3	2.3 ± 3
Dextromethorphan	0.31 - 0.6	0.44 ± 0.1	0.43 - 0.85	0.61 ± 0.15	0.43 - 0.85	0.61 ± 0.15
Dextropropoxyphene	1 - 1.9	1.4 ± 0.31	1.4 - 2.7	2 ± 0.48	1.4 - 2.7	2 ± 0.48
Diclofenac	13 - 53	28 ± 17	56 - 235	123 ± 60	26 - 83	54 ± 20
Etodolac	0.33 - 0.64	0.47 ± 0.1	0.46 - 0.91	0.65 ± 0.16	0.46 - 0.91	0.65 ± 0.16
Fentanyl	0.22 - 0.42	0.3 ± 0.07	0.3 - 0.59	0.42 ± 0.1	0.3 - 0.59	0.42 ± 0.1
Hydrocodone	0.49 - 120	54 ± 53	0.89 - 139	78 ± 53	0.45 - 0.89	0.64 ± 0
Hydromorphone	24 - 80	51 ± 19	27 - 104	55 ± 31	0.46 - 0.92	0.66 ± 0
Ibuprofen	0.54 - 454	109 ± 171	44 - 462	188 ± 144	0.82 - 37	25 ± 14
Ketoprofen	306 - 1,107	647 ± 328	478 - 1,376	874 ± 386	1.1 - 2.1	1.5 ± 0
Lidocaine	41 - 190	102 ± 51	46 - 126	95 ± 35	0.43 - 72	34 ± 26
Meloxicam	0.4 - 0.77	0.56 ± 0.12	0.55 - 1.1	0.78 ± 0.19	0.55 - 1.1	0.78 ± 0.19
Morphine	24 - 80	55 ± 22	27 - 104	58 ± 30	0.46 - 0.92	0.66 ± 0
<i>Morphine-6-β-D-glucuronide</i>	0.23 - 0.45	0.33 ± 0.07	0.32 - 0.64	0.46 ± 0.11	0.32 - 0.64	0.46 ± 0.11
Naproxen	0.23 - 0.45	0.33 ± 0.07	0.32 - 0.63	0.46 ± 0.11	0.32 - 0.63	0.46 ± 0.11
<i>Norfentanyl</i>	0.31 - 28	9.5 ± 9.6	0.32 - 30	9.7 ± 11	0.32 - 7.6	3 ± 3.1
<i>Norpethidine</i>	0.45 - 18	9.2 ± 7.7	0.57 - 16	5.5 ± 6.3	0.47 - 0.92	0.67 ± 0.16
<i>Norpropoxyphene</i>	0.34 - 0.65	0.48 ± 0.1	0.46 - 0.92	0.66 ± 0.16	0.46 - 0.92	0.66 ± 0.16
<i>O-Desmethyltramadol</i>	34 - 218	109 ± 74	72 - 252	151 ± 81	12 - 150	77 ± 63
Oxycodone	0.41 - 19	7.4 ± 8.9	0.53 - 29	13 ± 10	0.53 - 4.2	1.7 ± 2
Oxymorphone	0.74 - 21	9.8 ± 6.9	11 - 32	17 ± 9	0.53 - 1	0.75 ± 0
Pentazocine	0.25 - 0.48	0.35 ± 0.08	0.34 - 0.67	0.48 ± 0.12	0.34 - 0.67	0.48 ± 0.12
Pethidine	0.23 - 0.44	0.32 ± 0.07	0.32 - 0.63	0.45 ± 0.11	0.32 - 0.63	0.45 ± 0.11
Phenylbutazone	0.34 - 0.65	0.47 ± 0.1	0.46 - 0.92	0.66 ± 0.16	0.46 - 0.92	0.66 ± 0.16
Procaine	3.2 - 24	12 ± 8	3.7 - 71	28 ± 26	0.47 - 7.8	5.6 ± 3
Tolfenamic acid	0.25 - 0.49	0.36 ± 0.08	0.35 - 0.69	0.5 ± 0.12	0.35 - 0.69	0.5 ± 0.12
Tramadol	28 - 226	134 ± 81	136 - 281	192 ± 60	49 - 141	108 ± 39
Antiarrhythmic agents						
Amiodarone	0.53 - 1	0.75 ± 0.16	0.73 - 1.4	1 ± 0.25	0.73 - 1.4	1 ± 0.25

Table S20. (continued)

Compound	HWW (n = 6)		INF (n = 6)		MBRperm (n = 6)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Digitoxin	1.2 - 2.3	1.7 ± 0.37	1.7 - 3.3	2.4 ± 0.57	1.7 - 3.3	2.4 ± 0.57
Propafenone	11 - 52	31 ± 17	0.35 - 55	22 ± 20	0.26 - 6.6	1.4 ± 3
Strophanthidin	0.78 - 1.5	1.1 ± 0.24	1.1 - 2.1	1.5 ± 0.37	1.1 - 2.1	1.5 ± 0.37
Strophanthin	0.87 - 1.7	1.2 ± 0.27	1.2 - 147	26 ± 59	1.2 - 2.4	1.7 ± 0
Antibiotics						
2-NP-AOZ	0.39 - 0.75	0.55 ± 0.12	0.54 - 1.1	0.77 ± 0.19	0.54 - 1.1	0.77 ± 0.19
Amoxicillin	0.4 - 50	22 ± 18	0.55 - 41	31 ± 15	0.55 - 1.1	0.78 ± 0
Azithromycin	899 - 2,777	1,523 ± 760	783 - 2,106	1,333 ± 536	23 - 70	42 ± 16
Cinoxacin	0.22 - 0.42	0.31 ± 0.07	0.3 - 0.6	0.43 ± 0.1	0.3 - 0.6	0.43 ± 0.1
Ciprofloxacin	204 - 644	443 ± 184	171 - 436	357 ± 102	26 - 128	58 ± 37
Clarithromycin	67 - 197	128 ± 50	75 - 259	128 ± 66	5.4 - 22	14 ± 5
Doxycycline	0.29 - 0.55	0.4 ± 0.09	0.39 - 97	17 ± 39	0.39 - 0.78	0.56 ± 0
Enoxacin	0.53 - 357	65 ± 144	0.73 - 472	79 ± 192	0.73 - 1.4	1 ± 0
Erythromycin	247 - 549	388 ± 111	0.74 - 739	432 ± 287	1 - 101	21 ± 40
Flumequine	0.36 - 0.69	0.5 ± 0.11	0.49 - 0.98	0.7 ± 0.17	0.49 - 0.98	0.7 ± 0.17
Furazolidon	0.33 - 0.63	0.46 ± 0.1	0.45 - 0.9	0.65 ± 0.16	0.45 - 0.9	0.65 ± 0.16
Lomefloxacin	0.47 - 47	19 ± 22	0.64 - 74	25 ± 30	0.64 - 46	8.4 ± 18
Metronidazole	31 - 254	127 ± 85	5.9 - 209	55 ± 76	4.4 - 22	9.3 ± 6
Minocycline	0.68 - 185	55 ± 85	0.93 - 1.9	1.3 ± 0.32	0.93 - 1.9	1.3 ± 0.32
Nalidixic acid	0.69 - 1.3	0.97 ± 0.21	0.95 - 1.9	1.4 ± 0.33	0.95 - 1.9	1.4 ± 0.33
Norfloxacin	0.48 - 174	49 ± 70	0.65 - 253	56 ± 101	0.65 - 1.3	0.93 ± 0
Ofloxacin	248 - 588	429 ± 143	335 - 755	502 ± 148	24 - 505	292 ± 175
Oleandomycin	0.41 - 200	46 ± 81	0.57 - 282	67 ± 112	0.57 - 1.1	0.81 ± 0
Oxolinic acid	0.29 - 0.57	0.41 ± 0.09	0.4 - 0.8	0.58 ± 0.14	0.4 - 0.8	0.58 ± 0.14
Oxytetracycline	0.84 - 58	11 ± 23	1.2 - 24	5.4 ± 9.1	1.2 - 2.3	1.6 ± 0.4
Penicillin G	1.8 - 3.4	2.5 ± 0.54	2.4 - 4.8	3.4 ± 0.83	2.4 - 4.8	3.4 ± 0.83
Pipemidic acid	0.63 - 1.2	0.89 ± 0.19	0.87 - 1.7	1.2 ± 0.3	0.87 - 1.7	1.2 ± 0.3
Roxithromycin	0.82 - 253	131 ± 89	1.1 - 371	197 ± 159	1.1 - 96	28 ± 43
Silvadene	0.45 - 0.87	0.63 ± 0.14	0.62 - 9	2.2 ± 3.3	0.62 - 1.2	0.88 ± 0.21
Spiramycin	1.5 - 3	2.2 ± 0.47	2.1 - 4.2	3 ± 0.73	2.1 - 4.2	3 ± 0.73
Sulfabenzamide	0.63 - 1.2	0.89 ± 0.19	0.87 - 1.7	1.2 ± 0.3	0.87 - 1.7	1.2 ± 0.3
Sulfadimethoxine	0.41 - 0.8	0.58 ± 0.13	0.57 - 1.1	0.81 ± 0.2	0.57 - 1.1	0.81 ± 0.2
Sulfadimidine	0.39 - 0.74	0.54 ± 0.12	0.53 - 1.1	0.76 ± 0.18	0.53 - 1.1	0.76 ± 0.18
Sulfafurazole	0.75 - 1.4	1 ± 0.23	1 - 2	1.5 ± 0.35	1 - 2	1.5 ± 0.35
Sulfaguanidine	0.28 - 0.54	0.39 ± 0.09	0.38 - 0.76	0.55 ± 0.13	0.38 - 0.76	0.55 ± 0.13
Sulfamerazine	0.4 - 0.77	0.56 ± 0.12	0.55 - 1.1	0.79 ± 0.19	0.55 - 1.1	0.79 ± 0.19
Sulfamethizole	0.74 - 1.4	1 ± 0.23	1 - 2	1.4 ± 0.35	1 - 2	1.4 ± 0.35
Sulfamethoxazole	139 - 682	272 ± 204	85 - 650	270 ± 194	39 - 175	89 ± 57
Sulfamethoxydiazine	0.75 - 1.4	1.1 ± 0.23	1 - 2	1.5 ± 0.35	1 - 2	1.5 ± 0.35
Sulfamethoxypyridazine	0.22 - 0.42	0.31 ± 0.07	0.3 - 4.6	1.1 ± 1.7	0.3 - 0.6	0.43 ± 0.1
Sulfanilamide	0.65 - 1.3	0.91 ± 0.2	0.89 - 1.8	1.3 ± 0.31	0.89 - 1.8	1.3 ± 0.31
Sulfaphenazole	0.52 - 1	0.73 ± 0.16	0.71 - 1.4	1 ± 0.25	0.71 - 1.4	1 ± 0.25
Sulfapyridine	14 - 160	64 ± 56	0.75 - 153	62 ± 60	0.45 - 78	22 ± 30
Sulfathiazole	0.43 - 91	42 ± 36	0.57 - 218	51 ± 88	0.62 - 164	47 ± 64
Tinidazole	0.42 - 0.8	0.59 ± 0.13	0.57 - 1.1	0.82 ± 0.2	0.57 - 1.1	0.82 ± 0.2
Trimethoprim	42 - 293	110 ± 93	47 - 205	94 ± 60	4.3 - 23	12 ± 7

Table S20. (continued)

Compound	HWW (n = 6)		INF (n = 6)		MBRperm (n = 6)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Antifungals						
Sulfacetamide	0.34 - 0.66	0.48 ± 0.1	0.47 - 0.93	0.67 ± 0.16	0.47 - 0.93	0.67 ± 0.16
Terbinafine	0.3 - 0.57	0.41 ± 0.09	0.4 - 0.8	0.58 ± 0.14	0.4 - 0.8	0.58 ± 0.14
Tiabendazole	0.13 - 0.26	0.19 ± 0.04	0.18 - 0.36	0.26 ± 0.06	0.18 - 0.36	0.26 ± 0.06
Antihistamines						
Diphenhydramine	0.35 - 0.67	0.49 ± 0.11	0.48 - 0.95	0.68 ± 0.17	0.48 - 0.95	0.68 ± 0.17
Promethazine	0.58 - 1.1	0.82 ± 0.18	0.8 - 1.6	1.1 ± 0.28	0.8 - 1.6	1.1 ± 0.28
Antihypertensive						
Clonidine	0.05 - 0.1	0.07 ± 0.02	0.07 - 0.14	0.1 ± 0.02	0.07 - 0.14	0.1 ± 0.02
Antiparasitics						
Albendazole	0.28 - 0.54	0.39 ± 0.09	0.38 - 0.76	0.55 ± 0.13	0.38 - 0.76	0.55 ± 0.13
Flubendazole	0.64 - 1.2	0.9 ± 0.2	0.88 - 1.7	1.3 ± 0.3	0.88 - 1.7	1.3 ± 0.3
Levamisole	0.62 - 1.2	0.87 ± 0.19	0.85 - 1.7	1.2 ± 0.29	0.85 - 1.7	1.2 ± 0.29
Mebendazole	0.25 - 2.9	0.77 ± 1	0.34 - 0.67	0.48 ± 0.12	0.34 - 0.67	0.48 ± 0.12
Praziquantel	0.52 - 155	49 ± 58	0.71 - 129	50 ± 56	0.71 - 1.4	1 ± 0
Triclabendazole	0.2 - 0.38	0.28 ± 0.06	0.27 - 0.53	0.38 ± 0.09	0.27 - 0.53	0.38 ± 0.09
Antiseptic						
Nitrofurantoin	0.42 - 0.81	0.59 ± 0.13	0.58 - 1.1	0.83 ± 0.2	0.58 - 1.1	0.83 ± 0.2
Beta-blockers						
Atenolol	102 - 327	177 ± 79	112 - 392	261 ± 130	0.53 - 7.7	5.5 ± 3
Bisoprolol	28 - 70	40 ± 15	28 - 77	51 ± 19	0.69 - 19	4 ± 7
Metoprolol	49 - 129	92 ± 34	108 - 186	136 ± 29	37 - 334	162 ± 98
Calcium channel blocker						
Verapamil	0.23 - 19	11 ± 9	0.43 - 36	17 ± 12	0.31 - 0.63	0.45 ± 0
Diuretic						
Torsemide	0.47 - 0.91	0.66 ± 0.14	0.65 - 1.3	0.93 ± 0.22	0.65 - 1.3	0.93 ± 0.22
Hormones						
Fludrocortisone-acetate	0.75 - 1.4	1.1 ± 0.23	1 - 2	1.5 ± 0.35	1 - 2	1.5 ± 0.35
Flumethasone	0.58 - 1.1	0.82 ± 0.18	0.8 - 1.6	1.1 ± 0.28	0.8 - 1.6	1.1 ± 0.28
Hydrocortisone	0.39 - 58	10 ± 23	0.42 - 0.83	0.6 ± 0.14	0.42 - 0.83	0.6 ± 0.14
Methylprednisolone	1 - 1.9	1.4 ± 0.3	1.4 - 2.7	1.9 ± 0.47	1.4 - 2.7	1.9 ± 0.47
Mometasone furoate	0.4 - 0.76	0.56 ± 0.12	0.54 - 1.1	0.78 ± 0.19	0.54 - 1.1	0.78 ± 0.19
Prednicarbate	0.74 - 1.4	1 ± 0.23	1 - 2	1.5 ± 0.35	1 - 2	1.5 ± 0.35
Prednisolone	1.6 - 73	14 ± 29	1.8 - 3.5	2.5 ± 0.6	1.8 - 3.5	2.5 ± 0.6
Triamcinolone	0.19 - 0.37	0.27 ± 0.06	0.27 - 0.53	0.38 ± 0.09	0.27 - 0.53	0.38 ± 0.09
Triamcinolone acetonide	0.38 - 0.73	0.53 ± 0.12	0.52 - 1	0.74 ± 0.18	0.52 - 1	0.74 ± 0.18
Illicit drugs						
Amphetamine	21 - 114	64 ± 37	17 - 147	70 ± 51	0.55 - 24	4.6 ± 9
<i>Benzoyllecgonine</i>	63 - 211	155 ± 61	91 - 293	205 ± 81	0.52 - 1	0.74 ± 0
Cannabinol	0.89 - 31	6.2 ± 12	1.2 - 2.4	1.7 ± 0.42	1.2 - 2.4	1.7 ± 0.42
<i>Cocaeethylene</i>	0.1 - 54	20 ± 24	0.14 - 97	27 ± 43	0.14 - 0.28	0.2 ± 0
Cocaine	0.59 - 1.1	0.83 ± 0.18	0.81 - 1.6	1.2 ± 0.28	0.81 - 1.6	1.2 ± 0.28
<i>Ecgonine methyl ester</i>	0.95 - 191	72 ± 83	1.3 - 226	50 ± 90	1 - 2	1.5 ± 0
Ketamine	0.39 - 0.74	0.54 ± 0.12	0.53 - 1	0.75 ± 0.18	0.53 - 1	0.75 ± 0.18
MDA	14 - 343	73 ± 132	1.3 - 276	50 ± 111	1.2 - 209	52 ± 86
MDEA	0.33 - 0.64	0.47 ± 0.1	0.45 - 0.9	0.65 ± 0.16	0.45 - 0.9	0.65 ± 0.16
MDMA	3.1 - 43	19 ± 18	0.38 - 0.76	0.55 ± 0.13	0.38 - 0.76	0.55 ± 0.13

Table S20. (continued)

Compound	HWW (n = 6)		INF (n = 6)		MBRperm (n = 6)	
	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)
Methamphetamine	0.19 - 0.36	0.26 \pm 0.06	0.26 - 11	2.2 \pm 4.5	0.26 - 0.51	0.37 \pm 0.09
Phencyclidine	0.75 - 1.4	1 \pm 0.23	1 - 2	1.5 \pm 0.35	1 - 2	1.5 \pm 0.35
THC	0.57 - 25	14 \pm 11	0.78 - 1.6	1.1 \pm 0.27	0.78 - 1.6	1.1 \pm 0.27
Plastic additives						
Benzotriazole	476 - 4,458	2,678 \pm 1,448	480 - 5,499	3,449 \pm 1,939	149 - 2,992	1,961 \pm 1,065
p-Toluenesulfonamide	0.49 - 63	11 \pm 26	0.67 - 1.3	0.96 \pm 0.23	0.67 - 1.3	0.96 \pm 0.23
Psychiatric drugs						
10-Hydroxycarbazepine	0.35 - 184	86 \pm 94	0.36 - 400	160 \pm 180	0.36 - 0.72	0.52 \pm 0
7-Aminoclonazepam	0.16 - 0.31	0.22 \pm 0.05	0.22 - 0.43	0.31 \pm 0.08	0.22 - 0.43	0.31 \pm 0.08
7-Aminoflunitrazepam	0.16 - 0.31	0.22 \pm 0.05	0.22 - 0.43	0.31 \pm 0.08	0.22 - 0.43	0.31 \pm 0.08
Alprazolam	0.31 - 0.59	0.43 \pm 0.09	0.42 - 0.83	0.6 \pm 0.15	0.42 - 0.83	0.6 \pm 0.15
Amisulpride	0.39 - 7.3	2.7 \pm 2.8	0.5 - 11	7.1 \pm 4.2	0.4 - 9.5	2.7 \pm 3.7
Amitriptyline	0.26 - 0.5	0.36 \pm 0.08	0.35 - 0.7	0.51 \pm 0.12	0.35 - 0.7	0.51 \pm 0.12
Amoxapine	0.36 - 0.7	0.51 \pm 0.11	0.5 - 0.99	0.71 \pm 0.17	0.5 - 0.99	0.71 \pm 0.17
Bromazepam	0.37 - 0.71	0.52 \pm 0.11	0.51 - 6.8	1.7 \pm 2.5	0.51 - 1	0.73 \pm 0.18
Carbamazepine	22 - 66	43 \pm 15	57 - 153	105 \pm 32	24 - 104	58 \pm 35
Chlordiazepoxide	0.42 - 0.82	0.59 \pm 0.13	0.58 - 1.2	0.83 \pm 0.2	0.58 - 1.2	0.83 \pm 0.2
Chlorprothixene	0.65 - 1.3	0.91 \pm 0.2	0.89 - 1.8	1.3 \pm 0.31	0.89 - 1.8	1.3 \pm 0.31
Citalopram	12 - 20	15 \pm 4	0.85 - 27	12 \pm 11	0.63 - 1.3	0.91 \pm 0
Clobazam	0.27 - 0.51	0.37 \pm 0.08	0.36 - 0.72	0.52 \pm 0.13	0.36 - 0.72	0.52 \pm 0.13
Clomipramine	0.33 - 12	3.6 \pm 5.1	0.45 - 17	3.4 \pm 6.7	0.45 - 0.89	0.64 \pm 0.16
Clonazepam	0.47 - 0.91	0.67 \pm 0.14	0.65 - 1.3	0.93 \pm 0.22	0.65 - 1.3	0.93 \pm 0.22
Clorazepate	0.62 - 1.2	0.87 \pm 0.19	0.85 - 1.7	1.2 \pm 0.29	0.85 - 1.7	1.2 \pm 0.29
Clozapine	0.23 - 0.44	0.32 \pm 0.07	0.31 - 0.62	0.45 \pm 0.11	0.31 - 0.62	0.45 \pm 0.11
Desalkylflurazepam	0.17 - 0.33	0.24 \pm 0.05	0.23 - 0.46	0.33 \pm 0.08	0.23 - 0.46	0.33 \pm 0.08
Desipramine	0.79 - 1.5	1.1 \pm 0.24	1.1 - 2.1	1.5 \pm 0.37	1.1 - 2.1	1.5 \pm 0.37
Desvenlafaxine	5.6 - 32	15 \pm 9	15 - 61	31 \pm 16	0.32 - 25	15 \pm 9
Dexametasone	0.63 - 1.2	0.88 \pm 0.19	0.86 - 1.7	1.2 \pm 0.3	0.86 - 1.7	1.2 \pm 0.3
Diazepam	0.29 - 0.56	0.41 \pm 0.09	0.4 - 0.79	0.57 \pm 0.14	0.4 - 0.79	0.57 \pm 0.14
Dothiepin	0.47 - 0.91	0.66 \pm 0.14	0.65 - 1.3	0.92 \pm 0.22	0.65 - 1.3	0.92 \pm 0.22
Doxepin	0.33 - 0.63	0.46 \pm 0.1	0.45 - 0.88	0.64 \pm 0.15	0.45 - 0.88	0.64 \pm 0.15
EDDP	0.23 - 21	9.8 \pm 7.9	0.21 - 17	7.7 \pm 7.6	0.21 - 0.42	0.31 \pm 0.07
Felbamate	0.35 - 0.68	0.49 \pm 0.11	0.48 - 0.96	0.69 \pm 0.17	0.48 - 0.96	0.69 \pm 0.17
Fluoxetine	0.46 - 15	9 \pm 5.1	0.64 - 17	9.2 \pm 6.3	0.48 - 0.95	0.68 \pm 0.16
Flupentixol	0.31 - 0.6	0.44 \pm 0.1	0.43 - 0.85	0.61 \pm 0.15	0.43 - 0.85	0.61 \pm 0.15
Flurazepam	0.2 - 0.39	0.28 \pm 0.06	0.28 - 0.55	0.39 \pm 0.1	0.28 - 0.55	0.39 \pm 0.1
Fluvoxamine	0.28 - 0.54	0.4 \pm 0.09	0.39 - 0.77	0.55 \pm 0.13	0.39 - 0.77	0.55 \pm 0.13
Gabapentin	360 - 2,532	1,539 \pm 943	836 - 4,049	2,295 \pm 1,495	53 - 319	134 \pm 97
Haloperidol	0.24 - 0.46	0.34 \pm 0.07	0.33 - 0.65	0.47 \pm 0.11	0.33 - 0.65	0.47 \pm 0.11
Imipramine	0.1 - 0.19	0.14 \pm 0.03	0.13 - 0.26	0.19 \pm 0.05	0.13 - 0.26	0.19 \pm 0.05
Lamotrigine	29 - 81	47 \pm 20	76 - 193	135 \pm 48	45 - 190	115 \pm 54
Lorazepam	0.59 - 126	64 \pm 41	0.54 - 116	41 \pm 48	0.54 - 1.1	0.77 \pm 0
Maprotiline	0.29 - 20	7.1 \pm 7.8	0.36 - 15	5.3 \pm 5.6	0.26 - 0.53	0.38 \pm 0.09
Medazepam	0.58 - 1.1	0.81 \pm 0.18	0.79 - 1.6	1.1 \pm 0.27	0.79 - 1.6	1.1 \pm 0.27
Memantine	0.5 - 18	7.3 \pm 6.8	0.69 - 16	8 \pm 5.5	0.51 - 10	3.6 \pm 4.5
Methadone	0.63 - 6.2	1.8 \pm 2.2	0.86 - 1.7	1.2 \pm 0.3	0.86 - 1.7	1.2 \pm 0.3
Methylphenidate	0.82 - 1.6	1.2 \pm 0.25	1.1 - 2.2	1.6 \pm 0.39	1.1 - 2.2	1.6 \pm 0.39

Table S20. (continued)

Compound	HWW (n = 6)		INF (n = 6)		MBRperm (n = 6)	
	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)	Range (mg/d)	Average ± SD (mg/d)
Mianserin	0.3 - 0.57	0.41 ± 0.09	0.4 - 0.8	0.58 ± 0.14	0.4 - 0.8	0.58 ± 0.14
Mirtazapine	0.54 - 7.2	2.2 ± 2.7	0.55 - 8.4	2.1 ± 3.1	0.55 - 1.1	0.79 ± 0.19
Naltrexone	0.47 - 0.91	0.66 ± 0.14	0.64 - 1.3	0.92 ± 0.22	0.64 - 1.3	0.92 ± 0.22
<i>N-Desmethylozapine</i>	0.49 - 0.93	0.68 ± 0.15	0.66 - 1.3	0.95 ± 0.23	0.66 - 1.3	0.95 ± 0.23
Nitrazepam	0.59 - 1.1	0.82 ± 0.18	0.8 - 1.6	1.1 ± 0.28	0.8 - 1.6	1.1 ± 0.28
<i>Norbuprenorphine</i>	0.96 - 35	7 ± 14	1.3 - 2.6	1.9 ± 0.46	1.3 - 2.6	1.9 ± 0.46
Nordiazepam	0.22 - 0.42	0.3 ± 0.07	0.3 - 0.59	0.42 ± 0.1	0.3 - 0.59	0.42 ± 0.1
Nortriptyline	0.29 - 0.55	0.4 ± 0.09	0.39 - 0.78	0.56 ± 0.14	0.39 - 0.78	0.56 ± 0.14
Olanzapine	0.67 - 45	8.3 ± 18	0.91 - 46	8.8 ± 18	0.91 - 1.8	1.3 ± 0.32
Opipramol	0.25 - 0.49	0.35 ± 0.08	0.35 - 0.69	0.49 ± 0.12	0.35 - 0.69	0.49 ± 0.12
Oxazepam	0.21 - 0.4	0.29 ± 0.06	0.29 - 0.57	0.41 ± 0.1	0.29 - 0.57	0.41 ± 0.1
Oxcarbazepine	0.36 - 71	14 ± 28	0.49 - 0.98	0.7 ± 0.17	0.49 - 0.98	0.7 ± 0.17
Paliperidone	0.28 - 0.53	0.39 ± 0.08	0.38 - 0.75	0.54 ± 0.13	0.38 - 0.75	0.54 ± 0.13
Paroxetine	0.59 - 1.1	0.83 ± 0.18	0.81 - 1.6	1.2 ± 0.28	0.81 - 1.6	1.2 ± 0.28
Phenazepam	0.49 - 38	6.8 ± 15	0.67 - 1.3	0.96 ± 0.23	0.67 - 1.3	0.96 ± 0.23
Phenytoin	0.96 - 1.8	1.3 ± 0.29	1.3 - 26	5.9 ± 9.9	1.3 - 2.6	1.9 ± 0.45
Pipamperone	0.41 - 0.79	0.57 ± 0.13	0.56 - 1.1	0.8 ± 0.19	0.56 - 1.1	0.8 ± 0.19
Prazepam	0.23 - 0.45	0.33 ± 0.07	0.32 - 0.63	0.46 ± 0.11	0.32 - 0.63	0.46 ± 0.11
Promazine	0.77 - 1.5	1.1 ± 0.24	1.1 - 2.1	1.5 ± 0.36	1.1 - 2.1	1.5 ± 0.36
Protriptyline	0.24 - 0.47	0.34 ± 0.07	0.33 - 0.66	0.47 ± 0.11	0.33 - 0.66	0.47 ± 0.11
Quetiapine	0.38 - 15	8.4 ± 4.8	4.1 - 12	7.6 ± 3.1	0.39 - 0.78	0.56 ± 0.13
Risperidone	0.29 - 57	9.8 ± 23	0.4 - 0.79	0.57 ± 0.14	0.4 - 0.79	0.57 ± 0.14
<i>Ritalinic acid</i>	0.45 - 0.86	0.63 ± 0.14	0.61 - 1.2	0.88 ± 0.21	0.61 - 1.2	0.88 ± 0.21
Secobarbital	0.34 - 0.65	0.48 ± 0.1	0.46 - 0.92	0.66 ± 0.16	0.46 - 0.92	0.66 ± 0.16
Sertraline	0.55 - 1.1	0.77 ± 0.17	0.75 - 1.5	1.1 ± 0.26	0.75 - 1.5	1.1 ± 0.26
Temazepam	0.37 - 0.71	0.52 ± 0.11	0.51 - 1	0.73 ± 0.18	0.51 - 1	0.73 ± 0.18
Topiramate	0.45 - 0.87	0.64 ± 0.14	0.62 - 1.2	0.89 ± 0.21	0.62 - 1.2	0.89 ± 0.21
Trazodone	0.49 - 32	14 ± 10	0.68 - 39	16 ± 13	0.5 - 9	2.1 ± 3
Triazolam	0.24 - 0.47	0.34 ± 0.07	0.33 - 0.66	0.47 ± 0.11	0.33 - 0.66	0.47 ± 0.11
Trimipramine	0.58 - 1.1	0.81 ± 0.18	0.79 - 1.6	1.1 ± 0.27	0.79 - 1.6	1.1 ± 0.27
Venlafaxine	6 - 53	19 ± 17	14 - 74	32 ± 22	7.6 - 28	17 ± 9
Zolpidem	0.23 - 0.43	0.32 ± 0.07	0.31 - 0.61	0.44 ± 0.11	0.31 - 0.61	0.44 ± 0.11
Zopiclone	0.74 - 1.4	1 ± 0.23	1 - 2	1.5 ± 0.35	1 - 2	1.5 ± 0.35
<i>α-Hydroxyalprazolam</i>	0.51 - 0.99	0.72 ± 0.16	0.7 - 1.4	1 ± 0.24	0.7 - 1.4	1 ± 0.24
<i>α-Hydroxymidazolam</i>	2.2 - 6.2	3.9 ± 1.5	3.1 - 9.6	5.5 ± 2.5	0.19 - 4.5	1.8 ± 1.9
<i>α-Hydroxytriazolam</i>	0.35 - 0.68	0.5 ± 0.11	0.48 - 0.96	0.69 ± 0.17	0.48 - 0.96	0.69 ± 0.17
Receptor antagonists						
Atropine	0.4 - 0.77	0.56 ± 0.12	0.55 - 1.1	0.79 ± 0.19	0.55 - 1.1	0.79 ± 0.19
Flumazenil	0.76 - 1.5	1.1 ± 0.23	1 - 2.1	1.5 ± 0.36	1 - 2.1	1.5 ± 0.36
Stimulants						
Caffeine	726 - 1,498	1,019 ± 276	916 - 1,935	1,357 ± 355	29 - 48	36 ± 7
<i>Cotinine</i>	168 - 389	254 ± 73	233 - 579	389 ± 120	0.8 - 10	5 ± 4
Phentermine	0.5 - 0.96	0.7 ± 0.15	0.69 - 1.4	0.98 ± 0.24	0.69 - 1.4	0.98 ± 0.24
UV filter						
Octinoxate	0.45 - 32	17 ± 14	0.58 - 66	30 ± 22	0.47 - 17	4.4 ± 7
Veterinary drugs						
Carprofen	0.37 - 0.7	0.51 ± 0.11	0.5 - 0.99	0.72 ± 0.17	0.5 - 0.99	0.72 ± 0.17

Table S20. (continued)

Compound	HWW (n = 6)		INF (n = 6)		MBRperm (n = 6)	
	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)	Range (mg/d)	Average \pm SD (mg/d)
Diaveridine	0.32 - 423	178 \pm 140	0.44 - 585	246 \pm 197	0.44 - 35	21 \pm 16
Difloxacin	0.79 - 1.5	1.1 \pm 0.24	1.1 - 2.1	1.5 \pm 0.37	1.1 - 2.1	1.5 \pm 0.37
Dimetridazole	0.21 - 0.41	0.3 \pm 0.07	0.29 - 0.58	0.42 \pm 0.1	0.29 - 0.58	0.42 \pm 0.1
Enrofloxacin	0.42 - 0.81	0.59 \pm 0.13	0.57 - 1.1	0.82 \pm 0.2	0.57 - 1.1	0.82 \pm 0.2
Flunixin	0.34 - 0.66	0.48 \pm 0.11	0.47 - 0.93	0.67 \pm 0.16	0.47 - 0.93	0.67 \pm 0.16
Furaltadone	0.55 - 26	5.1 \pm 10	0.76 - 1.5	1.1 \pm 0.26	0.76 - 1.5	1.1 \pm 0.26
Iprnidazole	0.22 - 0.42	0.31 \pm 0.07	0.3 - 0.6	0.43 \pm 0.1	0.3 - 0.6	0.43 \pm 0.1
Marbofloxacin	0.7 - 1.4	0.99 \pm 0.22	0.96 - 1.9	1.4 \pm 0.33	0.96 - 1.9	1.4 \pm 0.33
Monensin	0.48 - 0.92	0.67 \pm 0.15	0.66 - 1.3	0.94 \pm 0.23	0.66 - 1.3	0.94 \pm 0.23
Orbifloxacin	0.45 - 0.87	0.64 \pm 0.14	0.62 - 1.2	0.89 \pm 0.21	0.62 - 1.2	0.89 \pm 0.21
Oxibendazole	0.19 - 0.36	0.27 \pm 0.06	0.26 - 0.51	0.37 \pm 0.09	0.26 - 0.51	0.37 \pm 0.09
Ronidazole	0.52 - 1	0.73 \pm 0.16	0.71 - 1.4	1 \pm 0.25	0.71 - 1.4	1 \pm 0.25
Salinomycin	1.6 - 3.1	2.2 \pm 0.49	2.2 - 4.3	3.1 \pm 0.76	2.2 - 4.3	3.1 \pm 0.76
Sarafloxacin	0.76 - 1.5	1.1 \pm 0.23	1 - 2.1	1.5 \pm 0.36	1 - 2.1	1.5 \pm 0.36
Sulfachlorpyridazine	0.22 - 11	2.1 \pm 4.4	0.29 - 0.58	0.42 \pm 0.1	0.29 - 0.58	0.42 \pm 0.1
Sulfaclozine	0.25 - 0.48	0.35 \pm 0.08	0.34 - 0.67	0.48 \pm 0.12	0.34 - 0.67	0.48 \pm 0.12
Sulfadoxine	0.54 - 1	0.75 \pm 0.16	0.74 - 1.5	1.1 \pm 0.25	0.74 - 1.5	1.1 \pm 0.25
Sulfamonomethoxine	0.33 - 0.63	0.46 \pm 0.1	0.45 - 0.89	0.64 \pm 0.16	0.45 - 0.89	0.64 \pm 0.16
Sulfanitran	0.43 - 0.83	0.61 \pm 0.13	0.59 - 1.2	0.84 \pm 0.2	0.59 - 1.2	0.84 \pm 0.2
Sulfaquinoxaline	0.29 - 29	9.6 \pm 14	0.4 - 0.8	0.57 \pm 0.14	0.4 - 0.8	0.57 \pm 0.14
Tilmicosin	0.75 - 1.4	1.1 \pm 0.23	1 - 2	1.5 \pm 0.36	1 - 2	1.5 \pm 0.36
X-ray contrast medium						
Iopromide	554 - 13,939	5,596 \pm 4,475	403 - 7,897	5,100 \pm 2,591	0.36 - 465	115 \pm 180

Text S7. Removal of key OMPs according to their properties.

The removal of OMPs found in wastewater greatly depends on the treatment configuration, operational conditions adopted in the bioreactor as well as the OMP physicochemical properties. Limiting the attention to the latter, it is well known the parameters involved in the removal are manyfold, and that the OMP charge and lipophilicity play an important role in hybrid systems such as a MBR coupled to PAC (Gutiérrez et al., 2022). At the range of pH in which the wastewater is commonly found, most of the OMPs of the current study are found to be in their ionic form (Table S3 and S4), which, to a certain degree, determines the interaction with the mixed liquor and the activated carbon. Besides, the octanol-water dissociation constant (D_{ow}), that is considered the effective hydrophobicity, is also fundamental in determining the predisposition of a substance to be sorbed into the activated carbon or in the sludge (Martínez-Alcalá et al., 2021).

In Figure S3, the average removal efficiencies of the key OMPs obtained in the 0.2PAC campaign are depicted with respect to their prevalent charge and $\log D_{ow}$ at pH = 7. Roughly speaking, cationic compounds containing aromatic rings exhibited better overall removal efficiencies and, in particular, the range of variability was reduced for those with $\log D_{ow} > 1$. In a previous study, the charge was found to be positively correlated with the removal of OMPs in hybrid MBRs coupled to PAC inside the bioreactor (Gutiérrez et al., 2022). As explained in many studies, among them Sipma et al., (2010) and Maillet et al., (2015), the PAC covered by organic matter from the mixed liquor acquires an overall negative surface charge that promotes positive

electrostatic interactions between the cationic compounds and surface of the adsorbent. However, other OMP properties may also influence the removal. For instance, the functional groups responsible for the electrostatic interaction between the OMPs and the surface of the activated carbon are not completely understood and are still under investigation, which may explain the unexpected behavior of certain charged compounds (Kovalova et al., 2013; Reif et al., 2023).

In the absence of adsorption mechanisms, the lipophilicity of the compounds may take the leading role in determining the tendency of an OMP to be sorbed to the activated carbon (with attached DOM) (de Ridder et al., 2011; Kovalova et al., 2013; Mailler et al., 2015). For the key OMPs, this fact did not occur. Uncharged compounds (among them, caffeine and iopromide) showed good overall removal efficiencies, whereas anionic compounds (e.g., ibuprofen and sulfamethoxazole) presented high variability. Since many other OMP parameters (e.g., molecular weight, presence of H-bonds and structure, etc.) as well as real wastewater characteristics, such as OMP load, seasonality and deconjugation of the metabolites, may influence the removal, the expected results may be shifted to a certain extent. Overall, the observed trends are in accordance with previous trends in the literature. However, it must be noted that the prediction of the removal in such a complex water matrix is not as accurate as it is in the case of PAC is used as a post-treatment (Kovalova et al., 2013).

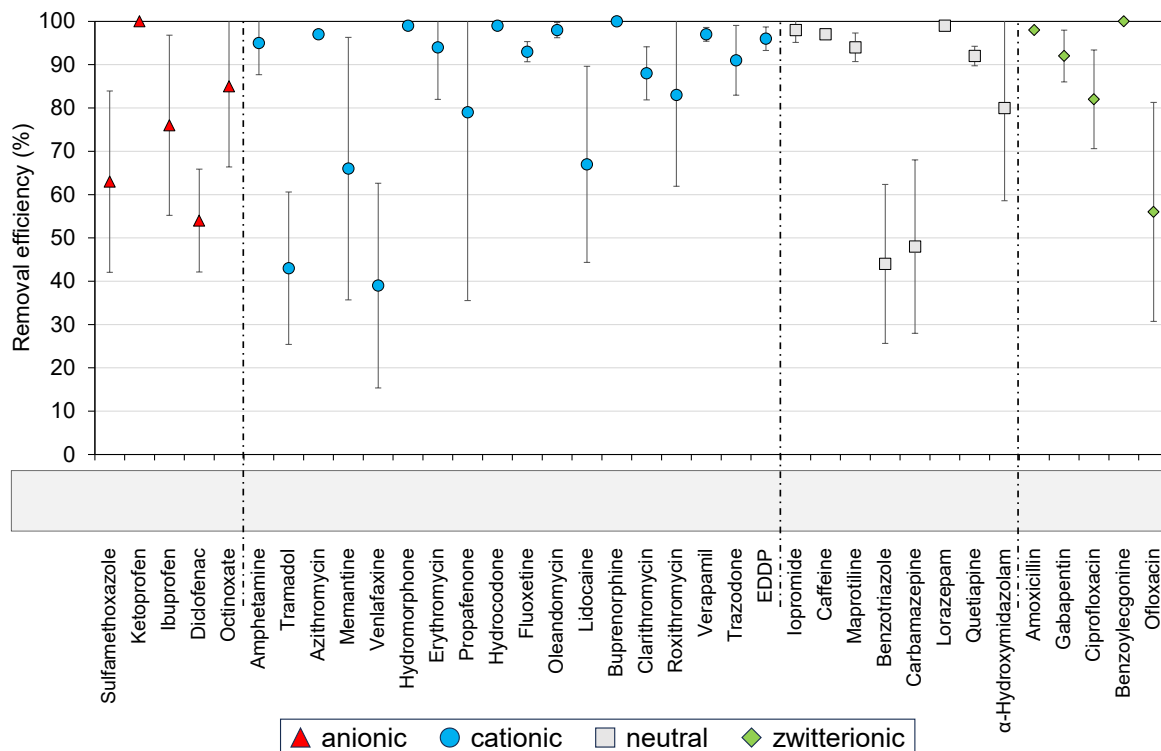


Figure S3. Average removal efficiencies and standard deviation during the 0.2PAC campaign of key OMPs, grouped by their prevalent charge and in increasing order according to their $\log D_{ow}$ at pH = 7.

Text S8. Removal of OMP classes.

The following analysis refers to the OMP classes, and the considerations regard set of compounds belonging to each of the classes, irrespective of the behavior of the single OMP which may differ from the class behavior. Bearing this in mind, the average removal efficiencies of the 20 OMP classes are displayed in Table S21, which refers to the whole list of target OMPs, with four exceptions. This is the case of nitrofurantoin (antiseptic), hydrocortisone (hormone), triamcinolone acetonide (hormone) and metoprolol (beta-blocker). They were discarded since they presented persistent negative and/or highly variably removals and significantly shifted the average removal of the class they pertain to (corresponding to those with a star in Table S21). In addition to these, three additional classes, i.e., antifungals, antihistamines and diuretics, did not have any compound over the LOD during the three campaigns, and thus the corresponding removal could not be calculated. Compounds pertaining to antihypertensives and receptor antagonist classes were only detected during the 0.1PAC campaign, and thus no comparison between the campaigns could be made.

No clear effect of the removal of analgesics/anti-inflammatories, beta-blockers, calcium channel blockers, UV filters and X-ray contrast media was shown due to the PAC addition into the MBR. They all presented very high removal efficiencies in MBR (> 90%), and thus the potential increase in their removal due to PAC addition is not significant. Furthermore, the effect of PAC on analgesics/anti-inflammatories depends on the compound analyzed, which is not the case for the other classes mentioned, including only one or two compounds. Benzotriazole was the compound that mainly influenced the significant decrease in the removal efficiencies obtained in the plastic additives class, since the other compound, *p*-toluenesulfonamide, had a low frequency of detection.

Except for the above-mentioned classes, the eight remaining ones (antiarrhythmic agents, antibiotics, antiparasitics, hormones, illicit drugs, psychiatric drugs, stimulants and veterinary drugs) increased their removal efficiencies during PAC campaigns and, in most cases, a positive correlation with the PAC dosage was observed. Four of these OMP classes contribute the most to the OMP load in the WWTP (Table S9, Figure S4A), and their removals increased between 10% and 35% during the PAC treatment. On the other hand, although the analgesics/anti-inflammatories class had the highest loads in the INF, the high removal efficiencies obtained in the three experimental campaigns significantly reduced their contribution to the load in the MBRperm (Figure S4B) compared to other classes. The same applies for X-ray contrast media, for which the contribution to the MBRperm load accounts for only between 0.4% and 3%. Apart from analgesics/anti-inflammatories, the MBRperm load therefore constituted of mainly antibiotics, psychiatric drugs and plastic additives, due to the high load of certain OMPs which presented low removals (e.g., ofloxacin and benzotriazole) despite the addition of activated carbon.

Table S21. Average removal efficiencies of the main classes of target OMPs analyzed in this study per experimental campaign. *m* represents the number of values (i.e., daily removal efficiencies) used to calculate the average. In brackets, the number of OMPs pertaining to each class. Classes with an * symbol do not consider all the OMPs pertaining to that class when calculating the removal. SD: standard deviation.

	noPAC		0.1PAC		0.2PAC	
	<i>m</i>	Average ± SD (%)	<i>m</i>	Average ± SD (%)	<i>m</i>	Average ± SD (%)
Analgesics/anti-inflammatories (39)	2	90 ± 2	8	87 ± 8	6	92 ± 3
Antiarrhythmic agents (5)	2	51 ± 7	8	74 ± 15	6	83 ± 41
Antibiotics (41)	2	59 ± 11	8	74 ± 9	6	82 ± 5
Antifungals (3)	0	–	0	–	0	–
Antihistamines (2)	0	–	0	–	0	–
Antihypertensive (1)	0	–	4	91 ± 2	0	–
Antiparasitics (6)	2	69 ± 24	7	85 ± 10	3	99.99
Antiseptic (1)*	0	–	0	–	0	–
Beta-blockers* (3)	2	98	8	96 ± 1	6	97 ± 2
Calcium channel blocker (1)	2	98 ± 1	7	99	5	99.99
Diuretic (1)	0	–	0	–	0	–
Hormones (9) *	2	41 ± 15	4	64 ± 29	0	–
Illicit drugs (13)	2	71 ± 3	8	83 ± 7	4	81 ± 22
Plastic additives (2)	2	85 ± 9	8	58 ± 9	6	44 ± 18
Psychiatric drugs (76)	2	48 ± 3	8	76 ± 7	6	83 ± 9
Receptor antagonists (2)	0	–	1	81	0	–
Stimulants (3)	2	68 ± 6	8	80 ± 16	6	98 ± 1
UV filter (1)	2	96 ± 4	8	99 ± 2	5	86 ± 20
Veterinary drugs (22)	2	72 ± 23	8	74 ± 8	5	86 ± 9
X-ray contrast medium (1)	2	99 ± 2	8	87 ± 18	6	98 ± 3

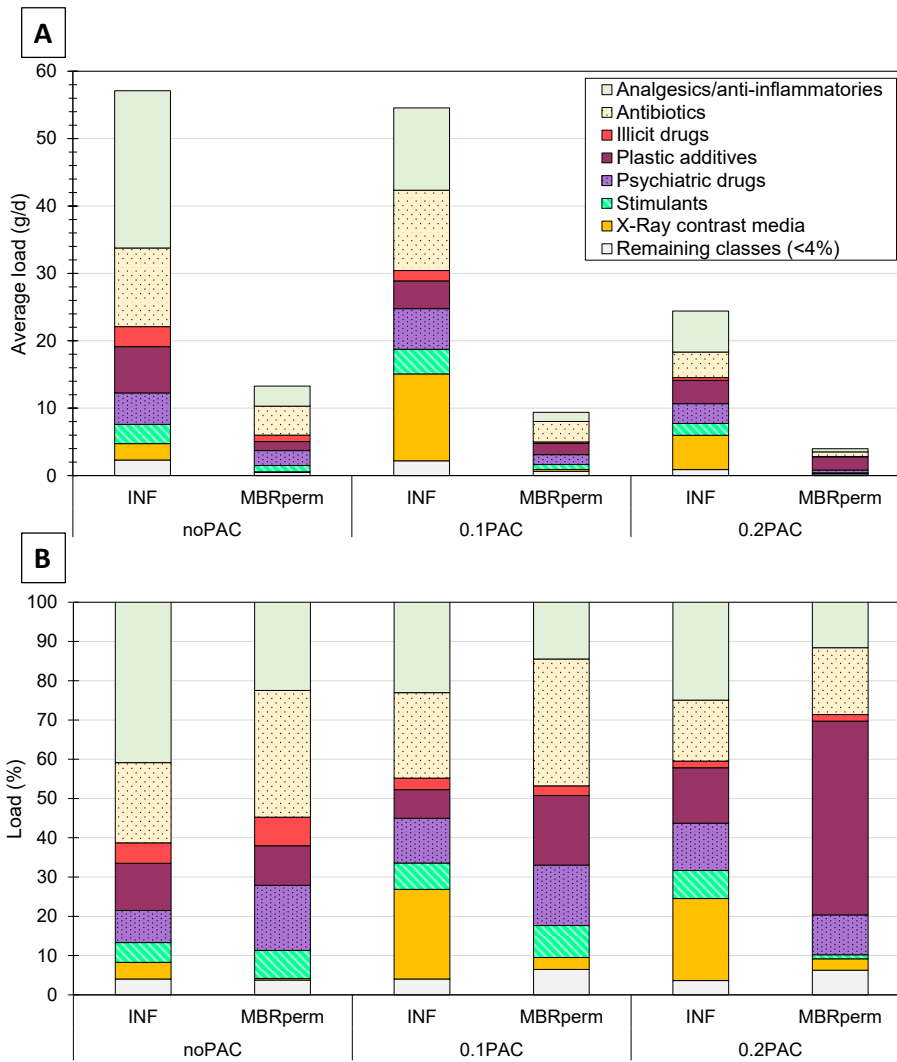


Figure S4. Average load of the main OMP classes (A) and contribution (%) of their loads (B) to the total one in the INF and MBRperm during the noPAC, 0.1PAC and 0.2PAC campaigns.

Text S9. Overall OMP load reduction.

As shown in Figure S5, the average load of OMPs reduced from 171 g/d in the INF to 27 g/d in the MBRperm during the noPAC campaign, from 441 g/d to 85 g/d during 0.1PAC and from 147 g/d to 24 g/d during 0.2PAC, which correspond to 80%, 81% and 84% of the average removal, respectively. Although the average removal was only increased by 4% with the highest dosage of PAC tested, a significant reduction for certain OMPs and OMP classes was described in the above sections, which may have a positive effect on the reduction of the environmental risk which will be discussed in section 3.5.

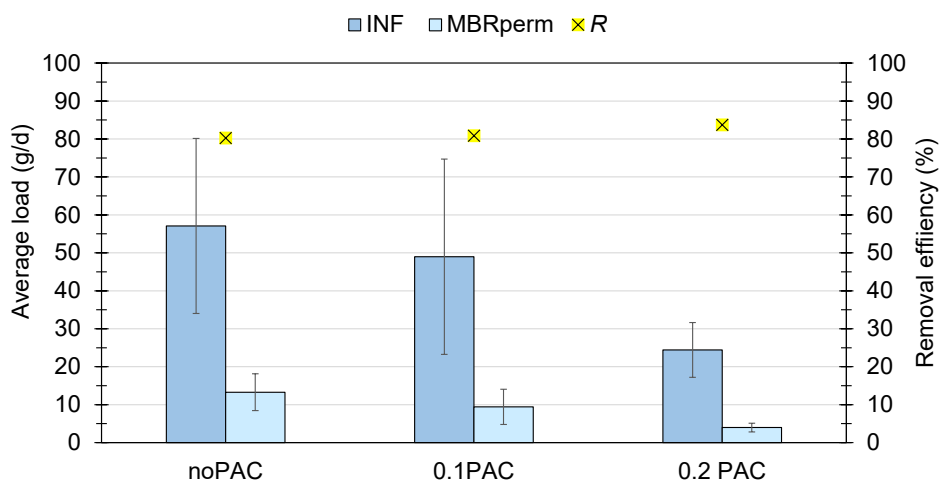


Figure S5. Average load of all target OMPs in the INF and MBRperm in each experimental campaign and corresponding removal efficiencies *R* (%).

Table S22. Frequency of detection and removal efficiencies in the MBRperm of the 90 non-target OMPs in the three experimental periods (i.e., noPAC, 0.1PAC and 0.2PAC), classified by class. Frequency of detection in HWW and INF consider the three experimental periods together. m is the number of values of removal efficiency taken into consideration to calculate the average. The transformation products are written in italics. SD: Standard deviation.

Compound	noPAC			0.1PAC			0.2PAC				
	HWW	INF	MBRperm	MBRperm		MBRperm		MBRperm			
	Freq (%)	Freq (%)	m Freq (%) Av. \pm SD (%)	m Freq (%) Av. \pm SD (%)	m Freq (%) Av. \pm SD (%)						
Analgesics/anti-inflammatories											
<i>2,6-Xylidine / Lidocaine-M / Dimethylaniline</i>	100	100	2	100	94 \pm 8	8	100	98 \pm 2	6	100	98 \pm 2
Azelastine	0	72	0	100	--	0	100	--	0	100	--
Benzocaine	100	100	2	100	93 \pm 7	6	100	64 \pm 37	6	100	87 \pm 10
<i>Depropionylbezitramide</i>	100	100	2	100	91 \pm 4	8	100	91 \pm 4	6	100	89 \pm 4
<i>Dimethylaminophenazone</i>	41	44	1	0	99.99	5	0	99.99	0	0	n.d.
Fenoprofen	94	83	2	0	99.99	8	22	99 \pm 3	3	0	99.99
Metaxalone	88	94	1	100	11	5	100	72 \pm 33	2	83	37 \pm 46
Niflumic acid	41	44	1	0	99.99	5	44	65 \pm 34	0	0	n.d.
Parsalimide	100	100	2	0	99.99	8	0	99.99	6	0	99.99
Propacetamol	82	89	2	0	99.99	6	0	99.99	6	100	79 \pm 12
Tapentadol	100	100	1	100	8	7	100	52 \pm 22	6	100	66 \pm 11
<i>Tramadol-N-oxide</i>	100	100	2	100	58 \pm 44	7	100	88 \pm 7	6	100	92 \pm 7
Antiacids											
Lansoprazole	100	100	2	100	97 \pm 2	8	78	99 \pm 1	6	17	99 \pm 3
Omeprazole	100	100	2	100	86 \pm 5	8	100	90 \pm 5	6	17	99 \pm 2
Troxipide	100	100	2	100	97 \pm 0	8	56	98 \pm 2	6	17	100 \pm 1
Antiarrhythmic agent											
Flecainide	100	100	0	100	--	8	100	45 \pm 15	6	100	43 \pm 19
Antibiotics											
<i>2-Hydroxyquinoline</i>	100	100	2	100	93 \pm 7	8	100	91 \pm 3	6	100	97 \pm 2
<i>Azithromycin 3'-N-oxide</i>	6	6	0	100	--	0	100	--	1	83	37
<i>Azithromycin N'-(Desmethyl)</i>	100	100	2	100	71 \pm 14	8	100	88 \pm 13	4	100	28 \pm 39
Cefalexin	100	100	2	100	97 \pm 2	8	89	99 \pm 1	6	17	99 \pm 3
Cefoxitin	88	89	2	100	29 \pm 27	6	100	50 \pm 35	4	17	91 \pm 17
<i>Clarithromycin-N-oxide</i>	100	100	2	100	88 \pm 8	8	100	85 \pm 6	6	100	94 \pm 5
<i>Erythromycin A enol ether</i>	100	100	2	100	73 \pm 17	8	100	94 \pm 4	5	100	84 \pm 10
Gatifloxacin	88	83	1	100	7	8	100	54 \pm 17	3	0	99.99
Moxifloxacin	76	67	1	100	40	7	89	52 \pm 28	3	17	91 \pm 16
N4-Acetylsulfamethoxazole	100	100	2	100	91 \pm 3	8	89	93 \pm 7	6	100	93 \pm 4
Pazufloxacin	65	67	0	100	--	3	89	78 \pm 7	2	50	58 \pm 59
Rifaximin	88	83	2	0	99.99	8	0	99.99	3	0	99.99
Anti-cancer drugs											
Cyclophosphamide	65	67	0	100	--	4	100	33 \pm 30	0	0	n.d.
Cytarabine	65	72	2	100	84 \pm 20	8	100	79 \pm 18	1	67	64
Flutamide	100	94	2	100	98 \pm 1	8	44	99 \pm 2	5	0	99.99
Lapatinib	76	78	2	0	99.99	8	0	99.99	2	0	99.99
Antidiabetic drugs											
Metformin	100	100	2	100	84 \pm 7	8	100	86 \pm 9	6	100	84 \pm 11
Sitagliptin	94	100	2	0	99.99	8	89	81 \pm 12	6	50	91 \pm 11

Table S22. (continued)

Compound	noPAC						0.1PAC			0.2PAC		
	HWW	INF	MBRperm			MBRperm			MBRperm			
	Freq (%)	Freq (%)	m	Freq (%)	Av. \pm SD (%)	m	Freq (%)	Av. \pm SD (%)	m	Freq (%)	Av. \pm SD (%)	
Antiemetic												
Metoclopramide	100	100	2	100	56 \pm 22	8	100	86 \pm 8	6	100	81 \pm 8	
Antigout preparation												
Allopurinol	94	89	2	100	99 \pm 1	8	100	96 \pm 2	3	83	91 \pm 5	
Antihistamine												
Fexofenadine	65	72	2	50	95 \pm 7	3	0	99.99	6	67	92 \pm 9	
Antihypertensives												
Candesartan	65	56	0	100	--	1	89	21	0	0	n.d.	
Irbesartan	100	100	1	100	8	3	100	41 \pm 26	6	100	62 \pm 24	
Losartan	65	56	2	0	99.99	7	0	99.99	0	0	n.d.	
Nitrendipin	100	100	2	100	39 \pm 8	8	100	63 \pm 22	6	100	84 \pm 6	
Olmesartan	100	100	0	100	--	3	100	15 \pm 3	6	100	29 \pm 11	
Sotalol	100	100	2	100	30 \pm 0	8	100	35 \pm 24	6	100	77 \pm 9	
Telmisartan	100	100	1	100	28	8	100	51 \pm 28	6	100	63 \pm 30	
Valsartan	100	100	2	100	97 \pm 0	8	89	86 \pm 9	6	0	99.99	
Antiparasitic												
Hydroxychloroquine	100	83	2	0	99.99	8	0	99.99	3	0	99.99	
Antiseptics												
4-Chloroaniline	94	50	0	0	n.d.	3	67	99.99	4	0	99.99	
Chlorhexidine	100	83	2	0	99.99	8	0	99.99	3	0	99.99	
Antithrombotics												
Clopidogrel	100	100	2	100	57 \pm 27	8	89	71 \pm 16	6	67	78 \pm 21	
Dabigatran	100	100	2	100	18 \pm 0	8	100	45 \pm 25	6	100	58 \pm 21	
Beta-blockers												
<i>Desacetylmepipranolol</i>	100	100	2	100	74 \pm 0	8	100	80 \pm 10	6	100	81 \pm 15	
<i>Metoprolol acid</i>	100	100	2	100	86 \pm 3	8	100	82 \pm 5	6	100	93 \pm 5	
Bronchodilators												
Terbutaline	100	100	0	100	--	4	89	86 \pm 13	1	100	53	
Theophylline	100	100	2	100	91 \pm 11	8	100	96 \pm 2	6	17	100 \pm 1	
Food additives												
Methylsalicylate	100	100	2	100	20 \pm 8	8	100	37 \pm 16	5	17	99.99	
Triethyl citrate	82	83	2	100	81 \pm 13	8	100	50 \pm 26	3	0	99.99	
Hormones												
Boldione	76	83	2	0	99.99	7	0	99.99	5	0	99.99	
Paramethasone acetate	100	94	1	100	9	0	100	--	2	83	76 \pm 35	
Illicit drug												
<i>Norcocaine</i>	100	100	2	50	99 \pm 1	8	78	98 \pm 2	6	0	99.99	
Lipid regulators												
Atorvastatin	100	100	2	0	99.99	8	0	99.99	6	0	99.99	
Bezafibrate	100	94	2	0	99.99	8	0	99.99	5	0	99.99	
Other												
1,2-Benzisothiazolinone	100	100	1	100	69	5	100	70 \pm 27	6	17	97 \pm 7	
1-Methylimidazole	100	100	1	100	6	4	100	56 \pm 46	6	83	86 \pm 17	
1-Naphthylamine	100	100	2	100	99 \pm 1	8	100	100 \pm 0	6	17	95 \pm 12	
2,2'-Oxamido bis-[ethyl-3-(3,5-di-t-butyl-4-hydroxyphenyl) propionate	100	100	2	100	90 \pm 2	8	100	92 \pm 4	6	100	87 \pm 3	

Table S22. (continued)

Compound	noPAC														
	HWW			INF			noPAC			0.1PAC			0.2PAC		
	Freq (%)	Freq (%)	m	Freq (%)	Av. \pm SD (%)	m	Freq (%)	Av. \pm SD (%)	m	Freq (%)	Av. \pm SD (%)	m	Freq (%)	Av. \pm SD (%)	
Indole	100	100	2	100	94 \pm 7	8	100	93 \pm 2	6	67	86 \pm 25				
MIT / Methylisothiazolinone	71	72	2	100	22 \pm 7	2	100	61 \pm 15	2	83	77 \pm 11				
NDEA / Nitrosodiethylamine	53	89	2	0	99.99	6	0	99.99	6	0	99.99				
Nicopholine	100	100	2	100	99 \pm 0	8	100	99 \pm 0	6	100	98 \pm 1				
Picaridin / Bayrepel / Icaridin	65	56	2	100	93 \pm 8	7	89	94 \pm 8	0	0	n.d.				
Pesticide															
DEET / Diethyltoluamide	100	100	2	100	73 \pm 15	7	100	81 \pm 8	6	100	85 \pm 6				
Plastic additive															
5-Methyl-1H-benzotriazole	100	100	2	100	76 \pm 3	7	100	67 \pm 17	6	100	69 \pm 11				
Psychiatric drugs															
10,11-Dihydro-10-hydroxycarbamazepine	88	94	2	100	88 \pm 1	8	89	84 \pm 10	5	0	99.99				
Acridine / Carbamazepine-M	100	100	1	100	3	3	100	26 \pm 33	5	100	21 \pm 17				
Carbamazepine 10,11-epoxide	94	100	1	100	9	6	100	35 \pm 30	6	100	61 \pm 9				
Levetiracetam	100	100	2	100	27 \pm 24	8	100	39 \pm 31	6	0	99.99				
Norcitalopram / Desmethylcitalopram	88	89	0	100	--	7	100	44 \pm 18	3	67	22 \pm 28				
Pregabalin	100	100	2	100	98 \pm 1	8	100	98 \pm 1	6	100	76 \pm 19				
Propyprone	100	100	2	100	88 \pm 4	8	100	87 \pm 5	6	100	86 \pm 2				
Sulpiride	100	100	0	100	--	7	100	57 \pm 26	6	100	59 \pm 24				
Stimulants															
3-Hydroxycotinine	100	100	2	100	99 \pm 0	8	100	99 \pm 1	6	100	99 \pm 1				
Nicotine	100	100	2	100	83 \pm 1	8	100	85 \pm 13	6	100	97 \pm 3				
Paraxanthine	100	100	2	100	91 \pm 11	8	100	96 \pm 2	6	17	99 \pm 4				
Theobromine	100	100	2	100	93 \pm 8	8	100	94 \pm 3	6	83	99 \pm 1				
Synthetic musks															
AHDI / Phantolide	82	72	2	100	73 \pm 33	8	89	92 \pm 10	1	0	99.99				
Celestolide	76	78	2	100	76 \pm 29	8	89	92 \pm 10	2	0	99.99				
UV filter															
Dioxybenzone / Benzophenone-8	100	100	2	100	15 \pm 12	8	100	46 \pm 22	6	100	68 \pm 11				
X-ray contrast media															
Diatrizoate / Amidotrizoic acid	100	100	0	100	--	1	100	25	3	100	17 \pm 22				
Iohexol	100	100	2	100	98 \pm 2	8	100	97 \pm 1	6	100	96 \pm 6				
Iopamidol	100	100	0	100	--	2	100	4 \pm 5	0	100	--				

Legend

“n.d.” indicates that the OMP is non-detected in both INF and MBRperm.

“--” indicates whether the average removal efficiency is negative or the OMP is not detected in the INF (MBRperm signal > INF signal)

Table S23. Scores assigned to Frequency F and persistence P, bioaccumulation B and toxicity T criteria to the 90 non-target OMPs in the MBRperm, as well as the final scores S attributed to each of them during noPAC, 0.1PAC and 0.2PAC campaigns.

Name	noPAC		0.1PAC		0.2PAC		B	T	FPBT final score S		
	F	P	F	P	F	P			noPAC	0.1PAC	0.2PAC
Analgesics/anti-inflammatories											
<i>2,6-Xylidine / Lidocaine-M / Dimethylaniline</i>	5	1	5	1	5	1	2	2	10	10	10
Azelastine	5	5	5	5	5	5	4	5	19	19	19
Benzocaine	5	1	5	2	5	1	2	5	13	14	13
<i>Depropionylbezitramide</i>	5	1	5	1	5	1	4	5	15	15	15
<i>Dimethylaminophenazone</i>	1	1	1	1	1	3	1	2	5	5	7
Fenoprofen	1	1	2	1	1	1	4	3	9	10	9
Metaxalone	5	5	5	2	5	4	2	2	14	11	13
Niflumic acid	1	1	3	2	1	3	4	4	10	13	12
Parsalmide	1	1	1	1	1	1	2	3	7	7	7
Propacetamol	1	1	1	1	5	2	2	3	7	7	12
Tapentadol	5	5	5	3	5	2	4	5	19	17	16
<i>Tramadol-N-oxide</i>	5	3	5	1	5	1	1	2	11	9	9
Antiacids											
Lansoprazole	5	1	4	1	1	1	3	4	13	12	9
Omeprazole	5	1	5	1	1	1	3	5	14	14	10
Troxipide	5	1	3	1	1	1	2	5	13	11	9
Antiarrhythmic agent											
Flecainide	5	5	5	3	5	3	4	4	18	16	16
Antibiotics											
<i>2-Hydroxyquinoline</i>	5	1	5	1	5	1	2	3	11	11	11
<i>Azithromycin 3'-N-oxide</i>	5	5	5	5	5	4	1	5	16	16	15
<i>Azithromycin N'-(Desmethyl)</i>	5	2	5	1	5	4	2	5	14	13	16
Cefalexin	5	1	5	1	1	1	1	3	10	10	6
Cefoxitin	5	4	5	3	1	1	1	3	13	12	6
<i>Clarithromycin-N-oxide</i>	5	1	5	1	5	1	1	3	10	10	10
<i>Erythromycin A enol ether</i>	5	2	5	1	5	1	4	5	16	15	15
Gatifloxacin	5	5	5	3	1	1	3	4	17	15	9
Moxifloxacin	5	3	5	3	1	1	3	5	16	16	10
N4-Acetylsulfamethoxazole	5	1	5	1	5	1	1	3	10	10	10
Pazufloxacin	5	5	5	2	3	3	1	3	14	11	10
Rifaximin	1	1	1	1	1	1	4	5	11	11	11
Anti-cancer drugs											
Cyclophosphamide	5	5	5	4	1	3	1	3	14	13	8
Cytarabine	5	1	5	2	4	2	1	2	9	10	9
Flutamide	5	1	3	1	1	1	4	3	13	11	9
Lapatinib	1	1	1	1	1	1	5	5	12	12	12
Antidiabetic drugs											
Metformin	5	1	5	1	5	1	1	5	12	12	12
Sitagliptin	1	1	5	1	3	1	3	5	10	14	12
Antiemetic											
Metoclopramide	5	3	5	1	5	1	3	3	14	12	12
Antigout preparation											
Allopurinol	5	1	5	1	5	1	1	2	9	9	9

Table S23. (continued)

Name	noPAC		0.1PAC		0.2PAC		B T		FPBT final score S		
	F	P	F	P	F	P	B	T	noPAC	0.1PAC	0.2PAC
Antihistamine											
Fexofenadine	3	1	1	1	4	1	4	5	13	11	14
Antihypertensives											
Candesartan	5	5	5	4	1	3	5	5	20	19	14
Irbesartan	5	5	5	3	5	2	5	5	20	18	17
Losartan	1	1	1	1	1	3	4	5	11	11	13
Nitrendipin	5	4	5	2	5	1	4	5	18	16	15
Olmesartan	5	5	5	5	5	4	3	5	18	18	17
Sotalol	5	4	5	4	5	2	1	3	13	13	11
Telmisartan	5	4	5	3	5	2	5	5	19	18	17
Valsartan	5	1	5	1	1	1	4	5	15	15	11
Antiparasitic											
Hydroxychloroquine	1	1	1	1	1	1	4	5	11	11	11
Antiseptics											
4-Chloroaniline	1	3	4	1	1	1	2	5	11	12	9
Chlorhexidine	1	1	1	1	1	1	5	5	12	12	12
Antithrombotics											
Clopidogrel	5	3	5	2	4	2	3	5	16	15	14
Dabigatran	5	5	5	3	5	3	2	5	17	15	15
Beta-blockers											
<i>Desacetylmepipranolol</i>	5	2	5	2	5	1	2	5	14	14	13
<i>Metoprolol acid</i>	5	1	5	1	5	1	1	2	9	9	9
Bronchodilators											
Terbutaline	5	5	5	1	5	3	1	5	16	12	14
Theophylline	5	1	5	1	1	1	1	2	9	9	5
Food additives											
Methylsalicylate	5	4	5	4	1	1	3	2	14	14	7
Triethyl citrate	5	1	5	3	1	1	2	2	10	12	6
Hormones											
Boldione	1	1	1	1	1	1	3	3	8	8	8
Paramethasone acetate	5	5	5	5	5	2	3	3	16	16	13
Illicit drug											
<i>Norcocaine</i>	3	1	4	1	1	1	2	3	9	10	7
Lipid regulators											
Atorvastatin	1	1	1	1	1	1	4	5	11	11	11
Bezafibrate	1	1	1	1	1	1	3	5	10	10	10
Other											
1,2-Benzisothiazolinone	5	2	5	2	1	1	2	3	12	12	7
1-Methylimidazole	5	5	5	3	5	1	1	2	13	11	9
1-Naphthylamine	5	1	5	1	1	1	3	4	13	13	9
2,2'-Oxamido bis-[ethyl-3-(3,5-di-t-butyl-4-hydroxyphenyl) propionate	5	1	5	1	5	1	5	3	14	14	14
Indole	5	1	5	1	4	1	3	3	12	12	11
MIT / Methylisothiazolinone	5	4	5	2	5	2	1	5	15	13	13
NDEA / Nitrosodiethylamine	1	1	1	1	1	1	1	2	5	5	5
Nicopholine	5	1	5	1	5	1	1	2	9	9	9
Picaridin / Bayrepel / Icaridin	5	1	5	1	1	3	2	5	13	13	11

Table S23. (continued)

Name	noPAC		0.1PAC		0.2PAC		B T		FPBT final score S		
	F	P	F	P	F	P	B	T	noPAC	0.1PAC	0.2PAC
Pesticides											
DEET / Diethyltoluamide	5	2	5	1	5	1	3	5	15	14	14
Plastic additives											
5-Methyl-1H-benzotriazole	5	2	5	2	5	2	2	5	14	14	14
Psychiatric drugs											
10,11-Dihydro-10-hydroxycarbamazepine	5	1	5	1	1	1	1	5	12	12	8
Acridine / Carbamazepine-M	5	5	5	4	5	4	4	4	18	17	17
Carbamazepine 10,11-epoxide	5	5	5	4	5	2	1	3	14	13	11
Levetiracetam	5	4	5	4	1	1	1	2	12	12	5
Norcitalopram / Desmethycitalopram	5	5	5	3	4	4	3	4	17	15	15
Pregabalin	5	1	5	1	5	2	2	5	13	13	14
Propyperone	5	1	5	1	5	1	4	5	15	15	15
Sulpiride	5	5	5	3	5	3	1	3	14	12	12
Stimulants											
3-Hydroxycotinine	5	1	5	1	5	1	1	3	10	10	10
Nicotine	5	1	5	1	5	1	1	5	12	12	12
Paraxanthine	5	1	5	1	1	1	1	2	9	9	5
Theobromine	5	1	5	1	5	1	1	5	12	12	12
Synthetic musks											
AHDI / Phantolide	5	2	5	1	1	1	5	5	17	16	12
Celestolide	5	2	5	1	1	1	4	5	16	15	11
UV filter											
Dioxybenzone / Benzophenone-8	5	5	5	3	5	2	4	4	18	16	15
X-ray contrast media											
Diatrizoate / Amidotrizoic acid	5	5	5	4	5	5	1	5	16	15	16
Iohexol	5	1	5	1	5	1	1	4	11	11	11
Iopamidol	5	5	5	5	5	5	1	5	16	16	16

Table S24. Range of variability and average concentration of target OMPs in the EFF during the noPAC and 0.1PAC campaigns, together with their \overline{RQ} values. At the end of the table, values of RQ_{mix} for the 232 target OMPs and 40 key OMPs¹ during noPAC and 0.1PAC campaigns. In red, $\overline{RQ} > 1$ (high risk). The transformation products are written in italics. SD: standard deviation.

Compound	noPAC			0.1PAC		
	Range (µg/L)	Average ± SD (µg/L)	\overline{RQ} EFF	Range (µg/L)	Average ± SD (µg/L)	\overline{RQ} EFF
Analgesics/anti-inflammatories						
<i>4-Acetylaminoantipyrine</i>	0.008 - 0.062	0.035 ± 0.027	3.46·10 ⁻⁴	0.013 - 0.103	0.043 ± 0.033	4.35·10 ⁻⁴
<i>4-Formylaminoantipyrine</i>	0.012 - 0.07	0.035 ± 0.031	3.49·10 ⁻⁵	<LOD - 0.079	0.035 ± 0.027	3.50·10 ⁻⁵
<i>6-Acetylmorphine</i>	0.007 - 0.013	0.009 ± 0.003	1.78·10 ⁻³	<LOD	<LOD	1.28·10 ⁻⁴
Acetaminophen	0.03 - 0.037	0.033 ± 0.003	2.48·10 ⁻⁴	<LOD - 0.065	0.038 ± 0.019	2.80·10 ⁻⁴
<i>Acetylcodeine</i>	<LOD	<LOD	8.65·10 ⁻⁴	<LOD - 0.012	0.004 ± 0.005	3.54·10 ⁻³
Acetylsalicylic acid	0.056 - 0.68	0.452 ± 0.345	2.44·10 ⁻²	0.126 - 0.547	0.245 ± 0.144	1.33·10 ⁻²
Alfentanil	<LOD - 0.005	0.002 ± 0.003	1.06·10 ⁻²	<LOD	<LOD	2.23·10 ⁻³
Aminopyrine	<LOD	<LOD	1.08·10 ⁻⁴	<LOD	<LOD	1.08·10 ⁻⁴
Betamethasone 17,21-dipropionate	<LOD	<LOD	4.36·10 ⁻⁴	<LOD - 0.028	0.004 ± 0.009	1.45·10 ⁻³
Buprenorphine	<LOD - 0.023	0.009 ± 0.013	3.90·10 ⁻²	<LOD - 0.046	0.02 ± 0.017	8.79·10 ⁻²
<i>Buprenorphine glucuronide</i>	<LOD - 0.15	0.051 ± 0.085	3.66·10 ⁻¹	<LOD	<LOD	1.33·10 ⁻²
Carisoprodol	<LOD - 0.257	0.133 ± 0.128	1.06·10 ⁻²	<LOD	<LOD	1.24·10 ⁻⁴
Codeine	<LOD - 0.037	0.021 ± 0.019	2.98·10 ⁻³	<LOD - 0.023	0.006 ± 0.008	8.55·10 ⁻⁴
Dextromethorphan	<LOD	<LOD	2.47·10 ⁻⁴	<LOD	<LOD	2.47·10 ⁻⁴
Dextropropoxyphene	<LOD	<LOD	5.72·10 ⁻³	<LOD	<LOD	5.72·10 ⁻³
Diclofenac	0.051 - 0.2	0.101 ± 0.086	2.02	0.036 - 0.188	0.11 ± 0.046	2.20
Etodolac	<LOD	<LOD	5.93·10 ⁻⁴	<LOD	<LOD	5.93·10 ⁻⁴
Fentanyl	<LOD	<LOD	3.24·10 ⁻³	<LOD	<LOD	3.24·10 ⁻³
Hydrocodone	<LOD - 0.03	0.012 ± 0.016	3.55·10 ⁻³	<LOD - 0.009	0.004 ± 0.003	1.15·10 ⁻³
Hydromorphone	<LOD - 0.004	0.002 ± 0.002	6.80·10 ⁻⁴	<LOD	<LOD	2.36·10 ⁻⁴
Ibuprofen	0.039 - 0.092	0.072 ± 0.029	7.23	0.021 - 0.121	0.087 ± 0.029	8.68
Ketoprofen	<LOD - 0.019	0.008 ± 0.01	3.72·10 ⁻³	<LOD - 0.054	0.03 ± 0.021	1.41·10 ⁻²
Lidocaine	0.074 - 0.269	0.193 ± 0.104	4.14·10 ⁻²	<LOD - 0.263	0.149 ± 0.082	3.19·10 ⁻²
Meloxicam	<LOD	<LOD	1.46·10 ⁻³	<LOD	<LOD	1.46·10 ⁻³
Morphine	<LOD	<LOD	1.60·10 ⁻⁴	<LOD	<LOD	1.60·10 ⁻⁴
<i>Morphine-6-β-D-glucuronide</i>	<LOD - 0.106	0.065 ± 0.056	3.01·10 ⁻²	<LOD - 0.201	0.023 ± 0.067	1.06·10 ⁻²
Naproxen	<LOD - 0.233	0.135 ± 0.12	7.43·10 ⁻²	<LOD	<LOD	3.26·10 ⁻⁴
<i>Norfentanyl</i>	0.046 - 0.065	0.056 ± 0.01	7.72·10 ⁻⁴	<LOD - 0.068	0.032 ± 0.022	4.36·10 ⁻⁴
<i>Norpethidine</i>	0.008 - 0.027	0.02 ± 0.01	6.85·10 ⁻⁴	<LOD - 0.024	0.012 ± 0.009	4.04·10 ⁻⁴
<i>Norpropoxyphene</i>	<LOD	<LOD	1.99·10 ⁻⁴	<LOD	<LOD	1.99·10 ⁻⁴
<i>O-Desmethyltramadol</i>	0.02 - 0.451	0.172 ± 0.242	1.70·10 ⁻²	0.011 - 0.389	0.102 ± 0.143	1.01·10 ⁻²
Oxycodone	<LOD - 0.01	0.004 ± 0.005	5.46·10 ⁻⁴	<LOD - 0.02	0.008 ± 0.007	1.03·10 ⁻³
Oxymorphone	<LOD	<LOD	2.13·10 ⁻⁴	<LOD - 0.012	0.005 ± 0.005	1.07·10 ⁻³
Pentazocine	<LOD	<LOD	1.24·10 ⁻³	<LOD	<LOD	1.24·10 ⁻³
Pethidine	<LOD - 0.012	0.004 ± 0.007	2.26·10 ⁻⁴	<LOD - 0.021	0.004 ± 0.007	2.12·10 ⁻⁴
Phenylbutazone	<LOD - 0.029	0.019 ± 0.016	1.75·10 ⁻²	<LOD - 0.017	0.004 ± 0.007	4.05·10 ⁻³
Procaine	<LOD - 0.013	0.008 ± 0.007	2.17·10 ⁻³	<LOD - 0.01	0.004 ± 0.004	1.06·10 ⁻³
Tolfenamic acid	<LOD	<LOD	3.40·10 ⁻³	<LOD	<LOD	3.40·10 ⁻³
Tramadol	0.141 - 0.489	0.33 ± 0.176	3.82·10 ⁻²	0.04 - 0.367	0.251 ± 0.097	2.90·10 ⁻²
Antiarrhythmic agents						
Amiodarone	<LOD	<LOD	1.23	<LOD - 0.005	<LOD	1.60

Table S24. (continued)

Compound	noPAC			0.1PAC		
	Range (µg/L)	Average ± SD (µg/L)	RQ EFF	Range (µg/L)	Average ± SD (µg/L)	RQ EFF
Digitoxin	<LOD	<LOD	3.50·10 ⁻³	<LOD	<LOD	3.50·10 ⁻³
Propafenone	<LOD - 0.026	0.015 ± 0.013	1.71·10 ⁻²	<LOD - 0.021	0.006 ± 0.007	6.50·10 ⁻³
Strophanthidin	<LOD	<LOD	3.43·10 ⁻⁵	<LOD	<LOD	3.43·10 ⁻⁵
Strophanthin	<LOD	<LOD	1.55·10 ⁻⁴	<LOD	<LOD	1.55·10 ⁻⁴
Antibiotics						
2-NP-AOZ	<LOD	<LOD	3.11·10 ⁻⁴	<LOD	<LOD	3.11·10 ⁻⁴
Amoxicillin	<LOD	<LOD	1.31·10 ⁻²	<LOD - 0.055	0.026 ± 0.02	3.36·10 ⁻¹
Azithromycin	0.013 - 0.058	0.035 ± 0.022	1.84	0.03 - 0.321	0.125 ± 0.092	6.58
Cinoxacin	<LOD - 0.017	0.008 ± 0.008	2.14·10 ⁻³	<LOD - 0.007	0.002 ± 0.003	6.66·10 ⁻⁴
Ciprofloxacin	0.093 - 0.58	0.366 ± 0.249	4.12	0.146 - 0.653	0.397 ± 0.164	4.46
Clarithromycin	0.008 - 0.036	0.023 ± 0.014	1.94·10 ⁻¹	<LOD - 0.075	0.028 ± 0.028	2.34·10 ⁻¹
Doxycycline	0.022 - 0.23	0.1 ± 0.113	2.17·10 ⁻¹	0.055 - 0.68	0.4 ± 0.2	8.69·10 ⁻¹
Enoxacin	<LOD - 0.073	0.043 ± 0.037	1.71·10 ⁻²	<LOD	<LOD	5.39·10 ⁻⁴
Erythromycin	<LOD - 0.174	0.072 ± 0.091	3.58·10 ⁻¹	<LOD - 0.216	0.07 ± 0.069	3.51·10 ⁻¹
Flumequine	<LOD	<LOD	6.09·10 ⁻⁴	<LOD	<LOD	6.09·10 ⁻⁴
Furazolidon	<LOD	<LOD	3.36·10 ⁻⁴	<LOD	<LOD	3.36·10 ⁻⁴
Lomefloxacin	0.05 - 0.202	0.143 ± 0.082	1.73·10 ⁻¹	<LOD - 0.098	0.061 ± 0.035	7.32·10 ⁻²
Metronidazole	0.016 - 0.053	0.04 ± 0.021	1.20·10 ⁻³	0.048 - 0.144	0.077 ± 0.031	2.32·10 ⁻³
Minocycline	<LOD	<LOD	4.23·10 ⁻²	<LOD - 0.041	0.01 ± 0.017	2.54·10 ⁻¹
Nalidixic Acid	<LOD - 0.043	0.016 ± 0.024	3.35·10 ⁻³	<LOD - 0.012	<LOD	6.27·10 ⁻⁴
Norfloxacin	<LOD	<LOD	1.56·10 ⁻³	<LOD - 0.013	0.003 ± 0.004	3.28·10 ⁻³
Ofloxacin	0.522 - 2.6	1.58 ± 1.039	11.3	0.428 - 1.504	1.063 ± 0.34	7.59
Oleandomycin	<LOD - 0.172	0.074 ± 0.088	8.56·10 ⁻²	<LOD - 0.179	0.067 ± 0.059	7.75·10 ⁻²
Oxolinic acid	<LOD	<LOD	5.00·10 ⁻⁵	<LOD	<LOD	5.00·10 ⁻⁵
Oxytetracycline	<LOD - 0.084	0.03 ± 0.047	9.23·10 ⁻²	<LOD - 0.157	0.056 ± 0.057	1.75·10 ⁻¹
Penicillin G	<LOD	<LOD	n.a.	<LOD	<LOD	n.a.
Pipemidic acid	<LOD	<LOD	1.70·10 ⁻³	<LOD	<LOD	1.70·10 ⁻³
Roxithromycin	<LOD - 0.127	0.046 ± 0.07	5.52·10 ⁻¹	<LOD - 0.231	0.062 ± 0.089	7.49·10 ⁻¹
Silvadene	<LOD	<LOD	2.49·10 ⁻⁴	<LOD - 0.456	0.052 ± 0.152	1.12·10 ⁻²
Spiramycin	<LOD - 0.1	0.036 ± 0.055	2.99·10 ⁻¹	<LOD - 0.123	0.027 ± 0.046	2.22·10 ⁻¹
Sulfabenzamide	<LOD - 0.975	0.326 ± 0.562	1.07·10 ⁻¹	<LOD - 1.697	0.878 ± 0.583	2.88·10 ⁻¹
Sulfadimethoxine	<LOD	<LOD	8.69·10 ⁻⁴	<LOD	<LOD	8.69·10 ⁻⁴
Sulfadimidine	<LOD	<LOD	8.79·10 ⁻⁴	<LOD - 0.02	0.003 ± 0.006	2.75·10 ⁻³
Sulfafurazole	<LOD	<LOD	4.11·10 ⁻⁴	<LOD	<LOD	4.11·10 ⁻⁴
Sulfaguanidine	<LOD	<LOD	6.72·10 ⁻⁵	<LOD	<LOD	6.72·10 ⁻⁵
Sulfamerazine	<LOD	<LOD	9.14·10 ⁻⁴	<LOD	<LOD	9.14·10 ⁻⁴
Sulfamethizole	<LOD	<LOD	1.25·10 ⁻³	<LOD	<LOD	1.25·10 ⁻³
Sulfamethoxazole	0.023 - 0.834	0.451 ± 0.407	7.52·10 ⁻¹	0.043 - 0.536	0.139 ± 0.153	2.31·10 ⁻¹
Sulfamethoxydiazine	<LOD	<LOD	1.85·10 ⁻³	<LOD	<LOD	1.85·10 ⁻³
Sulfamethoxypyridazine	<LOD	<LOD	4.06·10 ⁻⁴	<LOD	<LOD	4.06·10 ⁻⁴
Sulfanilamide	<LOD	<LOD	9.46·10 ⁻⁵	<LOD	<LOD	9.46·10 ⁻⁵
Sulfaphenazole	<LOD	<LOD	1.10·10 ⁻²	<LOD	<LOD	1.10·10 ⁻²
Sulfapyridine	<LOD - 0.025	0.011 ± 0.012	5.89·10 ⁻³	<LOD - 0.014	0.004 ± 0.005	1.93·10 ⁻³
Sulfathiazole	<LOD - 0.216	0.072 ± 0.124	3.77·10 ⁻²	<LOD - 0.499	0.182 ± 0.191	9.47·10 ⁻²
Tinidazole	<LOD	<LOD	7.28·10 ⁻⁵	<LOD	<LOD	7.28·10 ⁻⁵
Trimethoprim	0.014 - 0.074	0.038 ± 0.032	3.81·10 ⁻⁴	0.008 - 0.388	0.068 ± 0.121	6.77·10 ⁻⁴

Table S24. (continued)

Compound	noPAC			0.1PAC		
	Range (µg/L)	Average ± SD (µg/L)	RQ EFF	Range (µg/L)	Average ± SD (µg/L)	RQ EFF
Antifungals						
Sulfacetamide	<LOD	<LOD	6.09·10 ⁻⁵	<LOD	<LOD	6.09·10 ⁻⁵
Terbinafine	<LOD	<LOD	6.83·10 ⁻²	<LOD	<LOD	6.83·10 ⁻²
Tiabendazole	<LOD	<LOD	1.03·10 ⁻⁴	<LOD	<LOD	1.03·10 ⁻⁴
Antihistamines						
Diphenhydramine	<LOD - 0.019	0.007 ± 0.01	6.91·10 ⁻³	<LOD	<LOD	8.99·10 ⁻⁴
Promethazine	<LOD	<LOD	1.14·10 ⁻²	<LOD	<LOD	1.14·10 ⁻²
Antihypertensive						
Clonidine	<LOD	<LOD	4.65·10 ⁻⁵	<LOD	<LOD	4.65·10 ⁻⁵
Antihypertensive						
Albendazole	<LOD	<LOD	2.73·10 ⁻³	<LOD	<LOD	2.73·10 ⁻³
Flubendazole	<LOD	<LOD	6.78·10 ⁻³	<LOD	<LOD	6.78·10 ⁻³
Levamisole	<LOD - 0.011	0.005 ± 0.005	2.51·10 ⁻³	<LOD - 0.043	0.007 ± 0.014	3.97·10 ⁻³
Mebendazole	<LOD	<LOD	3.93·10 ⁻³	<LOD - 0.014	0.002 ± 0.005	1.33·10 ⁻²
Praziquantel	<LOD - 0.044	0.026 ± 0.022	1.17·10 ⁻²	<LOD - 0.023	0.006 ± 0.009	2.66·10 ⁻³
Triclabendazole	<LOD	<LOD	7.02·10 ⁻²	<LOD	<LOD	7.02·10 ⁻²
Antiseptic						
Nitrofurantoin	<LOD	<LOD	2.03·10 ⁻⁴	<LOD - 2.415	0.269 ± 0.805	5.09·10 ⁻²
Beta-blockers						
Atenolol	0.005 - 0.025	0.017 ± 0.011	1.14·10 ⁻⁴	<LOD - 0.059	0.02 ± 0.018	1.30·10 ⁻⁴
Bisoprolol	<LOD - 0.014	0.008 ± 0.006	2.48·10 ⁻³	<LOD - 0.061	0.015 ± 0.019	4.59·10 ⁻³
Metoprolol	0.037 - 0.083	0.053 ± 0.026	6.15·10 ⁻³	0.011 - 0.102	0.058 ± 0.034	6.69·10 ⁻³
Calcium channel blocker						
Verapamil	<LOD	<LOD	2.31·10 ⁻⁴	<LOD	<LOD	2.31·10 ⁻⁴
Diuretic						
Torsemide	<LOD	<LOD	2.46·10 ⁻³	<LOD	<LOD	2.46·10 ⁻³
Hormones						
Fludrocortisone-acetate	<LOD	<LOD	8.90·10 ⁻⁵	<LOD	<LOD	8.90·10 ⁻⁵
Flumethasone	<LOD	<LOD	7.66·10 ⁻⁵	<LOD	<LOD	7.66·10 ⁻⁵
Hydrocortisone	<LOD - 0.063	0.027 ± 0.032	9.21·10 ⁻⁴	<LOD - 0.122	0.035 ± 0.049	1.22·10 ⁻³
Methylprednisolone	<LOD	<LOD	1.46·10 ⁻⁴	<LOD	<LOD	1.46·10 ⁻⁴
Mometasone furoate	<LOD	<LOD	8.01·10 ⁻⁴	<LOD	<LOD	8.01·10 ⁻⁴
Prednicarbate	<LOD	<LOD	4.12·10 ⁻⁴	<LOD	<LOD	4.12·10 ⁻⁴
Prednisolone	<LOD	<LOD	1.33·10 ⁻⁴	<LOD	<LOD	1.33·10 ⁻⁴
Triamcinolone	<LOD	<LOD	1.97·10 ⁻⁵	<LOD	<LOD	1.97·10 ⁻⁵
Triamcinolone acetonide	<LOD - 0.804	0.345 ± 0.413	2.31·10 ⁻²	<LOD - 1.297	0.216 ± 0.429	1.45·10 ⁻²
Illicit drugs						
Amphetamine	0.045 - 0.365	0.225 ± 0.164	9.09·10 ⁻³	<LOD - 0.028	0.008 ± 0.011	3.04·10 ⁻⁴
<i>Benzoylcegonine</i>	<LOD	<LOD	n.a.	<LOD - 0.017	0.005 ± 0.007	n.a.
Cannabinol	<LOD	<LOD	2.84·10 ⁻²	<LOD	<LOD	2.84·10 ⁻²
<i>Cocaethylene</i>	<LOD - 0.002	0.001 ± 0.001	5.91·10 ⁻⁴	<LOD	<LOD	1.71·10 ⁻⁴
Cocaine	<LOD - 0.009	0.004 ± 0.004	1.59·10 ⁻³	<LOD - 0.019	0.003 ± 0.006	1.42·10 ⁻³
<i>Ecgonine methyl ester</i>	<LOD - 0.025	0.009 ± 0.013	1.06·10 ⁻⁴	<LOD - 0.078	0.01 ± 0.026	1.17·10 ⁻⁴
Ketamine	<LOD	<LOD	1.72·10 ⁻⁴	<LOD - 0.013	0.003 ± 0.005	5.94·10 ⁻⁴
MDA	0.345 - 0.596	0.464 ± 0.126	9.23·10 ⁻³	<LOD - 0.482	0.164 ± 0.187	3.25·10 ⁻³
MDEA	<LOD - 0.031	0.013 ± 0.016	4.98·10 ⁻⁴	<LOD - 0.036	0.014 ± 0.014	5.55·10 ⁻⁴
MDMA	<LOD - 0.004	0.002 ± 0.002	3.48·10 ⁻⁵	<LOD - 0.017	0.004 ± 0.005	7.45·10 ⁻⁵

Table S24. (continued)

Compound	noPAC			0.1PAC		
	Range (µg/L)	Average ± SD (µg/L)	RQ EFF	Range (µg/L)	Average ± SD (µg/L)	RQ EFF
Methamphetamine	<LOD	<LOD	4.90·10 ⁻⁵	<LOD	<LOD	4.90·10 ⁻⁵
Phencyclidine	<LOD	<LOD	1.12·10 ⁻²	<LOD	<LOD	1.12·10 ⁻²
THC	<LOD - 0.026	0.016 ± 0.013	2.28·10 ⁻¹	<LOD - 0.018	0.003 ± 0.006	4.63·10 ⁻²
Plastic additives						
Benzotriazole	0.678 - 1.924	1.22 ± 0.639	1.57·10 ⁻¹	0.477 - 2.745	1.704 ± 0.753	2.19·10 ⁻¹
p-Toluenesulfonamide	<LOD - 0.084	0.033 ± 0.044	2.22·10 ⁻⁴	<LOD - 0.373	0.081 ± 0.13	5.40·10 ⁻⁴
Psychiatric drugs						
10-Hydroxycarbazepine	<LOD	<LOD	1.67·10 ⁻⁴	<LOD - 0.394	0.136 ± 0.14	3.37·10 ⁻²
7-Aminoclonazepam	<LOD	<LOD	1.07·10 ⁻³	<LOD	<LOD	1.07·10 ⁻³
7-Aminoflunitrazepam	<LOD	<LOD	4.13·10 ⁻⁴	<LOD	<LOD	4.13·10 ⁻⁴
Alprazolam	<LOD	<LOD	1.02·10 ⁻²	<LOD	<LOD	1.02·10 ⁻²
Amisulpride	<LOD - 0.049	0.024 ± 0.024	1.65·10 ⁻²	<LOD - 0.111	0.015 ± 0.036	1.08·10 ⁻²
Amitriptyline	<LOD - 0.033	0.012 ± 0.019	8.25·10 ⁻²	<LOD - 0.03	0.006 ± 0.011	4.31·10 ⁻²
Amoxapine	<LOD	<LOD	2.21·10 ⁻³	<LOD	<LOD	2.21·10 ⁻³
Bromazepam	<LOD	<LOD	1.60·10 ⁻³	<LOD	<LOD	1.60·10 ⁻³
Carbamazepine	0.307 - 0.455	0.395 ± 0.078	7.91	0.018 - 0.302	0.188 ± 0.088	3.76
Chlordiazepoxide	<LOD	<LOD	1.89·10 ⁻³	<LOD	<LOD	1.89·10 ⁻³
Chlorprothixene	<LOD	<LOD	2.21·10 ⁻²	<LOD	<LOD	2.21·10 ⁻²
Citalopram	<LOD - 0.016	0.01 ± 0.008	6.12·10 ⁻⁴	<LOD - 0.022	0.008 ± 0.008	5.19·10 ⁻⁴
Clobazam	<LOD	<LOD	5.79·10 ⁻⁴	<LOD - 0.011	0.002 ± 0.003	1.55·10 ⁻³
Clomipramine	<LOD	<LOD	7.60·10 ⁻³	<LOD	<LOD	7.60·10 ⁻³
Clonazepam	<LOD	<LOD	4.02·10 ⁻³	<LOD	<LOD	4.02·10 ⁻³
Clorazepate	<LOD	<LOD	1.44·10 ⁻²	<LOD	<LOD	1.44·10 ⁻²
Clozapine	0.003 - 0.014	0.008 ± 0.006	4.22·10 ⁻²	<LOD - 0.009	0.003 ± 0.003	1.83·10 ⁻²
Desalkylflurazepam	<LOD	<LOD	5.52·10 ⁻⁴	<LOD	<LOD	5.52·10 ⁻⁴
Desipramine	<LOD	<LOD	6.92·10 ⁻³	<LOD	<LOD	6.92·10 ⁻³
Desvenlafaxine	0.011 - 0.081	0.051 ± 0.036	7.11·10 ⁻³	0.012 - 0.08	0.058 ± 0.02	8.10·10 ⁻³
Dexametasone	<LOD - 0.18	0.061 ± 0.103	2.48·10 ⁻³	<LOD	<LOD	6.51·10 ⁻⁵
Diazepam	<LOD	<LOD	2.55·10 ⁻³	<LOD	<LOD	2.55·10 ⁻³
Dothiepin	<LOD	<LOD	1.00·10 ⁻²	<LOD - 0.01	<LOD	1.86·10 ⁻²
Doxepin	<LOD	<LOD	2.30·10 ⁻³	<LOD	<LOD	2.30·10 ⁻³
EDDP	<LOD - 0.017	0.009 ± 0.008	6.35·10 ⁻²	<LOD - 0.018	0.009 ± 0.006	6.33·10 ⁻²
Felbamate	0.01 - 0.06	0.034 ± 0.025	3.06·10 ⁻³	<LOD	<LOD	8.08·10 ⁻⁵
Fluoxetine	<LOD - 0.012	0.007 ± 0.006	6.80·10 ⁻²	<LOD - 0.011	0.004 ± 0.004	3.62·10 ⁻²
Flupentixol	<LOD	<LOD	9.69·10 ⁻³	<LOD	<LOD	9.69·10 ⁻³
Flurazepam	<LOD - 0.014	0.005 ± 0.008	5.39·10 ⁻²	<LOD - 0.005	<LOD	1.07·10 ⁻²
Fluvoxamine	<LOD	<LOD	2.89·10 ⁻⁴	<LOD - 0.029	0.004 ± 0.009	1.80·10 ⁻³
Gabapentin	0.054 - 0.262	0.188 ± 0.116	1.88·10 ⁻²	0.161 - 0.654	0.309 ± 0.17	3.09·10 ⁻²
Haloperidol	<LOD	<LOD	8.06·10 ⁻⁴	<LOD	<LOD	8.06·10 ⁻⁴
Imipramine	<LOD	<LOD	1.30·10 ⁻³	<LOD	<LOD	1.30·10 ⁻³
Lamotrigine	0.195 - 0.441	0.332 ± 0.126	3.32·10 ⁻²	0.046 - 0.448	0.274 ± 0.125	2.74·10 ⁻²
Lorazepam	0.063 - 0.161	0.118 ± 0.05	1.23	<LOD - 0.087	0.037 ± 0.043	3.90·10 ⁻¹
Maprotiline	<LOD	<LOD	1.64·10 ⁻³	<LOD - 0.012	0.007 ± 0.005	2.20·10 ⁻²
Medazepam	<LOD	<LOD	7.03·10 ⁻³	<LOD	<LOD	7.03·10 ⁻³
Memantine	0.021 - 0.18	0.086 ± 0.084	4.66·10 ⁻²	0.009 - 0.102	0.037 ± 0.034	2.01·10 ⁻²
Methadone	<LOD	<LOD	1.90·10 ⁻³	<LOD	<LOD	1.90·10 ⁻³
Methylphenidate	<LOD - 0.05	0.026 ± 0.024	2.21·10 ⁻³	<LOD - 0.035	0.007 ± 0.011	5.89·10 ⁻⁴

Table S24. (continued)

Compound	noPAC			0.1PAC		
	Range (µg/L)	Average ± SD (µg/L)	RQ EFF	Range (µg/L)	Average ± SD (µg/L)	RQ EFF
Mianserin	<LOD	<LOD	2.35·10 ⁻³	<LOD	<LOD	2.35·10 ⁻³
Mirtazapine	<LOD	<LOD	1.03·10 ⁻³	<LOD	<LOD	1.03·10 ⁻³
Naltrexone	<LOD	<LOD	6.24·10 ⁻⁴	<LOD - 0.018	0.003 ± 0.006	1.62·10 ⁻³
<i>N-Desmethylozapine</i>	<LOD	<LOD	2.29·10 ⁻²	<LOD	<LOD	2.29·10 ⁻²
Nitrazepam	<LOD - 0.014	0.006 ± 0.007	1.13·10 ⁻²	<LOD - 0.092	0.032 ± 0.033	6.57·10 ⁻²
<i>Norbuprenorphine</i>	<LOD	<LOD	2.31·10 ⁻³	<LOD	<LOD	2.31·10 ⁻³
Nordiazepam	<LOD	<LOD	1.28·10 ⁻³	<LOD	<LOD	1.28·10 ⁻³
Nortriptyline	<LOD	<LOD	3.86·10 ⁻³	<LOD	<LOD	3.86·10 ⁻³
Olanzapine	<LOD	<LOD	3.14·10 ⁻²	<LOD	<LOD	3.14·10 ⁻²
Opipramol	<LOD	<LOD	1.29·10 ⁻³	<LOD - 0.024	0.005 ± 0.008	9.24·10 ⁻³
Oxazepam	<LOD	<LOD	1.44·10 ⁻³	<LOD	<LOD	1.44·10 ⁻³
Oxcarbazepine	0.032 - 0.095	0.073 ± 0.035	2.46·10 ⁻²	<LOD - 0.072	0.032 ± 0.026	1.08·10 ⁻²
Paliperidone	<LOD	<LOD	1.15·10 ⁻³	<LOD	<LOD	1.15·10 ⁻³
Paroxetine	<LOD	<LOD	1.07·10 ⁻³	<LOD	<LOD	1.07·10 ⁻³
Phenazepam	<LOD	<LOD	3.91·10 ⁻³	<LOD - 0.111	0.036 ± 0.052	1.12·10 ⁻¹
Phenytoin	0.018 - 0.407	0.175 ± 0.205	2.02·10 ⁻¹	<LOD - 0.259	0.1 ± 0.074	1.15·10 ⁻¹
Pipamperone	<LOD	<LOD	6.28·10 ⁻⁴	<LOD	<LOD	6.28·10 ⁻⁴
Prazepam	<LOD	<LOD	2.83·10 ⁻³	<LOD	<LOD	2.83·10 ⁻³
Promazine	<LOD	<LOD	1.63·10 ⁻²	<LOD	<LOD	1.63·10 ⁻²
Protriptyline	<LOD	<LOD	1.67·10 ⁻³	<LOD	<LOD	1.67·10 ⁻³
Quetiapine	<LOD	<LOD	5.19·10 ⁻³	<LOD	<LOD	5.19·10 ⁻³
Risperidone	<LOD	<LOD	1.94·10 ⁻³	<LOD	<LOD	1.94·10 ⁻³
<i>Ritalinic acid</i>	<LOD - 0.062	0.021 ± 0.035	1.51·10 ⁻³	<LOD - 0.153	0.038 ± 0.054	2.69·10 ⁻³
Secobarbital	<LOD	<LOD	2.04·10 ⁻⁴	<LOD	<LOD	2.04·10 ⁻⁴
Sertraline	<LOD	<LOD	1.54·10 ⁻²	<LOD	<LOD	1.54·10 ⁻²
Temazepam	0.017 - 0.02	0.019 ± 0.002	2.61·10 ⁻¹	<LOD - 0.014	0.005 ± 0.006	6.64·10 ⁻²
Topiramate	<LOD	<LOD	7.55·10 ⁻⁵	<LOD	<LOD	7.55·10 ⁻⁵
Trazodone	<LOD	<LOD	5.85·10 ⁻²	<LOD	<LOD	5.85·10 ⁻²
Triazolam	<LOD	<LOD	2.13·10 ⁻²	<LOD	<LOD	2.13·10 ⁻²
Trimipramine	<LOD - 0.054	0.019 ± 0.03	1.12·10 ⁻¹	<LOD	<LOD	8.69·10 ⁻³
Venlafaxine	0.032 - 0.106	0.066 ± 0.037	1.75	0.004 - 0.095	0.052 ± 0.035	1.38
Zolpidem	<LOD	<LOD	3.18·10 ⁻³	<LOD	<LOD	3.18·10 ⁻³
Zopiclone	<LOD	<LOD	2.45·10 ⁻²	<LOD	<LOD	2.45·10 ⁻²
<i>α-Hydroxyalprazolam</i>	<LOD	<LOD	4.21·10 ⁻³	<LOD	<LOD	4.21·10 ⁻³
<i>α-Hydroxymidazolam</i>	0.007 - 0.009	0.008 ± 0.001	5.46·10 ⁻²	<LOD - 0.015	0.007 ± 0.004	4.59·10 ⁻²
<i>α-Hydroxytriazolam</i>	<LOD - 0.105	0.036 ± 0.06	4.08·10 ⁻¹	<LOD	<LOD	1.03·10 ⁻²
Receptor antagonists						
Atropine	<LOD	<LOD	8.88·10 ⁻⁵	<LOD	<LOD	8.88·10 ⁻⁵
Flumazenil	<LOD	<LOD	1.14·10 ⁻³	<LOD	<LOD	1.14·10 ⁻³
Stimulants						
Caffeine	0.268 - 2.065	1.021 ± 0.933	8.51·10 ⁻¹	0.092 - 1.753	0.867 ± 0.708	7.23·10 ⁻¹
<i>Cotinine</i>	<LOD - 0.023	0.012 ± 0.011	1.16·10 ⁻³	<LOD - 0.033	0.016 ± 0.01	1.60·10 ⁻³
Phentermine	<LOD	<LOD	7.73·10 ⁻⁵	<LOD	<LOD	7.73·10 ⁻⁵
UV filter						
Octinoxate	<LOD - 0.04	0.014 ± 0.023	5.38·10 ⁻¹	<LOD - 0.006	<LOD	5.65·10 ⁻²
Veterinary drugs						
Carprofen	<LOD	<LOD	4.90·10 ⁻³	<LOD	<LOD	4.90·10 ⁻³

Table S24. (continued)

Compound	noPAC			0.1PAC		
	Range (µg/L)	Average ± SD (µg/L)	\overline{RQ} EFF	Range (µg/L)	Average ± SD (µg/L)	\overline{RQ} EFF
Diaveridine	0.041 - 0.061	0.048 ± 0.011	1.33·10 ⁻¹	<LOD - 0.067	0.033 ± 0.022	9.24·10 ⁻²
Difloxacin	<LOD - 0.255	0.086 ± 0.146	5.57·10 ⁻²	<LOD	<LOD	1.29·10 ⁻³
Dimetridazole	<LOD	<LOD	1.85·10 ⁻⁵	<LOD	<LOD	1.85·10 ⁻⁵
Enrofloxacin	<LOD	<LOD	6.63·10 ⁻⁴	<LOD	<LOD	6.63·10 ⁻⁴
Flunixin	<LOD - 0.066	0.039 ± 0.034	2.44·10 ⁻¹	<LOD - 0.098	0.038 ± 0.033	2.40·10 ⁻¹
Furaltadone	<LOD	<LOD	7.35·10 ⁻⁵	<LOD	<LOD	7.35·10 ⁻⁵
Iprnidazole	<LOD	<LOD	8.44·10 ⁻⁵	<LOD	<LOD	8.44·10 ⁻⁵
Marbofloxacin	<LOD - 0.418	0.175 ± 0.217	2.25·10 ⁻²	<LOD - 0.314	0.124 ± 0.133	1.60·10 ⁻²
Monensin	<LOD	<LOD	8.98·10 ⁻⁴	<LOD	<LOD	8.98·10 ⁻⁴
Orbifloxacin	<LOD	<LOD	4.82·10 ⁻²	<LOD - 0.008	<LOD	7.82·10 ⁻²
Oxibendazole	<LOD	<LOD	3.70·10 ⁻⁴	<LOD	<LOD	3.70·10 ⁻⁴
Ronidazole	<LOD	<LOD	7.95·10 ⁻⁵	<LOD	<LOD	7.95·10 ⁻⁵
Salinomycin	<LOD	<LOD	2.54·10 ⁻²	<LOD	<LOD	2.54·10 ⁻²
Sarafloxacin	<LOD	<LOD	1.03·10 ⁻³	<LOD	<LOD	1.03·10 ⁻³
Sulfachlorpyridazine	<LOD	<LOD	7.50·10 ⁻⁴	<LOD - 0.012	0.002 ± 0.004	2.56·10 ⁻³
Sulfaclozine	<LOD	<LOD	5.78·10 ⁻⁴	<LOD	<LOD	5.78·10 ⁻⁴
Sulfadoxine	<LOD	<LOD	9.31·10 ⁻⁴	<LOD	<LOD	9.31·10 ⁻⁴
Sulfamonomethoxine	<LOD	<LOD	4.47·10 ⁻⁴	<LOD	<LOD	4.47·10 ⁻⁴
Sulfanitran	<LOD	<LOD	1.23·10 ⁻³	<LOD	<LOD	1.23·10 ⁻³
Sulfaquinoxaline	<LOD	<LOD	5.32·10 ⁻³	<LOD	<LOD	5.32·10 ⁻³
Tilmicosin	<LOD	<LOD	2.77·10 ⁻²	<LOD	<LOD	2.77·10 ⁻²
X-ray contrast medium						
Iopromide	<LOD	<LOD	3.59·10 ⁻³	<LOD - 0.826	0.269 ± 0.268	1.92
			noPAC	0.1PAC		
			<i>RQ</i> _{mix, 232}	47		
			<i>RQ</i> _{mix, 40}	1.0		

Legend

n.a.: PNEC value was not available in the NORMAN database, and thus the RQ calculation.

¹ 40 key OMPs refer to the 41 key OMPs selected in section 3.1.1 of the manuscript, with the exception of benzoylcgonine, for which the calculation of the RQ value was not possible.

5. References

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Table S24. (continued)

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