SUPPLEMENTARY INFORMATION

a) General information

General information S1. UPLC-QqTOF-MS analysis for water samples

A liquid chromatography-quadrupole time-of-flight mass spectrometry (UPLC-QqTOF-MS) system was used for target and non-target analysis. Specifically, LC separation was achieved using an ACQUITY I-Class UPLC system (Waters Corporation, Milford, MA, USA) coupled with an ACQUITY BEH C18 (100 mm x 2.1 mm, 1.7 μm) column. Mobile phases were 0.1% formic acid in MilliQ water (solvent A) and 0.1 % formic acid in MeOH (solvent B). The gradient used ranged from 5% to 95% of solvent B: Initially was increased from 5% to 25% in 1.50 min, after increased from 25% to 80%, kept at 80% during 1 min, increased in 8 min and from 80% to 95% in 1 min and finally returned to its initial conditions in 4 min. The total analysis run time was 15.50 min. The flow rate was adjusted at 0.25 mL/min and 10 μL of sample was injected. The LC system was connected to a Bruker Daltonics, maXis q-TOF mass spectrometer equipped with an electrospray ion source (Bruker Daltonics, Bremen, Germany). The ion source settings were as follows: nitrogen was used as nebulizer, drying and collision gas; the nebulizer pressure was 2 bars, the drying gas flow was 8 L/min, the dry gas temperature was 200 ºC and the capillary voltage was 4500 V. The system worked via TOF MS survey scan (resolving power ≥ 55000 FWHM). The chromatographic peaks were identified and reported from accurate-mass scan data using the software Target Analysis (1.3) and Data Analysis (4.2) from Bruker. In order to simplify, all analysis was performed in positive ionization mode.

General information S2. Solid-phase extraction (SPE) protocol

SPE was performed with commercial Oasis® HLB (200 mg, 6 cm^3) using a Visiprep vacuum manifold. Before use, the cartridges were conditioned with 4 ml of methanol and 4 ml of Milli-Q water (pH adjusted to 8, same pH as the real water samples, in order not to alter their composition). Samples (100 ml) were passed through the cartridges at a flow rate of 1 ml/min. The cartridges were then rinsed with 4 ml of ultrapure water and vacuum dried for 10 min to remove excess of water. Finally, the retained compounds were eluted with 8 ml MeOH (4 + 4). The extracts were evaporated to dryness under a gentle nitrogen stream and reconstituted with 1 ml of H_2O/MeOH (95:5, *v/v)* containing 0.1% formic acid. Final extracts were filtered through a 0.22 μm PTFE filter.

b) Tables

Table S1. Inlet wastewater characterization (n=20)

ANALYSED PARAMETERS		VALUES
Physico-chemical	pH	7.4 ± 0.2
	Turbidity (NTU)	4.8 ± 2.7
	Temperature (ºC)	20.0 ± 5.0
	Electrical Conductivity (EC, dS/m)	1.6 ±0.2
	5-day Biochemical Oxygen Demand (BOD_5, mg/L)	15.3 ± 3.1
	Chemical oxygen demand (COD, mg/L)	75.2 ± 12.2
	Total Nitrogen (TN, mg/L)	9.4 ± 1.8
	Dissolved Organic Carbon (DOC, mg/L)	30.1 ± 4.9
	Total Solids (TSS, mg/L)	6.0 ± 4.5
	Transmittance (%)	53.7 ± 4.6
	F^- (mg/L)	0.2 ± 0.03
	Cl^- (mg/L)	243.6 ± 47.1
	NO_2^-(mg/L)	1.4 ± 0.1
	Br^- (mg/L)	0.4 ± 0.1
	NO_3^- (mg/L)	9.9 ± 5.7
	PO_4^{3-} (mg/L)	9.1 ±2.9
	SO_4^{2-} (mg/L)	200.8 ± 30.9
	Sodium adsorption Ratio (SAR, meq/L)	4.9 ± 1.0
Microbiological	*E. Coli* (CFU/100 mL)	$2.3 \times 10^4 \pm 1.1 \times 10^4$
	Clostridium perfringens spores (CFU/100 mL)	800.0 ± 141.0

Table S2. Suspect list developed under literature research

Pharmaceutical	TP	FORMULA	REF.	Pharmaceutical	TP	FORMULA	REF.
AMOXICILLIN (AMX)	TPA1	C10H12N2O3	[46]	ERYTHROMYCIN (*ERY*)	TPE1	C18H26O4	[47]
	TPA2	C12H15NSO4			TPE2	C27H40O7	
	TPA3	C12H16N2SO4			TPE3	C29H50O11	
	TPA4	C13H12O7SN3			TPE4	C34H61NO13	
	TPA5	C14H17N2SO4			TPE5	C36H65NO13	
	TPA6	C14H19N3SO4			TPE6	C37H67NO14	
	TPA7	C16H17N3SO9		KETOPROFEN (KTP)	TPK1	C10H14O9	[48]
	TPA8	C9H13N3SO2			TPK2	C10H8O8	
CARBAMAZEPINE (CBZ)	TPC1	C13H9NO	[49-51]		TPK3	C12H10O5	
	TPC2	C11H10N2O6			TPK4	C14H14O11	
	TPC3	C14H10N2O2			TPK5	C14H14O5	
	TPC4	C14H11NO2			TPK6	C14H14O6	
	TPC5	C14H11NO3			TPK7	C15H14O11	
	TPC6	C14H11NO4			TPK8	C15H16O7	
	TPC7	C14H9NO			TPK9	C16H14O3	
	TPC8	C14H9NO2			TPK10	C16H14O5	
	TPC9	C14H9NO2			TPK11	C16H8O12	
	TPC10	C14H9NO3			TPK12	C4H4O5	
	TPC11	C15H10N2O2			TPK13	C5H8O4	
	TPC12	C15H10N2O3			TPK14	C5H8O6	
	TPC13	C15H10N2O4			TPK15	C6H7O4	
	TPC14	C15H12N2O2			TPK16	C9H9O3	
	TPC15	C15H12N2O2		NAPROXEN (NPX)	TPN1	C10H10O2	[48]
	TPC16	C15H12N2O3			TPN2	C10H8O	
	TPC17	C15H12N2O4			TPN3	C10H8O2	
	TPC18	C15H14N2O5			TPN4	C11H10O2	
	TPC19	C8H6N2O			TPN5	C12H10O2	
	TPC20	C8H6N2O2			TPN6	C13H12O3	
	TPC21	C8H8N2O3			TPN7	C13H14O	
	TPC22	C9H8N2O			TPN8	C14H11O5	
DICLOFENAC (DCF)	TPD1	C10H7Cl2NO3	[49, 52-53]		TPN9	C14H13O6	
	TPD2	C10H9Cl2NO3			TPN10	C14H14O5	
	TPD3	C12H9Cl2NO			TPN11	C14H14O7	
	TPD4	C12H9Cl2NO4			TPN12	C14H16O5	
	TPD5	C13H9Cl2NO3			TPN13	C5H8O4	
	TPD6	C14H11Cl2NO3			TPN14	C7H10O5	
	TPD7	C14H11Cl2NO5			TPN15	C7H6O2	

	TPD8	C14H9Cl2NO3			TPN16	C7H6O3	
	TPD9	C37H67NO14			TPN17	C8H6O4	
	TPD10	C6H5Cl2N					
Pharmaceutical	**TP**	**FORMULA**	**REF.**	**Pharmaceutical**	**TP**	**FORMULA**	**REF.**
SULFAMETOXAZOLE (SMX)	TPS1	C10H10N2SO5	[49, 53-54]	**TETRACYCLINE (TCL)**	TPTE1	C20H17NO9	[55]
	TPS2	C10H10N3SO5			TPTE2	C20H19NO10	
	TPS3	C10H11N3SO3			TPTE3	C20H21NO11	
	TPS4	C10H9N3SO5			TPTE4	C20H21NO13	
	TPS5	C11H15NO			TPTE5	C20H21NO14	
	TPS6	C6H6N2SO4			TPTE6	C22H26N2O13	
	TPS7	C6H8N2O2			TPTE7	C22H27N2O9	
	TPS8	C7H5N3SO4			TPTE8	C22H28N2O10	
	TPS9	C8H7NO			TPTE9	C22H28N2O12	

Table S3. Transformation products detected under experimental conditions.

Workflow (L/h)	Ozone supply gO_3/h	Compound	Formula	Exact mass	Retention time (min)	Score	Mass error	Proposed name
2000	4.5	CBZ	$C_{14}H_{11}NO_2$	225.07	8.67	100	-1.7	TPC4-8,67
	11.4	CBZ	$C_{14}H_{11}NO_2$	225.07	8.67	100	-3.6	TPC4-8,67
	15.9	CBZ	$C_{15}H_{12}N_2O_2$	252.09	9.45	100	3.3	TPC13-9,45
	15.9	CBZ	$C_{14}H_{11}NO_2$	225.07	8.67	100	-1.7	TPC4-8,67
	15.9	DCF	$C_{14}H_{11}Cl_2NO_3$	311.01	9.08	100	4.9	TPD6-9,08
	22.8	CBZ	$C_{14}H_{11}NO_2$	225.07	8.67	100	-1.5	TPC4-8,67
1200	4.5	CBZ	$C_{14}H_9NO_3$	250.07	6.54	100	-0.3	TPC10-6,54
	11.4	CBZ	$C_{14}H_9NO_3$	250.07	6.54	100	1.9	TPC10-6,54
500	4.5	NPX	$C_{10}H_{10}O_2$	162.06	10.83	100	0.8	TPN1-10,83