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Supplementary Material

for

Monitoring of a broad set of pharmaceuticals in wastewaters by high-resolution mass spectrometry and evaluation of heterogenous catalytic ozonation for their removal in a pre-industrial level unit

C. Nannou[1,2], E. Kaprara[3], S. Psaltou[4], M. Salapasidou[5], P.-A. Palasantza[5], P. Diamantopoulos[5], D. A. Lambropoulou[1,2], M. Mitrakas[3], A. Zouboulis[4*]

[1] Laboratory of Environmental Pollution Control, Department of Chemistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece; chnannou@chem.auth.gr; dlambro@chem.auth.gr
[2] Center for Interdisciplinary Research and Innovation (CIRI-AUTH), Balkan Center, Thessaloniki GR-57001, Greece; chnannou@chem.auth.gr; dlambro@chem.auth.gr
[3] Department of Chemical Engineering, Aristotle University of Thessaloniki, GR-54124, Thessaloniki, Greece
[4] Department of Chemistry, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece
[5] AKTOR S.A., Wastewater Treatment Plant of Touristic Area of Thessaloniki "AINEIA", N. Michaniona, Thessaloniki, Greece
* Correspondence zoubouli@chem.auth.gr

Contents of the Supplementary Material

Section S1. Description of the four distinct operating sections of the pre-industrial level unit

Section S2. Supplementary Tables

Section S3. Supplementary Figures

Section S1. Description of the four distinct operating sections of the pre-industrial level unit

(a) Post-filtration

The first treatment stage includes a fixed-bed column (D=480mm, H=3000mm) packed with sand and activated carbon (i. 10 cm sand 1,0-1,6 mm, ii. 80 cm sand 0,4-0,8 mm and iii. 40 cm activated carbon) for the filtration of the secondary effluent of WWTP that serves the removal of suspended solids and the improvement of quality characteristics of treated waste, prior to its introduction to the following sections of the unit.

(b) Ozone dilution

The treated wastewater, after the first treatment stage, is inserted to a custom-made porous PTFE hollow fiber membrane module (provided by Markel Corporation, PA, USA) used for the contact/dissolution of ozone gas to the liquid phase. The specifications of the membrane are listed in Table S1. To achieve maximum efficiency in ozone dissolution to wastewater hollow fiber membrane operates in a dead-end function, so that the gas phase is completely transported to the liquid one and maximum ozone exploitation is achieved. In addition, the ozone gas is introduced to the shell side and the liquid phase to the lumen side of the hollow fibre membrane.

(c) Catalytic ozonation

Catalytic ozonation is performed in a fixed-bed column (D=200mm, H=3000mm) packed with an appropriate solid material, applied as potential catalyst for the ozonation treatment of CECs (i. 10 cm sand 1,0-1,6 mm, ii. 100 cm catalyst). Materials tested as catalysts were zeolite and PET as they presented the highest efficiency in catalysing CECs' ozonation when applied in laboratory scale experiments in a pilot unit operating correspondingly to the pre-industrial unit. Table S2 summarizes the main physicochemical characteristics of these materials.

(d) Biological stabilisation

The last treatment stage of the pre-industrial unit includes a sand/activated carbon column (D=200mm, H=3000mm) for the final biological stabilisation of treated wastewater (i. 10 cm sand 1,0-1,6 mm, ii. 70 cm sand 0,4-0,8 mm and iii. 40 cm activated carbon). This step aims to further improve the quality characteristics of the treated wastewater through the removal of CECs' transformation products.

The secondary (biologically treated) effluent of WWTP is introduced into the pilot unit at a flow rate of 200 L/h, while ozone gas supply is provided by the existing generator, used to disinfect the treated wastewaters before disposal to the sea, which can produce 190 g O_3/Nm^3.

Section S2. Supplementary Tables

Table S1 Specifications of the membrane module used

Membrane	PTFE Hollow Fiber
Inner Diameter (mm)	1.47
Outer Diameter (mm)	1.88
Density (g/cm^3)	0.97
Porosity (%)	53
Pure Water Flux (L/min/m^2 @ 2 bar)	180
Water Entry Pressure (bar)	1.93
Maximum Pore Diameter (μm)	0.741
Mean Pore Diameter (μm)	0.589
Minimum Pore Diameter (μm)	0.52
Length, L (m)	0.96
Effective Contact Area (m^2)	4.8
Number of fibers	846

Table S2 Main physicochemical characteristics of materials tested as catalysts

Catalyst	PET	Zeolite
PZC	6.8	6.2
IEP	2.2	
S_{BET}, m^2/g	21	
Pore volume, mL/g	0.164	
Granule size, mm		0.8-2.5

Table S3 Sampling Points

Name	Description
WWTP Influent	Influent wastewater
WWTP Effluent	Effluent wastewater after conventional disinfection (simple ozonation), discharged at the receiver
P0-Secondary effluent	- Secondary treatment effluent wastewater before conventional disinfection (simple ozonation) and - Influent wastewater to the pre-industrial pilot unit
P1-1st Bed effluent	Effluent wastewater after the post filtration (1st Fix-Bed) in the pre-industrial pilot unit
P3-2nd Bed effluent	Effluent wastewater after the catalytic ozonation (2nd Fix-Bed) in the pre-industrial pilot unit
P4-3rd Bed effluent	Effluent wastewater after the biological stalilization (3rd Fix-Bed) in the pre-industrial pilot unit

Table S4 Physicochemical properties of the studied PPCPs

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	$\log K_{ow}$	pK_a
Antibiotics						
Amoxicillin	26787-78-0	$C_{16}H_{19}N_3O_5S$	365.10	3430	0.87	2.8; 7.3
Ampicillin	69-53-4	$C_{16}H_{19}N_3O_4S$	349.11	1.01×10^4	1.35	2.5; 7.3
Azithromycin	83905-01-5	$C_{38}H_{72}N_2O_{12}$	748.51	7.09	4.02	8.7
Ciprofloxacin	85721-33-1	$C_{17}H_{18}FN_3O_3$	331.13	3×10^4	0.28	6.1
Clarithromycin	81103-11-9	$C_{38}H_{69}NO_{13}$	747.48	0.342	3.16	9.0
Erythromycin	114-07-8	$C_{37}H_{67}NO_{13}$	733.93	1.44	3.06	8.9
Isoniazid	54-85-3	$C_6H_7N_3O$	137.06	1.4×10^5	-0.70	1.8
Levofloxacin	100986-85-4	$C_{18}H_{20}FN_3O_4$	361.14	insoluble	-0.39	6.2
Lincomycin	154-21-2	$C_{18}H_{34}N_2O_6S$	406.21	927	0.56	7.6
Metronidazole	443-48-1	$C_6H_9N_3O_3$	171.06	9500	-0.02	2.6;15.4
Moxifloxacin	354812-41-2	$C_{21}H_{24}FN_3O_4$	401.18	1146	2.90	6.3; 9.3
Norfloxacin	70458-96-7	$C_{16}H_{18}FN_3O_3$	319.13	1.78×10^5	-1.03	5.8
Roxithromycin	80214-83-1	$C_{41}H_{76}N_2O_{15}$	836.52	0.0189	1.70	12.5 ;9.1
Sulfadiazine	68-35-9	$C_{10}H_{10}N_4O_2S$	250.05	77	-0.09	6.4
Sulfamethoxazole	723-46-6	$C_{10}H_{11}N_3O_3S$	253.28	610	0.89	6.2; 2
Trimethoprim	738-70-5	$C_{14}H_{18}N_4O_3$	290.14	400	0.91	7.1
NSAIDs						
Aceclofenac	89796-99-6	$C_{16}H_{13}Cl_2NO_4$	354.18	insoluble	2.17	4.7
Celecoxib	169590-42-5	$C_{17}H_{14}F_3N_3O_2S$	381.37	slightly soluble	3.53	11.1
Diclofenac	15307-86-5	$C_{14}H_{11}Cl_2NO_2$	296.15	2.37	4.51	4.2
Etoricoxib	202409-33-4	$C_{18}H_{15}ClN_2O_2S$	358.84	3.28	0.88	4.5
Indomethacin	53-86-1	$C_{19}H_{16}ClNO_4$	357.79	0.937	4.27	4.5
Ketoprofen	22071-15-4	$C_{16}H_{14}O_3$	254.28	51	3.12	4.5

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	logKow	pKa
Lornoxicam	70374-39-9	$C_{13}H_{10}ClN_3O_4S_2$	371.82	15.5	2.62	4.7
Naproxen	22204-53-1	$C_{14}H_{14}O_3$	230.26	15.9	3.18	4.2
Nimesulide	51803-78-2	$C_{13}H_{12}N_2O_5S$	308.31	26.9	2.60	6.5
Piroxicam	36322-90-4	$C_{15}H_{13}N_3O_4S$	331.35	23	3.06	6.3
Tolfenamic acid	13710-19-5	$C_{14}H_{12}ClNO_2$	261.70	1000	5.17	5.1
Anxiolytics-Sedatives						
Alprazolam	28981-97-7	$C_{17}H_{13}ClN_4$	308.76	40	2.12	
Bromazepam	1812-30-2	$C_{14}H_{10}BrN_3O$	316.15	175	2.05	2.7
Buspirone	36505-84-7	$C_{21}H_{31}N_5O_2$	385.25	21.4	2.63	7.6
Clobazam	22316-47-8	$C_{16}H_{13}ClN_2O_2$	300.74	266.9	1.69	6.7
Diazepam	439-14-5	$C_{16}H_{13}ClN_2O$	284.74	50	2.82	3.4
Flunitrazepam	1622-62-4	$C_{16}H_{12}FN_3O_3$	313.28	8.58	2.06	1.8
Lorazepam	846-49-1	$C_{15}H_{10}Cl_2O_2N_2$	321.16	80	2.39	13
Midazolam	59467-70-8	$C_{18}H_{13}ClFN_3$	325.77	24	4.33	5.5
Oxazepam	604-75-1	$C_{15}H_{11}ClN_2O_2$	286.71	179	2.24	10.6; -1.5
Triazolam	28911-01-5	$C_{17}H_{12}Cl_2N_4$	343.21	4.53	2.42	4.3
Antidepressants						
Amitriptyline	549-18-8	$C_{20}H_{23}N$*HCl	313.86	9.71	4.92	9.8
Bupropion	34911-55-2	$C_{13}H_{18}ClNO$	239.11	140	3.85	8.2
Citalopram	59729-33-8	$C_{20}H_{21}FN_2O$	324.16	5.9	3.50	9.8
Doxepin	1668-19-5	$C_{19}H_{21}NO$	279.16	31.6	4.29	9.8
Duloxetine	116539-59-4	$C_{18}H_{19}NOS$	297.12	13	4.68	9.7
Fluvoxamine	54739-18-3	$C_{15}H_{21}F_3N_2O_2$	318.16	7.34	3.20	9.2
Sertraline	79617-96-2	$C_{17}H_{17}Cl_2N$	305.07	3.5	5.29	9.9
Venlafaxine	93413-69-5	$C_{17}H_{27}NO_2$	277.20	267	3.28	8.9

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	logKow	pKa
Antineoplastics						
Capecitabine	154361-50-9	$C_{15}H_{22}FN_3O_6$	359.35	26000	0.40	1.9
Cyclophosphamide	50-18-0	$C_7H_{15}Cl_2N_2O_2P$	260.02	40000	0.63	2.8
Cytarabine	147-94-4	$C_9H_{13}N_3O_5$	243.09	1000000	-2.8	4.2
Dacarbazine	04/03/4342	$C_6H_{10}N_6O$	182.18	4220	-0.24	4.4
Doxorubicin	23214-92-8	$C_{27}H_{29}NO_{11}$	543.17	2600	1.27	7.3;8.5;9.5
Methotrexate	59-05-2	$C_{20}H_{22}N_8O_5$	454.17	2600	-1.85	4.7
Tamoxifen citrate	10540-29-1	$C_{26}H_{29}NO$	371.52	1.02	6.3	8.7
Viblastine	865-21-4	$C_{46}H_{58}N_4O_9$	810.42	$4{,}46\times10^{-2}$	3.7	5.4;7.4
Beta-blockers						
Atenolol	29122-68-7	$C_{14}H_{22}N_2O_3$	266.16	13300	0.16	9.6
Bisoprolol	66722-44-9	$C_{18}H_{31}NO_4$	325.23	2240	1.87	9.3; 14.1
Carvedilol	72956-09-3	$C_{24}H_{26}N_2O_4$	406.47	0.583	4.19	7.8
Metoprolol	51384-51-1	$C_{15}H_{25}NO_3$	267.18	16900	1.88	14.1
Pindolol	13523-86-9	$C_{14}H_{20}N_2O_2$	248.15	7880	1.75	9.3
Propranolol	525-66-6	$C_{16}H_{21}NO_2$	259.16	61.7	3.48	9.4
Timolol	26839-75-8	$C_{13}H_{24}N_4O_3S$	316.16	2740	1.83	9.2
Antihypertensives						
Enalapril	75847-73-3	$C_{20}H_{28}N_2O_5$	376.2	16400	2.00	3; 5.4
Irbesartan	138402-11-6	$C_{25}H_{28}N_6O$	428.23	0.059	6.00	4.1; 4.3
Losartan	114798-26-4	$C_{22}H_{23}ClN_6O$	422.16	0.82	6.10	5.5
Ramipril	87333-19-5	$C_{23}H_{32}N_2O_5$	416.23	3.5	3.32	3.7; 5.2
Telmisartan	144701-48-4	$C_{33}H_{30}N_4O_2$	514.62	insoluble	7.70	3.6; 6.1
Valsartan	137862-53-4	$C_{24}H_{29}N_5O_3$	435.23	1406	5.80	3.6
Antidiabetics						

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	logKow	pKa
Glibenclamide	10238-21-8	$C_{23}H_{28}ClN_3O_5S$	494.00	4	4.79	4.3; -1.2
Gliclazide	21187-98-4	$C_{15}H_{21}N_3O_3S$	323.13	190	2.12	5.8
Glimepiride	93479-97-1	$C_{24}H_{34}N_4O_5S$	490.22	insoluble	3.50	5.0
Glipizide	29094-61-9	$C_{21}H_{27}N_5O_4S$	445.18	37.2	1.91	5.9
Metformin	657-24-9	$C_4H_{11}N_5$	129.10	1.06×10^6	-1.00	12.0
Repaglinide	135062-02-1	$C_{27}H_{36}N_2O_4$	452.27	2.94	5.90	3.7
Urinary tract pharmaceuticals						
Alfuzosin	81403-80-7	$C_{19}H_{27}N_5O_4$	389.21	92	1.40	8.1
Finasteride	98319-26-7	$C_{23}H_{36}N_2O_2$	372.28	11,7	3.03	4.9; 6.2
Progesterone	57-83-0	$C_{21}H_{30}O_2$	314.22	8.81	3.87	18.9; -4.8
Raloxifene	84449-90-1	$C_{28}H_{27}NO_4S$	473.17	0.25	6.09	8; 8.9; 9.9
Sildenafil	139755-83-2	$C_{22}H_{30}N_6O_4S$	474.20	3500	2.75	6.0
Analgesics and muscle relaxants						
Acetaminophen	103-90-2	$C_8H_9NO_2$	151.16	1.40×10^4	0.46	9.4
Orphenadrine	4682-36-4	$C_{24}H_{31}NO_8$	461.20	30	3.77	8.9
Thiocolchicoside	602-41-5	$C_{27}H_{33}NO_{10}S$	563.62	10000	0.34	12.7
Tizanidine	51322-75-9	$C_9H_8ClN_5S$	253.71	133	1.40	7.5
Tramadol	27203-92-5	$C_{16}H_{25}NO_2$	263.38	1151	3.00	9.4
Antipsychotic drugs						
Amisulpride	71675-85-9	$C_{17}H_{27}N_3O_4S$	369.48	293	1.06	9.0
Olanzapine	132539-06-1	$C_{17}H_{20}N_4S$	312.43	39.88	3.00	4.0; 7.2; 14.2
Quetiapine	111974-72-2	$C_{21}H_{25}N_3O_2S$	383.51	0.5869	2.80	7.1
Risperidone	106266-06-2	$C_{23}H_{27}FN_4O_2$	410.48	2330	3.49	8.8
Anticonvulsants						
Carbamazepine	298-46-4	$C_{15}H_{12}N_2O$	236.09	17.7	2.45	3.8

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	$\log K_{ow}$	pK_a
Gabapentin	60142-96-3	$C_9H_{17}NO_2$	171.24	4490	1.10	3.7
Lamotrigine	84057-84-1	$C_9H_7Cl_2N_5$	256.09	170	2.50	8.5; 9.2
Pregabalin	148553-50-8	$C_8H_{17}NO_2$	159.23	12000	-1.35	4.2; 10.6
Lipid regulators						
Atorvastatin	134523-00-5	$C_{33}H_{35}FN_2O_5$	558.25	1.12×10^{-3}	6.00	4.3 ; 14.9
Bezafibrate	41859-67-0	$C_{19}H_{20}ClNO_4$	361.11	1.55	4.00	3.8; -0.8
Clofibric acid (TP of clofibrate)	882-09-7	$C_{10}H_{11}ClO_3$	214.65	583	2.57	3.2
Rosuvastatin	287714-41-4	$C_{22}H_{28}FN_3O_6S$	481.17	17.96	0.13	4.0
Antihistamines						
Cetirizine dihydrochloride	83881-51-0	$C_{21}H_{25}ClN_2O_3$	388.16	101	2.80	2.7; 3.6; 7.6
Desloratadine (TP of loratadine)	100643-71-8	$C_{19}H_{19}ClN_2$	310.12	3.95	3.20	9.7
Ebastine	90729-43-4	$C_{32}H_{39}NO_2$	469.30	2	7.20	8.2
Methdilazine	1982-37-2	$C_{18}H_{20}N_2S$	296.13	0.348	5.23	7.5
Proton pump inhibitors						
Lansoprazole	103577-45-3	$C_{16}H_{14}F_3N_3O_2S$	369.08	0,97	1.90	1.1; 6.9; 12
Omeprazole	73590-58-6	$C_{17}H_{19}N_3O_3S$	345.11	359	2.23	1.2; 7.4
Pantoprazole	102625-70-7	$C_{16}H_{15}F_2N_3O_4S$	383.08	48	0.50	3.9; 8.2
Antidiarrheals						
Loperamide	53179-11-6	$C_{29}H_{33}ClN_2O_2$	476.22	405	5.15	9.4; 14
Rifaximin	80621-81-4	$C_{43}H_{51}N_3O_{11}$	785.35	7.38	2.60	11.9
Antivirals						
Abacavir sulphate	188062-50-2	$C_{14}H_{18}N_6O$	286.33	77000	1.20	5.8; 15.4
Adefovir	106941-25-7	$C_8H_{12}N_5O_4P$	273.06	7.64×10^{4}	-2,28	2.0; 6.8
Diuretics						
Furosemide	54-31-9	$C_{12}H_{11}ClN_2O_5S$	330.74	73.1	2.03	3.9
Indapamide	26807-65-8	$C_{16}H_{16}ClN_3O_3S$	365.06	75	2.00	8.8

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	$\log K_{ow}$	pK_a
Cardiovascular agents						
Dopamine	62-31-7	$C_8H_{12}ClNO_2$	189.06	1×10^6	-0.98	8.93
Trimetazidine	5011-34-7	$C_{14}H_{22}N_2O_3$	266.16	754	1.04	4.5; 9.1
Antifungals						
Fluconazole	86386-73-4	$C_{13}H_{12}F_2N_6O$	306.10	1	0.40	2.3
Voriconazole	137234-62-9	$C_{16}H_{14}F_3N_5O$	349.12	610	1.00	1.8
Anti-vertigo						
Betahistine	5638-76-6	$C_8H_{12}N_2$	136.10	1×10^6	0.68	10.1
Cinnarizine	298-57-7	$C_{26}H_{28}N_2$	368.23	750	5.77	2 ; 7.5
Corticosteroids						
Prednisolone	50-24-8	$C_{21}H_{28}O_5$	360.44	223	1.62	12.6; -2.9
Fluticasone propionate	80474-14-2	$C_{25}H_{31}F_3O_5S$	500.57	0.51	3.40	13.6
Antiulcer agents						
Cimetidine	51481-61-9	$C_{10}H_{16}N_6S$	252.12	9380	0.40	6.8
Ranitidine	66357-35-5	$C_{13}H_{22}N_4O_3S$	314.14	24700	0.27	8.2 ;2.7
Anesthetics						
Lidocaine	137-58-6	$C_{14}H_{22}N_2O$	234.34	4100	2.44	7.9
Prilocaine	721-50-6	$C_{13}H_{20}N_2O$	220.16	541	2.11	7.9
Calcium channel blockers						
Diltiazem	42399-41-7	$C_{22}H_{26}N_2O_4S$	414.16	465	2.80	8.1
Nifedipine	21829-25-4	$C_{17}H_{18}N_2O_6$	346.12	1.7×10^{-5}	2.20	3.9
Laxative						
Bisacodyl	603-50-9	$C_{22}H_{19}NO_4$	361.13	1.27	3.00	4.7
Mucolytic agent						
Bromhexine	611-75-6	$C_{14}H_{21}Br_2ClN_2$	409.98	3.62	4.30	9.3

PPCPs	CAS No	Molecular formula	MW (g/mol)	Water solubility (mg/L, 25°C)	$\log K_{ow}$	pK_a
Anti-Parkinson						
Pramipexole	104632-25-9	$C_{10}H_{17}N_3S$	211.33	3900	0.40	4.7 ; 10.3; 17.7
β_2 adrenergic receptor agonist						
Salbutamol	18559-94-9	$C_{13}H_{21}NO_3$	239.15	1.41×10^{4}	1.40	10.3
Antiplatelet agent						
Clopidogrel	113665-84-2	$C_{16}H_{16}ClNO_2S$	321.06	50.78	3.80	5.3
Thyroid hormone						
Levothyroxine	51-48-9	$C_{15}H_{11}I_4NO_4$	776.69	1.05×10^{-4}	4.12	0.3; 7.4; 9.4
Stimulant						
Caffeine	58-08-2	$C_8H_{10}N_4O_2$	194.08	2.16×10^{4}	-0.07	10.4
Antiseptic/antibacterial						
Triclosan	3380-34-5	$C_{12}H_7Cl_3O_2$	287.95	10	4.76	7.9
Boosting supplement						
Caffeic acid	331-39-5	$C_9H_8O_4$	180.04	5.41×10^{4}	1.15	4.62
Insect repellent						
DEET	134-62-3	$C_{12}H_{17}NO$	191.13	912	2.02	-1.4
UVA/UVB filters						
BP-1	119-61-9	$C_{13}H_{10}O_3$	182.22	137	3.18	n.a.
BP-2	131-55-5	$C_{13}H_{10}O_5$	246.22	8821	2.78	7.1; 7.9
BP-3	131-57-7	$C_{14}H_{12}O_3$	228.08	3.7	3.79	7.1
PABA	150-13-0	$C_7H_7NO_2$	137.05	6110	0.83	2.4

Table S5 Instrumental Parameters in LC–Orbitrap MS/MS

Time (min)	Flow (mL min^{-1})	MeOH + 0.1% FA	H_2O + 0.1% FA
0.0	0.200	10.0	90.0
1.5	0.200	10.0	90.0
4.0	0.200	60.0	40.0
8.0	0.200	70.0	30.0
11.0	0.200	100.0	0.0
13.0	0.200	100.0	0.0
14.0	0.350	10.0	90.0
15.0	0.350	10.0	90.0

HESI Parameters	Value
Tube lens (V)	110
Sheath gas flow rate	45
Auxiliary gas flow rate	10
Sweep gas fow rate	2
Spray voltage (|kV|)	2.5
Cap. Temperature (°C)	320
S-lens RF	50
Heater temperature (°C)	400

MS Parameters	Value
Polarity	Negative
Resolution	70,000
Scan Range	100–1000 m/z
AGC Target	10^6
Maximum IT	auto
Microscan	1

MS/MS Parameters	Value
Resolution	17,500
Isolation window	1 m/z
CE/(N)CE	15-30-50
AGC target	2*10^5
Maximum IT	auto
Apex trigger	2-5 s

LC Parameters	Value
Injection volume (µL)	5
Column temperature (°C)	40

Table S6 LC-Orbitrap MS/MS data for the target PhACs

PhACs	Formula	RT	ESI	Adduct Ion	m/z (theor)	m/z (exp.)	Δ (ppm)	Fragments			
Amoxicillin	$C_{16}H_{19}N_3O_5S$	5.07	+	M+H	**366.1118**	398.1379	-0.2512	321.0900	211.0711	208.0415	160.0425
	$C_{16}H_{19}N_3O_4S$			M+CH3OHOH+H	398.138						
Ampicillin	$C_{38}H_{72}N_2O_{12}$	6.11	+	M+H	**350.1169**	350.1173	1.0826	106.0655	192.0475	160.0429	174.0548
	$C_{17}H_{18}FN_3O_3$			M+CH3OHOH+H	382.1431						
Azithromycin	$C_{38}H_{69}NO_{13}$	7.04	+	M+H	**749.5158**	749.5143	-2.0250	591.4199	278.2111		
Ciprofloxacin	$C_{37}H_{67}NO_{13}$	6.24	+	M+H	**332.1405**	332.1411	1.7546	231.0562	245.1082	288.1500	249.0663
Clarithromycin	$C_{37}H_{65}NO_{12}$	9.19	+	M+H	**748.4842**	748.4850	1.1308	158.1176	83.0498	590.3898	116.1074
Erythromycin	$C_6H_7N_3O$	8.20	+	M-H2O+H	**716.4580**	716.4570	-0.2792	158.1176	83.0498	127.0754	116.0706
	$C_{18}H_{20}FN_3O_4$			M+H	734.4685						
Isoniazid	$C_{18}H_{34}N_2O_6S$	1.38	+	M+H	**138.0662**	138.0668	4.3292	57.0706			
Levofloxacin	$C_6H_9N_3O_3$	6.13	+	M+H	**362.1511**	362.1510	-0.2734	731.6874	323.9638	633.7614	
Lincomycin	$C_{21}H_{24}FN_3O_4$	5.53	+	M+H	**407.2210**	407.2218	1.8952	266.1538	210.1276		
Metronidazole	$C_{16}H_{18}FN_3O_3$	3.10	+	M+H	**172.0717**	172.0720	1.9540	261.1034	382.1755	358.1924	305.0940
Moxifloxacin	$C_{41}H_{76}N_2O_{15}$	6.78	+	M+H	**402.1824**	402.1831	1.7541	261.1035	382.1745	110.0968	82.0812
Norfloxacin	$C_{10}H_{10}N_4O_2S$	6.19	+	M+H	**320.1405**	320.1414	2.7736	233.1083	148.0555	219.0925	
Roxithromycin	$C_{10}H_{11}N_3O_3S$	9.41	+	M+H	**837.5319**	837.5320	0.2310	158.1175	649.4368	83.0498	116.1072
Sulfadiazine	$C_{14}H_{18}N_4O_3$	3.43	+	M+H	**251.0597**	251.0600	1.1055	108.0446	65.0392	156.0106	
Sulfamethoxazole	$C_{16}H_{13}Cl_2NO_4$	5.94	+	M+H	**254.0594**	254.0599	2.1512	108.0448	65.0393	92.0500	156.0117
Trimethoprim	$C_{17}H_{14}F_3N_3O_2S$	5.70	+	M+H	**291.1452**	291.1457	1.7892	123.0667	161.0822	245.1031	230.1160
Aceclofenac	$C_{14}H_{11}Cl_2NO_2$	10.20	+	M+H	**354.0294**	354.0299	1.4327	214.0416	215.0490	250.0182	
Celecoxib	$C_{18}H_{15}ClN_2O_2S$	9.940	-	M-H	**380.0686**	380.0691	1.2137	68.9944	316.1071	276.0941	247.1109
Diclofenac	$C_{19}H_{16}ClNO_4$	10.43	+	M+H	**296.0240**	296.0245	1.8431	278.0131	250.0182	215.0494	
Etoricoxib	$C_{16}H_{14}O_3$	7.08	+	M+H	**359.0616**	359.0620	1.3709	312.0656	279.0681	243.0913	
Indomethacin	$C_{13}H_{10}ClN_3O_4S_2$	10.45	+	M+H	**358.0841**	358.0849	2.3191	207.0914	195.1490	180.0805	84.0813
Ketoprofen	$C_{14}H_{14}O_3$	8.39	+	M+H	**255.1016**	255.1020	1.7052	210.9820	108.9843	58.0408	166.0294
Lornoxicam	$C_{13}H_{12}N_2O_5S$	7.98	+	M+H	**371.9874**	371.9882	2.0409	207.0915	180.0805	152.0619	
Naproxen	$C_{15}H_{13}N_3O_4S$	10.65	-	M-H	**229.0870**	229.0865	-2.1276	254.1039	211.0861	195.0918	239.0806
Nimesulide	$C_{14}H_{12}ClNO_2$	8.19	-	M-H	**307.0394**	307.0402	2.6777	229.0618	214.9259	198.0553	241.5405

PhACs	Formula	RT	ESI	Adduct Ion	m/z (theor)	m/z (exp.)	Δ (ppm)	Fragments			
Piroxicam	$C_{15}H_{22}FN_3O_6$	7.78	+	M+H	**332.0700**	332.0705	1.6430	95.0609	121.0399	91.0549	
Tolfenamic Acid	$C_7H_{15}Cl_2N_2O_2P$	12.15	-	M-H	**260.0483**	260.0486	1.3268	244.0525	246.0493	209.1196	159.0611
Capecitabine	$C_9H_{13}N_3O_5$	7.48	+	M+H	**360.1565**	360.1570	1.2547	130.0413	174.0311	244.1093	
Cyclophosphamide	$C_6H_{10}N_6O$	6.95	+	M+H	**261.0321**	261.0324	1.0694	140.0032	106.0418	233.0017	
Cytarabine	$C_{27}H_{29}NO_{11}$	1.21	+	M+H	**244.0928**	244.0937	3.6419	112.0508	95.0245		
Dacarbazine	$C_{20}H_{22}N_8O_5$	2.58	+	M+H	**183.0989**	183.0996	3.6243	65.0142	123.0428	90.9482	
Doxorubicin	$C_{26}H_{29}NO$	8.13	+	M+H	**544.1813**	544.1822	1.5619	361.0693	86.0605	321.0749	130.0861
Methotrexate	$C_{46}H_{58}N_4O_9$	6.01	+	M+H	**455.1786**	455.1808	4.7577	94.0656	106.0655	170.0366	
Tamoxifen	$C_{17}H_{13}ClN_4$	11.68	+	M+H	**372.2322**	372.2328	1.4979	321.6286	72.0815		
Viblastine	$C_{14}H_{10}BrN_3O$	7.11	+	M+H	**811.4277**	811.4280	0.3432	224.1274	751.4069	355.2013	542.3049
Alprazolam	$C_{21}H_{31}N_5O_2$	8.42	+	M+H	**309.0902**	309.0902	0.0000	281.0703	205.0705	274.1207	
Bromazepam	$C_{16}H_{13}ClN_2O_2$	7.42	+	M+H	**316.0080**	316.0085	1.7244	182.0839	209.0946	261.0022	288.0131
Buspirone	$C_{16}H_{13}ClN_2O$	6.79	+	M+H	**386.2551**	386.2555	1.2263	122.0714	148.0870	222.1489	265.1910
Clobazam	$C_{16}H_{12}FN_3O_3$	9.46	+	M+H	**301.0738**	301.0738	0.0000	185.0961	141.0698	170.0725	71.9526
Diazepam	$C_{15}H_{10}Cl_2O_2N_2$	9.12	+	M+H	**285.0789**	285.0793	1.4933	154.0417	257.0838	193.0886	222.1150
Flunitrazepam	$C_{18}H_{13}ClFN_3$	7.80	+	M+H	**314.0936**	314.0935	0.3184	300.0894	183.0600		
Lorazepam	$C_{15}H_{11}ClN_2O_2$	8.06	+	M+H	**321.0192**	321.0191	0.3115	275.0128	292.9292	229.0521	
Midazolam	$C_{17}H_{12}Cl_2N_4$	7.46	+	M+H	**326.0855**	326.0854	0.3067	291.1162	222.0713	183.0606	109.0452
Oxazepam	$C_{20}H_{28}N_2O_5$	8.08	+	M+H	**287.0581**	287.0582	-0.3484	241.0524	104.0499	231.0681	118.0527
Triazolam	$C_{25}H_{28}N_6O$	8.60	+	M+H	**343.0512**	343.0509	0.8745	308.0820	315.0319	239.0368	
Enalapril	$C_{22}H_{23}ClN_6O$	7.18	+	M+H	**377.2071**	377.2078	1.7594	91.0548	234.1487	117.0701	160.1120
Irbesartan	$C_{23}H_{32}N_2O_5$	8.44	+	M+H	**429.2397**	429.2404	1.7426	111.0318	121.0398	93.0452	
Losartan	$C_{33}H_{30}N_4O_2$	8.11	+	M+H	**423.1695**	423.1701	1.5018	207.0922	180.0813	171.0689	405.1605
Ramipril	$C_{24}H_{29}N_5O_3$	8.15	+	M+H	**417.2384**	417.2391	1.6171	234.1487	117.0701	130.0864	160.1119
Telmisartan	$C_{20}H_{23}N$*HCl	8.97	+	M+H	**515.2442**	515.2453	2.1355	185.0956	276.1360	170.0721	261.1125
Valsartan	$C_{13}H_{18}ClNO$	9.07	+	M+H	**436.2343**	436.2358	3.3441	207.0916	180.0807	235.0991	291.1488
Amitriptyline	$C_{20}H_{21}FN_2O$	8.41	+	M+H	**278.1903**	278.1908	1.7844	91.0548	105.0703	117.0701	191.0852
Bupropion	$C_{19}H_{21}NO$	6.83	+	M+H	**240.1150**	240.1154	1.9272	131.0730	166.0419	139.0309	184.0525
Citalopram	$C_{18}H_{19}NOS$	7.21	+	M+H	**325.1711**	325.1716	1.5371	109.0452	262.1019	116.0498	
Doxepin	$C_{15}H_{21}F_3N_2O_2$	7.44	+	M+H	**280.1696**	280.1702	2.0560	107.0495	141.0697	117.0700	84.0813

PhACs	Formula	RT	ESI	Adduct Ion	m/z (theor)	m/z (exp.)	Δ (ppm)	Fragments			
Duloxetine	$C_{17}H_{17}Cl_2N$	8.20	+	M+H	**298.1260**	298.1266	1.8328	144.1382	100.1125		
Fluvoxamine	$C_{17}H_{27}NO_2$	8.49	+	M+H	**319.1628**	319.1633	1.6922	71.0499	200.0680	228.0988	87.0808
Sertraline	$C_{14}H_{22}N_2O_3$	9.07	+	M+H	**306.0811**	306.0817	2.1108	275.0383	196.9916	158.9761	129.0698
Venlafaxine	$C_{18}H_{31}NO_4$	7.04	+	M+H	**278.2115**	278.2119	1.5224	58.0659	121.0650	121.0650	147.0806
Atenolol	$C_{24}H_{26}N_2O_4$	3.57	+	M+H	267.1703	267.1707	1.4797	225.1229	190.0860	116.1071	98.0967
Bisoprolol	$C_{15}H_{25}NO_3$	6.97	+	M+H	**326.2326**	326.2331	1.6668	116.1073	74.0608	98.0966	
Carvedilol	$C_{14}H_{20}N_2O_2$	7.51	+	M+H	**407.1965**	407.1971	1.5068	100.0762	222.0914	283.1440	194.0966
Metoprolol	$C_{16}H_{21}NO_2$	6.38	+	M+H	**268.1907**	268.1910	1.1933	62.9469	115.9702	128.0458	
Pindolol	$C_{13}H_{24}N_4O_3S$	5.53	+	M+H	**249.1598**	249.1602	1.8142	67.0550			
Propranolol	$C_{23}H_{28}ClN_3O_5S$	7.21	+	M+H	**260.1645**	260.1650	2.0720	116.1074	155.0856	183.0806	56.0503
Timolol	$C_{15}H_{21}N_3O_3S$	6.33	+	M+H	**317.1642**	317.1647	1.7148	244.0749	188.0489	74.0608	56.0503
Glibenclamide	$C_{24}H_{34}N_4O_5S$	9.91	+	M+H	**494.1511**	494.1519	1.5906	304.0730			
Gliclazide	$C_{21}H_{27}N_5O_4S$	8.35	+	M+H	**324.1376**	324.1382	1.7063	110.0965	127.1228	153.1019	156.0191
Glimepiride	$C_4H_{11}N_5$	10.48	+	M+H	**491.2323**	491.2342	3.9124	292.0995	276.1928	271.1433	
Glipizide	$C_{27}H_{36}N_2O_4$	8.06	+	M+H	**446.1857**	446.1865	1.7771	167.0162	111.0556	103.0547	286.0643
Metformin	$C_{19}H_{27}N_5O_4$	1.19	+	M+H	**130.1087**	130.1092	3.3924	98.0969	180.0806	96.0814	237.0603
Repaglinide	$C_{23}H_{36}N_2O_2$	8.92	+	M+H	**453.2748**	453.2755	1.6838	230.1903	86.0971	162.1277	174.1278
Alfuzosin	$C_{21}H_{30}O_2$	6.71	+	M+H	**390.2136**	390.2141	1.2834	71.0499	156.1020	235.1188	275.1494
Finasteride	$C_{28}H_{27}NO_4S$	9.90	+	M+H	**373.2850**	373.2857	2.0241	305.2582	317.2217		
Progesterone	$C_{22}H_{30}N_6O_4S$	11.48	+	M+H	**315.2319**	315.2324	1.4619	97.0654	109.0653	123.0807	81.0706
Raloxifene	$C_8H_9NO_2$	7.35	+	M+H	**474.1734**	474.1743	1.8683	112.1124	84.0814	269.0266	
Sildenafil Citrate	$C_{24}H_{31}NO_8$	7.68	+	M+H	**475.2122**	475.2134	2.6092	58.0659	100.1000		
Acetaminophen	$C_{27}H_{33}NO_{10}S$	3.17	+	M+H	**152.0706**	152.0710	2.7597	110.0600	73.0648	59.0494	
Orphenadrine	$C_9H_8ClN_5S$	7.84	+	M+H	**270.1852**	270.1857	1.8135	165.0699	181.1011	115.0545	141.0698
Thiocolchicoside	$C_{16}H_{25}NO_2$	6.46	+	M+H	**564.1898**	564.1913	2.6484	402.1363	360.1260	89.0603	
Tizanidine	$C_{17}H_{27}N_3O_4S$	4.83	+	M+H	**254.0262**	254.0267	1.9796	55.9351	186.9353		
Tramadol	$C_{17}H_{20}N_4S$	6.35	+	M+H	**264.1958**	264.1964	2.0443	58.0659	246.18623.		
Amisulpride	$C_{21}H_{25}N_3O_2S$	5.85	+	M+H	**370.1795**	370.1803	2.0729	242.0479	112.1124	155.1177	129.1386
Olanzapine	$C_{23}H_{27}FN_4O_2$	5.48	+	M+H	**313.1481**	313.1486	1.6625	256.9010	282.1057	84.0814	115.0545
Quetiapine	$C_{15}H_{12}N_2O$	7.44	+	M+H	**384.1740**	384.1747	1.7768	253.0790	221.1070	279.0950	

PhACs	Formula	RT	ESI	Adduct Ion	m/z (theor)	m/z (exp.)	Δ (ppm)	Fragments			
Risperidone	$C_9H_{17}NO_2$	6.88	+	M+H	**411.2191**	411.2198	1.8692	191.1177	110.0605		
Carbamazepine	$C_9H_7Cl_2N_5$	7.66	+	M+H	**237.1022**	237.1025	1.1326	194.0966	179.0730	165.0700	
Gabapentin	$C_8H_{17}NO_2$	5.18	+	M+H	**172.1332**	172.1337	2.8322	62.9468			
Lamotrigine	$C_{33}H_{35}FN_2O_5$	6.47	+	M+H	**256.0151**	256.0156	1.8143	119.0606	136.0757	234.0193	252.0298
Pregabalin	$C_{19}H_{20}ClNO_4$	5.07	+	M+H	**160.1332**	160.1335	2.0915	72.9377	55.9350	56.9429	51.9407
Atorvastatin	$C_{10}H_{11}ClO_3$	10.00	+	M+H	**559.2603**	559.2620	3.0091	440.2231	466.2022	292.1494	380.1643
Bezafibrate	$C_{22}H_{28}FN_3O_6S$	8.79	+	M+H	**362.1154**	362.1160	1.6757	138.9947	121.0650	161.0960	316.1089
Clofibric Acid	$C_{14}H_{18}N_6O$	8.54	-	M-H	**213.0323**	213.0325	0.7297	91.0178	126.9946	135.0076	65.0020
Rosurvastatin	$C_8H_{12}N_5O_4P$	8.07	+	M+H	**482.1756**	482.1754		446.1541	464.1648	376.1489	133.0446
Abacavir	$C_{21}H_{25}ClN_2O_3$	5.82	+	M+H	**287.1615**	287.1621	2.1221	191.1039	79.0549	150.0649	174.0776
Adefovir	$C_{19}H_{19}ClN_2$	8.15	+	M+H	**502.2061**	502.2072	2.1582	57.0707	274.0696	162.0774	358.1271
Cetirizine	$C_{32}H_{39}NO_2$	8.53	+	M+H	**389.1627**	389.1631	1.2770	201.0461	166.0779		
Desloratadine	$C_{18}H_{20}N_2S$	7.28	+	M+H	**311.1310**	311.1314	1.3136	259.1353	279.0805	242.0962	217.0888
Ebastine	$C_8H_{12}ClNO_2$	11.68	+	M+H	**470.3054**	470.3062	1.6847	167.0854	203.1428	161.0959	
Methdilazine	$C_{14}H_{22}N_2O_3$	8.20	+	M+H	**297.1420**	297.1425	1.8429	308.1249	175.0726	134.0600	
Dopamine	$C_{12}H_{11}ClN_2O_5S$	1.22	+	M+H	**154.0863**	154.0865	1.4720	91.0547	65.0393	55.9352	119.0493
Trimetazidine	$C_{16}H_{16}ClN_3O_3S$	3.57	+	M+H	**267.1703**	267.1707	1.4797	145.0644	74.0404	56.0501	98.9756
Furosemide	$C_{29}H_{33}ClN_2O_2$	6.98	-	M-H	**329.0004**	329.0012	2.4018	204.9839	77.9643	126.0105	
Indapamide	$C_{43}H_{51}N_3O_{11}$	7.08	+	M+H	**366.0674**	366.0687	3.5364	298.1682	316.1796	284.1551	280.1597
Loperamide	$C_{16}H_{14}F_3N_3O_2S$	8.70	+	M+H	**477.2303**	477.2312	1.8244	121.0396	95.0607		
Rifaximin	$C_{17}H_{19}N_3O_3S$	9.95	+	M+H	**786.3596**	786.3594	-0.2085	754.3322	362.1130	151.0753	123.0806
Lansoprazole	$C_{16}H_{15}F_2N_3O_4S$	7.64	+	M+H	**370.0832**	370.0835	0.8257	261.1032	318.1609	122.0403	
Omeprazole	$C_{13}H_{12}F_2N_6O$	8.36	+	M+H	**346.1220**	346.1223	0.9967	136.0757	180.0476	151.0992	108.0811
Pantoprazole	$C_{16}H_{14}F_3N_5O$	7.20	+	M+H	**384.0824**	384.0830	1.5825	138.0549	200.0375	154.0498	
Fluconazole	$C_8H_{12}N_2$	6.40	+	M+H	**307.1113**	307.1118	1.6506	238.0784	220.0679	169.0459	127.0355
Voriconazole	$C_{26}H_{28}N_2$	8.25	+	M+H	**350.1223**	350.1230	2.0761	127.0356	281.0896	224.0628	
Betahistine	$C_{21}H_{28}O_5$	1.29	+	M+H	**137.1073**	137.1077	2.7808	94.0656	72.9373	90.9483	55.9352
Cinnarizine	$C_{25}H_{31}F_3O_5S$	9.26	+	M+H	**369.2325**	369.2332	1.8561	167.0855	152.0620	165.0701	
Prednisolone	$C_{10}H_{16}N_6S$	7.63	+	M+H	**361.2010**	361.2013	0.8138	174.0806	121.0646	91.0551	173.0965
Fluticasone	$C_{13}H_{22}N_4O_3S$	10.38	+	M+H	**501.1917**	501.1928	2.1949	293.1530	275.1430	313.1601	

PhACs	Formula	RT	ESI	Adduct Ion	m/z (theor)	m/z (exp.)	Δ (ppm)	Fragments			
Cimetidine	$C_{14}H_{22}N_2O$	3.45	+	M+H	**253.1230**	253.1234	1.4303	95.0610	117.0485	159.0701	99.0671
Ranitidine	$C_{13}H_{20}N_2O$	3.76	+	M+H	**315.1485**	315.1491	1.7083	176.0491	130.0560	102.0376	125.0057
Lidocaine	$C_{22}H_{26}N_2O_4S$	5.92	+	M+H	**235.1805**	235.1810	2.1026	100.0761	222.0912	56.0503	
Prilocaine	$C_{17}H_{18}N_2O_6$	6.08	+	M+H	**221.1648**	221.1653	2.0729	86.0970			
Diltiazem	$C_{22}H_{19}NO_4$	7.58	+	M+H	**415.1686**	415.1692	1.4198	178.0321	137.0595	150.0372	
Nifedipine	$C_{14}H_{21}Br_2ClN_2$	8.34	+	M+H	**347.1238**	347.1232	-1.7027	333.1079	138.0551	315.0973	
Bisacodyl	$C_{10}H_{17}N_3S$	7.93	+	M+H	**362.1387**	362.1392	1.3259	184.0757	167.0729	226.0864	320.1274
Bromhexine	$C_{13}H_{21}NO_3$	7.86	+	M+H	**375.0066**	375.0073	1.9312	263.8752	261.8773	114.1262	
Pramipexole	$C_{16}H_{16}ClNO_2S$	1.21	+	M+H	**212.1216**	212.1220	1.7608	111.0443	103.0546	166.0860	131.0492
Salbutamol	$C_{15}H_{11}I_4NO_4$	3.03	+	M+H	**240.1594**	240.1598	1.7314	148.0756	166.0862	222.1486	
Clopidogrel	$C_8H_{10}N_4O_2$	9.55	+	M+H	322.0663	322.0661		212.0473	184.0516	125.0154	155.0248
Levothyroxine	$C_{12}H_7Cl_3O_2$	8.95	+	M+H	**777.6940**	777.6958	2.3155	86.0970	731.6902	604.7806	
Caffeine	$C_9H_8O_4$	5.99	+	M+H	**195.0877**	195.0882	2.7977	138.0663	110.0716	83.0610	69.0455
Triclosan	$C_{12}H_{17}NO$	11.93	-	M-H	**286.9438**	286.9438	-0.1530	307.4193	255.2432	191.3187	174.6795
Caffeic Acid	$C_{13}H_{10}O_3$	5.81	-	M-H	**179.0349**	179.0345	-2.4892	135.0442	133.0292	89.0383	
DEET	$C_{13}H_{10}O_5$	8.17	+	M+H	**192.1383**	192.1387	2.2531	119.0494	109.0652	91.0548	65.0393
BP1	$C_{14}H_{12}O_3$	8.47	-	M-H	**213.0557**	213.0555	-1.1713	91.0178	126.9946	153.0186	135.0076
BP2	$C_7H_7NO_2$	7.12	-	M-H	**245.0455**	245.0457	0.8787	109.0284	91.0178	153.0181	65.0385
BP3	$C_{19}H_{21}NO_4$	8.70	+	M+H	**229.0859**	229.0870	4.9594	169.0645	158.0359		
PABA	$C_{16}H_{14}FN_3O$	3.00	+	M+H	**138.0550**	138.0554	2.8206	65.0393	92.0500		

*Quantitation ions in bold

Table S7 Summary of mean recoveries (%R), precision (%RSD$_R$, n=6) and method quantification limits (MQL) in the two different matrices and matrix effect study results on effluents

Compounds	Influent					Effluent				
	50 ng L^{-1}		100 ng L^{-1}		MQL	50 ng L^{-1}		100 ng L^{-1}		MQL
	% R	%RSD$_R$	% R	%RSD$_R$	(ng/L)	% R	%RSD$_R$	% R	%RSD$_R$	(ng/L)
Amoxicillin	50	20	51	27	10.0	55	20	53	21	10.0
Ampicillin	47	28	58	21	20.0	43	17	55	18	20.0
Azithromycin	70	14	74	15	10.0	68	9	72	11	10.0
Ciprofloxacin	96	35	99	27	3.8	98	31	104	31	3.9
Clarithromycin	70	15	64	9	10.0	62	9	65	10	10.0
Erythromycin	60	10	72	11	0.1	55	11	72	10	0.1
Isoniazide	<30	22	31	19	25.0	<30	20	31	16	25.0
Levofloxacin	38	10	39	10	10.0	33	10	35	10	10.0
Lincomycin	75	30	82	23	0.1	79	27	85	26	0.1
Metronidazole	92	35	98	26	1.0	97	30	105	28	1.1
Moxifloxacin	51	10	65	10	1.1	53	10	60	10	1.1
Norfloxacin	39	6	45	7	7.1	45	7	49	3	7.9
Roxithromycin	70	10	68	10	20.0	72	10	67	10	1.0
Sulfadiazine	115	35	121	27	1.1	118	31	126	31	1.1
Sulfamethoxazole	92	25	97	20	0.4	97	23	105	19	0.4
Trimethoprim	124	28	132	21	0.0	130	24	139	22	0.0
Aceclofenac	113	15	130	13	2.8	122	14	132	10	2.9
Celecoxib	72	11	71	13	0.5	76	12	81	7	0.6
Diclofenac	94	31	97	23	5.0	103	27	111	21	5.0
Etoricoxib	95	13	104	11	0.1	101	12	108	9	0.1
Indomethacin	96	16	104	14	1.0	101	15	108	13	1.0
Ketoprofen	139	36	150	30	0.5	144	33	153	31	0.5
Lornoxicam	73	16	79	13	1.1	79	14	86	10	1.2
Naproxen	106	8	108	7	1.0	109	8	117	6	1.0
Nimesulide	44	10	47	10	10.0	51	17	53	10	10.0
Piroxicam	49	15	55	12	1.9	55	14	60	10	2.1
Tolfenamic Acid	83	7	88	5	0.7	89	6	95	4	0.7
Alprazolam	102	17	107	14	0.6	106	15	113	13	0.6
Bromazepam	84	16	91	13	0.9	93	14	101	7	1.0
Buspirone	64	26	75	20	0.1	69	23	74	23	0.1
Clobazam	102	19	88	10	5.0	102	16	121	12	5.8
Diazepam	103	15	112	15	0.1	111	15	119	8	0.1
Flunitrazepam	120	12	95	11	6.4	88	8	122	8	6.2
Lorazepam	102	14	85	13	0.7	89	11	106	13	0.8
Midazolam	64	11	71	10	0.4	81	8	84	6	0.5
Oxazepam	88	15	95	13	2.7	92	11	109	10	3.0
Triazolam	107	14	113	11	10.0	114	13	123	8	10.0
Amitriptyline	51	25	63	21	1.0	60	23	66	19	1.2
Bupropion	72	33	82	24	0.1	77	28	83	28	0.1
Citalopram	63	38	71	26	0.1	68	32	73	31	0.2
Doxepin	45	15	47	9	10.0	50	10	48	11	10.0
Duloxetine	82	12	85	11	5.0	71	10	75	11	5.0

Compounds	Influent					Effluent				
	50 ng L^{-1}		100 ng L^{-1}		MQL	50 ng L^{-1}		100 ng L^{-1}		MQL
	% R	%RSD$_R$	% R	%RSD$_R$	(ng/L)	% R	%RSD$_R$	% R	%RSD$_R$	(ng/L)
Fluvoxamine	34	38	49	30	2.7	39	34	43	33	2.7
Sertraline	36	27	42	20	5.5	43	23	48	20	5.5
Venlafaxine	92	36	101	27	0.1	98	27	106	21	0.1
Capecitabine	98	14	102	11	10.0	105	13	113	8	10.0
Cyclophosphamide	100	14	111	14	0.1	106	14	114	11	0.1
Cytarabine	<30	10	<30	10	10.0	<30	10	<30	10	10.0
Dacarbazine	88	34	92	24	10.0	95	29	103	25	10.0
Doxorubicin	<30	23	36	19	3.4	34	21	38	17	3.9
Methotrexate	81	21	84	15	1.9	85	18	92	16	2.0
Tamoxifen	<30	10	<30	11	7.0	<30	10	<30	11	7.0
Viblastine	<30	10	<30	9	10.0	<30	10	<30	11	10.0
Atenolol	56	21	60	15	0.1	63	18	69	14	0.1
Bisoprolol	76	18	77	13	0.1	82	16	89	12	0.1
Carvedilol	<30	19	<30	15	0.1	<30	17	33	13	0.1
Metoprolol	84	18	87	14	0.1	88	16	95	14	0.1
Pindolol	86	29	88	20	0.1	89	24	95	24	0.1
Propranolol	114	33	120	23	0.2	123	28	133	23	0.2
Timolol	101	21	107	17	0.3	106	19	114	16	0.3
Enalapril	93	10	96	9	0.3	96	9	103	8	0.3
Irbesartan	91	17	93	14	0.1	98	16	105	10	0.1
Losartan	87	15	93	13	0.3	92	14	99	11	0.3
Ramipril	99	12	105	11	0.3	106	12	113	7	0.3
Telmisartan	93	28	96	21	0.7	97	24	104	23	0.7
Valsartan	88	14	90	12	1.1	97	13	105	6	1.1
Glibenclamide	99	19	107	18	5.5	105	19	113	13	5.5
Gliclazide	67	26	70	19	0.3	73	23	80	19	0.4
Glimepiride	95	10	96	8	4.1	101	9	109	5	4.1
Glipizide	98	10	99	7	0.8	103	9	111	6	0.9
Metformin	<30	9	<30	9	1.1	<30	9	<30	7	1.2
Repaglinide	87	10	89	7	0.2	90	9	96	9	0.2
Alfuzosin	81	8	87	6	0.1	85	7	92	5	0.1
Finasteride	97	10	101	8	0.2	104	9	112	5	0.2
Progesterone	94	17	99	15	0.2	99	16	106	13	0.2
Raloxifene	<30	25	34	20	0.3	34	22	39	16	0.4
Sildenafil	<30	15	40	12	1.2	34	14	39	10	1.3
Acetaminophen	105	25	111	19	1.2	115	22	125	14	1.3
Orphenadrine	32	29	43	25	0.5	36	27	39	25	0.5
Thiocolchicoside	77	21	80	16	0.8	81	18	87	18	0.9
Tizanidine	104	34	111	26	0.4	106	30	113	31	0.4
Tramadol	83	26	87	19	0.1	88	22	94	21	0.1
Amisulpride	82	29	90	23	0.2	90	26	97	22	0.2
Olanzapine	90	10	96	9	6.6	82	10	89	10	6.6
Quetiapine	<30	10	<30	9	10.0	<30	10	<30	9	10.0
Risperidone	49	23	56	19	0.1	53	21	58	19	0.1
Carbamazepine	92	9	97	8	0.7	98	8	106	5	0.7

Compounds	Influent					Effluent				
	50 ng L^{-1}		100 ng L^{-1}		MQL	50 ng L^{-1}		100 ng L^{-1}		MQL
	% R	%RSD_R	% R	%RSD_R	(ng/L)	% R	%RSD_R	% R	%RSD_R	(ng/L)
Gabapentin	<30	10	<30	9	10.0	<30	10	<30	10	10.0
Lamotrigine	94	15	103	14	0.1	103	14	112	7	0.1
Pregabalin	<30	8	<30	8	2.1	<30	8	<30	2	3.1
Atorvastatin	58	10	63	9	1.5	64	9	69	6	1.7
Bezafibrate	105	15	112	13	0.5	110	14	118	12	0.5
Clofibric acid	94	14	89	15	0.5	95	15	101	11	0.5
Rosurvastatin	96	17	98	13	21.7	101	15	108	12	23.5
Cetirizine	69	26	75	21	1.9	73	23	79	22	2.0
Desloratadine	<30	16	31	13	0.9	30	15	34	11	1.1
Ebastine	<30	15	<30	11	0.3	<30	13	<30	13	0.3
Methdilazine	58	9	64	9	10.0	50	10	59	10	10.0
Lansoprazole	65	29	69	22	3.4	71	25	78	22	3.7
Omeprazole	83	28	82	19	22.3	87	24	93	24	24.3
Pantoprazole	79	26	82	19	0.2	83	22	89	21	0.3
Loperamide	79	38	89	29	0.9	85	34	91	32	0.9
Rifaximin	31	20	43	19	5.6	34	19	37	18	5.4
Abacavir	86	13	87	11	0.3	89	12	96	11	0.3
Adefovir	86	7	91	6	1.0	92	6	99	3	1.1
Furosemide	87	8	93	7	1.1	91	8	97	6	1.1
Indapamide	71	21	72	16	0.5	75	18	80	18	0.6
Dopamine	<30	9	<30	9	10.0	<30	10	<30	10	10.0
Trimetazidine	82	28	87	22	1.2	88	25	95	21	1.3
Fluconazole	104	13	111	11	0.4	110	12	118	9	0.4
Voriconazole	107	15	114	13	0.1	109	14	117	13	0.1
Betahistine	35	10	48	10	0.7	40	10	44	8	0.7
Cinnarizine	73	9	80	9	10.0	68	10	72	10	10.0
Prednisolone	90	19	99	17	0.7	94	18	101	10	0.7
Fluticasone	92	18	103	16	10.0	95	17	102	15	10.0
Cimetidine	<30	9	39	9	10.0	<30	10	41	10	10.0
Ranitidine	48	9	49	9	10.0	54	10	57	10	10.0
Lidocaine	78	35	81	26	0.1	81	30	87	31	0.1
Prilocaine	66	19	76	16	0.1	73	18	79	13	0.1
Diltiazem	41	9	40	9	10.0	42	10	40	10	10.0
Nifedipine	39	10	50	11	3.0	46	10	51	5	3.2
Bisacodyl	78	14	87	12	0.1	88	13	95	8	0.1
Bromhexine	46	19	54	14	0.4	52	16	57	13	0.4
Pramipexole	45	18	51	15	1.3	47	16	51	16	1.3
Salbutamol	60	9	58	9	10.0	60	10	65	10	10.0
Clopidogrel	71	13	75	11	0.1	73	12	78	12	0.1
Levothyroxine (T4)	41	20	45	14	49.0	44	17	48	17	44.0
Caffeine	138	32	143	22	0.5	143	27	153	26	0.5
Triclosan	73	6	77	6	0.5	79	6	85	2	0.5
Caffeic acid	40	9	39	9	10.0	42	10	40	10	10.0
DEET	90	22	97	18	0.1	96	20	104	16	0.1
BP1	69	5	66	6	0.4	72	5	77	2	0.4

Compounds	Influent					Effluent				
	50 ng L^{-1}		100 ng L^{-1}		MQL	50 ng L^{-1}		100 ng L^{-1}		MQL
	% R	%RSD_R	% R	%RSD_R	(ng/L)	% R	%RSD_R	% R	%RSD_R	(ng/L)
BP2	50	13	54	13	0.2	54	13	59	9	0.2
BP3	86	14	89	11	0.7	91	12	98	9	0.7
PABA	71	33	77	26	6.3	77	30	83	26	6.8

Table S8 Occurrence (ng/L) for PhACs detected in the effluents of the studied WWTP. Concentrations (ng/L) are calculated as the minimum, maximum and average from all sampling campaigns

PhACs	Min.	Max.	Mean	(%) Detection frequency
Ciprofloxacin	<MDL	119.7	49.04	82
Erythromycin	<MDL	0.1	<MQL	38
Trimethoprim	<MDL	12.9	<MQL	64
Clarithromycin	<MDL	14.0	<MQL	30
Azithromycin	<MDL	25.4	<MQL	34
Sulfadiazine	<MDL	5.7	<MQL	5
Sulfamethoxazole	<MDL	2.5	0.49	14
Roxithromycin	<MDL	11.9	<MQL	17
Levofloxacin	<MDL	68.3	26.41	55
Clindamycin	<MDL	<MDL	<MQL	0
Norfloxacin	<MDL	44.9	9.06	27
Moxifloxacin	<MDL	44.2	17.67	55
Lincomycin	<MDL	102.3	4.03	14
Metronidazole	<MDL	14.5	3.79	14
Amoxicillin	<MDL	<MDL	<MQL	0
Ampicillin	<MDL	<MDL	<MQL	0
Cefadroxil	<MDL	<MDL	<MQL	0
Rifaximin	<MDL	<MDL	<MQL	5
Piroxicam	<MDL	4.1	<MQL	14
Lornoxicam	<MDL	<MDL	<MQL	0
Nimesulide	<MDL	5.0	<MQL	50
Naproxen	<MDL	14.8	2.29	27
Diclofenac	<MDL	118.8	42.42	95
Ketoprofen	<MDL	33.7	18.27	68
Aceclofenac	<MDL	<MDL	<MQL	0
Indomethacin	<MDL	<MDL	<MQL	0
Celecoxib	<MDL	<MDL	<MQL	14
TolfenamicAcid	<MDL	205.2	8.64	14
Etoricoxib	<MDL	0.1	<MQL	100
SalicylicAcid	<MDL	148.3	34.21	100
Paracetamol	<MDL	32.5	13.73	100
Tramadol	<MDL	70.6	27.18	77
Thiocolchicoside	<MDL	<MDL	<MQL	0
Tizanidine	<MDL	16.1	<MQL	5
Doxepin	<MDL	<MDL	<MQL	0
Amitriptyline	<MDL	<MDL	<MQL	0

PhACs	Min.	Max.	Mean	(%) Detection frequency
Duloxetine	<MDL	17.2	<MQL	0
Bupropion	<MDL	0.1	<MQL	0
Fluvoxamine	<MDL	<MDL	<MQL	0
Citalopram	<MDL	<MDL	<MQL	0
Venlafaxine	<MDL	9.6	<MQL	68
Triazolam	<MDL	<MDL	<MQL	0
Sertraline	<MDL	<MDL	<MQL	5
Amisulpride	<MDL	0.1	<MQL	36
Quetiapine	<MDL	<MDL	<MQL	0
Risperidone	<MDL	0.1	<MQL	50
Olanzapine	<MDL	<MDL	<MQL	0
Alprazolam	<MDL	<MDL	<MQL	0
Diazepam	<MDL	0.1	<MQL	0
Bromazepam	<MDL	<MDL	<MQL	0
Buspirone	<MDL	<MDL	<MQL	0
5-Fluorouracil	<MDL	<MDL	<MQL	0
Tamoxifen	<MDL	20.2	<MQL	34
Cyclophosphamide	<MDL	759.9	25.92	5
Cytarabine	<MDL	32.6	<MQL	17
Etoposide	<MDL	<MDL	<MQL	0
Viblastine	<MDL	<MDL	<MQL	0
Capecitabine	<MDL	<MDL	<MQL	0
Dacarbazine	<MDL	<MDL	<MQL	0
Methotrexate	<MDL	<MDL	<MQL	0
Doxorubicin	<MDL	<MDL	<MQL	0
Telmisartan	<MDL	133.2	75.53	86
Valsartan	<MDL	3340.2	1398.32	86
Losartan	<MQL	27.0	9.45	68
Irbesartan	184.1	2452.2	1816.87	100
Captopril	<MDL	<MDL	<MQL	0
Methyldopa	<MDL	<MDL	<MQL	0
Ramipril	<MDL	<MDL	<MQL	9
Enalapril	<MDL	<MDL	<MQL	0
Carvedilol	<MDL	<MDL	<MQL	0
Atenolol	<MQL	53.7	6.68	73
Propranolol	<MQL	0.1	<MQL	0
Timolol	<MDL	<MDL	<MQL	0
Bisoprolol	<MQL	13.8	1.77	64
Pindonol	<MDL	<MDL	<MQL	0
Metoprolol	<MDL	11.4	5.18	68
Glibenclamide	<MDL	<MDL	<MQL	0
Gliclazide	<MDL	<MDL	<MQL	0
Glimepiride	<MDL	<MDL	<MQL	0
Glipizide	<MDL	<MDL	<MQL	0
Metformin	<MQL	37.4	15.53	100
Repaglinide	<MDL	<MDL	<MQL	0
Guanylurea (TP)	<MDL	141.1	52.21	100

PhACs	Min.	Max.	Mean	(%) Detection frequency
Ranitidine	<MDL	<MDL	<MQL	0
Cimetidine	<MDL	<MDL	<MQL	0
Cinnarizine	<MDL	<MDL	<MQL	0
Desloratadine	<MDL	14.8	<MQL	5
Cetirizine	<MQL	509.8	190.94	64
Methdilazine	<MDL	<MDL	<MQL	0
Ebastine	<MDL	<MDL	<MQL	0
Gabapentin	<MDL	640.4	84.42	27
Pregabalin	<MQL	11.1	<MQL	0
Carbamazepine	<MDL	192.8	45.21	77
Lamotrigine	<MDL	237.9	80.30	73
Clofibricacid	<MDL	<MDL	<MQL	0
Atorvastatin	<MDL	0.4	<MQL	17
Bezafibrate	<MDL	<MDL	<MQL	0
BP-1	<MDL	<MDL	<MQL	0
BP-2	<MDL	<MDL	<MQL	0
BP-3	<MDL	56.4	13.87	59
PABA	<MDL	68.6	11.56	14
Abacavir	<MDL	<MDL	<MQL	5
Acyclovir	<MDL	<MDL	<MQL	0
Adefovir	<MDL	<MDL	<MQL	0
Valganciclovir	<MDL	<MDL	<MQL	0
Lansoprazole	<MDL	<MDL	<MQL	0
Omeprazole	<MDL	9.2	<MQL	23
Pantoprazole	<MQL	0.2	<MQL	0
Finasteride	<MDL	<MDL	<MQL	0
Prednisolone	<MDL	<MDL	<MQL	0
Progesterone	<MDL	0.1	<MQL	5
Orphenadrine	<MDL	26.3	9.14	50
Solifenacin	<MDL	<MDL	<MQL	18
Lidocaine	<MQL	4.2	0.19	14
Prilocaine	<MQL	0.1	<MQL	5
Prednisolone	<MDL	6.3	<MQL	9
Loperamide	<MDL	8.3	2.29	50
Fluconazole	<MDL	352.5	176.35	86
Voriconazole	<MDL	<MDL	<MQL	0
Nifedipine	<MDL	<MDL	<MQL	0
Diltiazem	<MQL	5.0	<MQL	0
Indapamide	<MDL	<MDL	<MQL	0
Furosemide	<MDL	25.4	2.09	32
Caffeine	<MDL	144.8	37.40	100
Pramipexole	<MDL	<MDL	<MQL	0
Betahistine	<MDL	118.7	42.39	55
Bromhexine	<MDL	<MDL	<MQL	0
Fluticasone	<MDL	<MDL	<MQL	0
Levothyroxine (T4)	<MDL	<MDL	<MQL	0

PhACs	Min.	Max.	Mean	(%) Detection frequency
Bisacodyl	<MDL	<MDL	<MQL	0
Alfuzosin	<MDL	4.8	1.66	50
Trimetazidine	<MDL	<MDL	<MQL	0
Raloxifene	<MDL	<MDL	<MQL	0
DEET	<MDL	522.0	186.78	82
Triclosan	<MDL	6.4	1.02	9
Ergonovine	<MDL	<MDL	<MQL	0
Caffeicacid	<MDL	35.6	<MQL	17
Clopidogrel	<MDL	<MDL	<MQL	0
Sildenafil	<MDL	6.2	<MQL	17
Dopamine	<MDL	91.9	18.97	41
Salbutamol	<MDL	<MDL	<MQL	0

MDL: Method Detection Limit

MQL: Method Quantification Limit

Table S9 Measured effluent concentrations (ng/L) for the PhACs (i) before (P0), (ii) after the conventional disinfection (by ozonation), and (iii) after different treatment stages (P1, P2, P3) of the pre-industrial level unit (catalyst: zeolite).

PhAC	Therapeutic class	Before ozonation (P0)	After ozonation	P1	P3	P4
Acetaminophen	Analgesics/ muscle relaxant	104.7	<MDL	59.1	<MQL	<MDL
Alfuzosin	Urinary tract drug	16.7	<MDL	4.7	<MDL	<MDL
Amisulpride	Antipsychotic	538.4	<MQL	265.9	<MDL	<MDL
Amitriptyline	Antidepressant	<MQL	<MDL	<MQL	<MDL	<MDL
Atenolol	Beta-blocker	135.5	6.7	66.5	<MDL	1.8
Azithromycin	Antibiotic	137	<MDL	121.1	<MDL	<MDL
Bisoprolol	Beta-blocker	40	<MQL	19.6	<MDL	<MQL
BP1	UV filters	<MQL	<MQL	<MQL	<MDL	<MQL
Bromazepam	Anxiolytic-Sedative	2.8	<MDL	<MDL	<MDL	<MDL
Bupropion	Antidepressant	<MQL	<MQL	<MQL	<MDL	<MDL
Caffeic acid	Boosting supplement	33.3	<MDL	21.7	<MDL	<MDL
Caffeine	Stimulant	268.9	12.8	137.5	<MDL	91.2
Carbamazepine	Anticonvulsant	233.8	<MDL	136.7	<MDL	<MQL
Celecoxib	NSAID	<MQL	<MDL	<MQL	<MDL	<MDL
Cetirizine	Antihistamine	536	<MQL	412.7	<MDL	<MQL
Ciprofloxacin	Antibiotic	158.8	21.5	147	21.4	21.4
Citalopram	Antidepressant	31.1	<MDL	10	<MDL	<MDL
Clarithromycin	Antibiotic	102.4	<MDL	97.3	<MDL	<MDL
Clindamycin	Antibiotic	20	<MDL	13	<MDL	<MDL
Clopidogrel	Antiplatelet	10.6	<MDL	2.8	<MDL	<MDL
DEET	Insect repellent	2.6	2.7	14.5	<MQL	0.7

PhAC	Therapeutic class	Before ozonation (P0)	After ozonation	P1	P3	P4
Diazepam	Anxiolytic-Sedative	<MQL	<MQL	<MQL	<MQL	<MQL
Diclofenac	NSAID	555.7	<MDL	334.1	<MDL	<MDL
Diltiazem	Calcium channel blocker	<MQL	<MQL	<MQL	<MDL	<MQL
Erythromycin	Antibiotic	112.5	<MDL	91.1	<MDL	<MQL
Etoricoxib	NSAID	<MQL	<MQL	<MQL	<MDL	<MQL
Fluconazole	Antifungal	199.2	106.4	162	<MDL	65.7
Furosemide	Diuretic	721.9	<MDL	398.8	<MDL	<MDL
Gliclazide	Antidiabetic	5.8	<MDL	<MQL	<MDL	<MDL
Glimepiride	Antidiabetic	<MDL	<MDL	<MDL	<MDL	<MDL
Glipizide	Antidiabetic	<MDL	<MDL	<MDL	<MDL	2.8
Ibuprofen	NSAID	<MQL	<MQL	<MQL	<MDL	<MQL
Irbesartan	Antihypertensive	5565.4	1829.3	4904.8	<MQL	867.8
Ketoprofen	NSAID	18	21.1	0.8	<MQL	<MQL
Lamotrigine	Anticonvulsant	529.5	237.9	334	<MDL	27.9
Levofloxacin	Antibiotic	69.2	<MDL	44.7	<MDL	<MDL
Levothyroxine (T4)	Thyroid hormone	<MDL	<MDL	<MDL	<MDL	<MDL
Lidocaine	Anesthetic	88.8	<MQL	42.8	<MQL	<MQL
Lincomycin	Antibiotic	<MQL	<MDL	<MQL	<MDL	<MDL
Losartan	Antihypertensive	188.5	<MDL	125.8	<MDL	<MDL
Metformin	Antidiabetic	<MQL	<MQL	6.4	<MDL	29.4
Metronidazole	Antibiotic	35.1	12.6	29.7	<MDL	7.6
Moxifloxacin	Antibiotic	21.8	<MDL	23.2	<MDL	27.8
Naproxen	NSAID	<MDL	<MDL	<MQL	<MQL	<MQL
Nimesulide	NSAID	<MQL	<MQL	<MQL	<MDL	<MQL
Omeprazole	Proton pump inhibitor	2547.7	<MDL	1029.5	<MDL	<MDL
Orphenadrine	Analgesics/ muscle relaxant	105.6	<MDL	53	<MDL	<MDL
Pantoprazole	Proton pump inhibitor	11.8	<MQL	3.8	<MDL	<MDL
Pindolol	Beta-blocker	<MQL	<MQL	<MQL	<MDL	<MQL
Pregabalin	Anticonvulsant	<MQL	<MQL	<MQL	<MDL	<MDL
Prilocaine	Anesthetic	<MQL	<MQL	<MQL	<MDL	<MQL
Progesterone	Urinary tract drug	1.2	<MQL	2	<MDL	<MQL
Propranolol	Beta-blocker	<MQL	<MQL	<MQL	<MDL	<MQL
Repaglinide	Antidiabetic	<MDL	<MDL	<MDL	<MDL	<MDL
Risperidone	Antipsychotic	<MQL	<MQL	<MQL	<MQL	<MQL
Rosurvastatin	Lipid regulator	83.3	13.4	60.4	<MDL	10.7
Sertraline	Antidepressant	<MQL	<MDL	<MQL	<MDL	<MDL
Sulfamethoxazole	Antibiotic	40.5	2.5	80.8	<MDL	<MDL
Telmisartan	Antihypertensive	77.1	33.8	72.5	<MQL	<MQL

PhAC	Therapeutic class	Before ozonation (P0)	After ozonation	P1	P3	P4
Triclosan	Antiseptic	45.6	6.4	15.4	<MQL	5.8
Trimethoprim	Antibiotic	<MQL	<MQL	<MQL	<MQL	<MQL
Valsartan	Antihypertensive	4829.5	1351.6	1965.2	<MQL	336.3
Venlafaxine	Antidepressant	270.4	<MQL	182	<MQL	<MQL

P1: Effluent wastewater after the post filtration (1st Fix-Bed) in the pre-industrial pilot unit
P3: Effluent wastewater after the catalytic ozonation (2nd Fix-Bed) in the pre-industrial pilot unit
P4: Effluent wastewater after the biological stalilization (3rd Fix-Bed) in the pre-industrial pilot unit
MDL: Method Detection Limit
MQL: Method Quantification Limit

Table S10 Measured effluent concentrations (ng/L) for the PhACs (i) before (P0), (ii) after the conventional disinfection (by ozonation), and (iii) after different treatment stages (P1, P2, P3) of the pre-industrial level unit (catalyst: PET).

Emerging contaminant	Therapeutic class	Before ozonation (P0)	After ozonation	P1	P3	P4
Acetaminophen	Analgesics/ muscle relaxant	68.7	20.9	34.8	149.9	34.8
Alfuzosine	α1-antagonist	<MQL	<MDL	<MDL	<MDL	<MDL
Amisulpride	Antipsychotic	732.4	<MDL	428.1	<MDL	<MDL
Amitriptyline	Antidepressant	<MQL	<MDL	<MDL	<MDL	<MDL
Amoxicillin	Antibiotic	<MDL	<MDL	<MQL	<MDL	<MDL
Atenolol	Beta-blocker	60.4	<MQL	66.1	268.0	<MQL
Azithromycin	Antibiotic	<MDL	<MDL	<MDL	<MDL	<MDL
Bisoprolol	Beta-blocker	53.4	13.8	31.7	<MDL	<MDL
BP1	UV filters	<MQL	<MDL	<MDL	<MDL	<MQL
Caffeine	Stimulant	386.6	58.5	186.4	33.0	92.3
Carbamazepine	Anticonvulsant	655.4	192.8	423.1	128.4	76.6
Cetirizine	Antihistamine	600.5	<MDL	495.2	<MDL	<MDL
Ciprofloxacin	Antibiotic	77.1	<MDL	60.2	37.5	<MDL
Citalopram	Antidepressant	103.3	<MDL	4.5	36.2	<MDL
Clarithromycin	Antibiotic	45.2	<MDL	29.7	<MDL	<MDL
Clofibric Acid	Lipid regulator	11.7	12.2	12.1	11.9	12.4
Cytarabine	Cytostatic	<MDL	13.8	<MDL	10.9	<MDL
DEET	Insect repellent	37.1	4.4	27.8	1.8	1.7
Desloratadine	Antihistamine	58.8	<MDL	24.5	<MDL	21.9
Diclofenac	NSAID	4154.0	<MQL	4485.0	266.7	0.2
Dopamine	Neuromodulatory	734.7	490.1	574.0	<MDL	<MDL
Duloxetine	Antidepressant	<MDL	17.2	<MDL	3.9	9.6
Erythromycin-H2O	Antibiotic	<MDL	<MQL	<MQL	<MQL	<MQL
Fluconazole	Antifungal	234.9	146.1	192.4	149.5	101.3
Gabapentin	Anticonvulsant	1493.2	640.4	655.6	1893.6	934.2
Glibenclamide	Antidiabetic	<MQL	<MDL	<MQL	<MQL	<MDL

Emerging contaminant	Therapeutic class	Before ozonation (P0)	After ozonation	P1	P3	P4
Glimepiride	Antidiabetic	<MQL	<MDL	<MQL	<MDL	<MQL
Ibuprofen	NSAID	<MQL	<MQL	<MQL	<MQL	<MQL
Indomethacin	NSAID	5.9	<MDL	<MQL	<MQL	<MDL
Irbesartan	Antihypertensive	7464.4	2161.8	6613.7	2174.5	830.7
Ketoprofen	NSAID	37.5	26.0	15.4	753.3	15.2
Lamotrigine	Anticonvulsant	372.9	199.8	246.9	266.2	54.0
Lansoprazole	Antiulcer	135.2	<MDL	36.1	<MDL	<MDL
Levofloxacin	Antibiotic	54.0	<MDL	39.0	<MDL	<MDL
Lidocaine	Anesthetic	146.4	<MQL	80.7	<MQL	<MQL
Losartan	Antihypertensive	268.1	<MQL	213.4	<MQL	<MQL
Metformin	Antidiabetic	<MQL	<MQL	<MQL	<MQL	<MQL
Metoprolol	β blocker	313.9	<MDL	186.7	<MDL	<MDL
Metronidazole	Antibiotic	79.8	14.5	123.7	311.9	2.1
Moxifloxacin	Antibiotic	2015.2	9.5	40.6	55.9	9.6
Naproxen	NSAID	34.9	14.8	27.5	16.3	17.7
Norfloxacin	Antibiotic	42.7	44.9	39.9	42.6	<MDL
Orphenadrine	Analgesics/ muscle relaxant	156.7	<MDL	81.0	<MDL	<MDL
PABA	UV-filter	47.2	68.6	16.2	71.1	15.1
Piracetam	Nootropic	335.2	231.7	247.9	286.3	178.9
Prednisolone	Corticosteroid hormone	<MDL	<MDL	<MDL	120.8	<MDL
Pregabalin	Anticonvulsant	60.7	11.1	33.4	14.1	10.0
Prilocaine	Anesthetic	<MQL	<MDL	<MDL	<MDL	<MDL
Progesterone	Urinary tract drug	<MDL	<MQL	<MDL	<MQL	38.5
Propranolol	Beta-blocker	<MQL	<MDL	<MDL	<MDL	<MDL
Quetiapine	Antipsychotic	<MDL	<MDL	<MDL	<MDL	<MDL
Ramipril	Antihypertensive	<MDL	<MDL	<MDL	<MDL	<MDL
Rosurvastatin	Lipid regulator	526.6	80.4	348.5	40.1	<MDL
Salbutamol	β2 antagonist	<MDL	15.8	<MDL	26.2	23.5
Sulfamethoxazole	Antibiotic	65.9	<MDL	75.0	<MDL	<MDL
Tamoxifen	Cytostatic	<MDL	<MDL	<MDL	<MDL	<MDL
Telmisartan	Antihypertensive	1146.8	96.4	916.3	15.3	0.1
Tramadol	Analgesic	874.9	<MDL	646.5	<MDL	<MDL
Trimethoprim	Antibiotic	<MQL	<MQL	<MQL	399.4	<MQL
Valsartan	Antihypertensive	11364.0	3340.2	8494.1	2975.4	849.7
Venlafaxine	Antidepressant	352.1	<MDL	234.1	240.3	<MDL

P1: Effluent wastewater after the post filtration (1st Fix-Bed) in the pre-industrial pilot unit

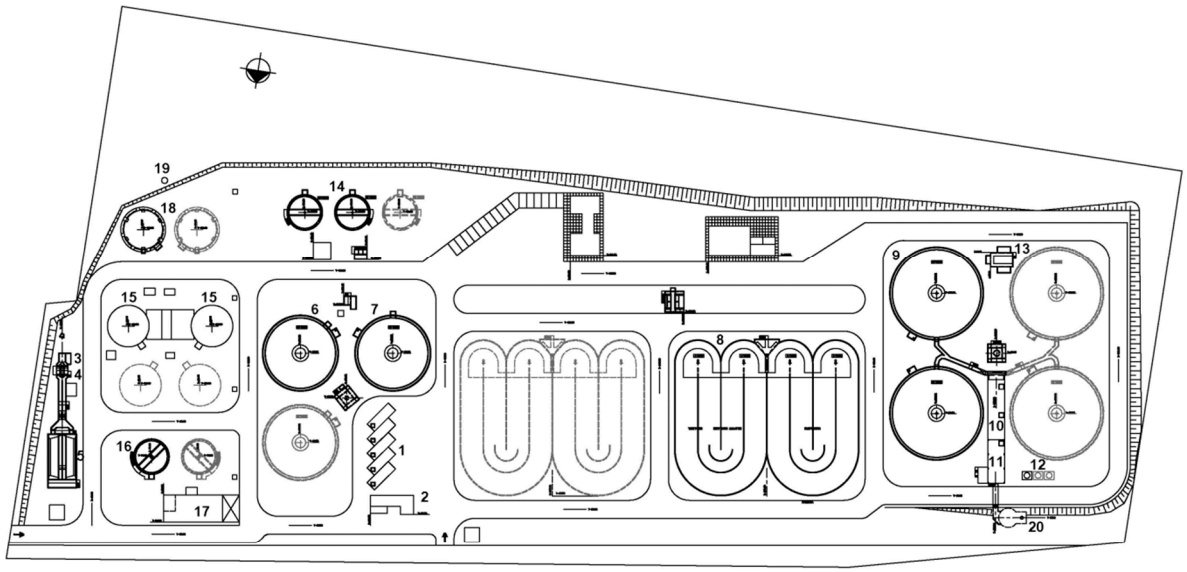
P3: Effluent wastewater after the catalytic ozonation (2nd Fix-Bed) in the pre-industrial pilot unit

P4: Effluent wastewater after the biological stalilization (3rd Fix-Bed) in the pre-industrial pilot unit

MDL: Method Detection Limit

MQL: Method Quantification Limit

Section S3. Supplementary Figures



GENERAL ARRANGEMENT PLAN LEGEND

1	SEPTIC WASTEWATER RECEPTION STATION
2	SEPTIC WASTEWATER PRETREATMENT UNIT
3	INFLOW CHAMBER
4	SCREENING STATION
5	GRIT & GREASE REMOVAL
6	PST (PRIMARY SEDIMENTATION TANK)
7	SEPTIC WASTEWATER BALANCING TANK
8	BIOREACTOR
9	FST (FINAL SEDIMENTATION TANK)
10	OZONE CONTACT UNIT
11	OZONE PRODUCTION STATION
12	LIQUID OXYGEN STORAGE TANK
13	RAS & SAS PUMPING STATION
14	SLUDGE THICKENERS
15	ANAEROBIC SLUDGE DIGESTERS
16	SLUDGE POST-THICKENER
17	SLUDGE DEWATERING STATION
18	GAS HOLDER
19	GAS FLARE
20	EFFLUENT CHAMBER

LINE'S LEGEND

———— OPERATING UNITS
- - - - - - - - - - FUTURE UNITS

(a)

(b)

Figure S1 Diagram (a) and view (b) of wastewater treatment plant "AINEIAS"

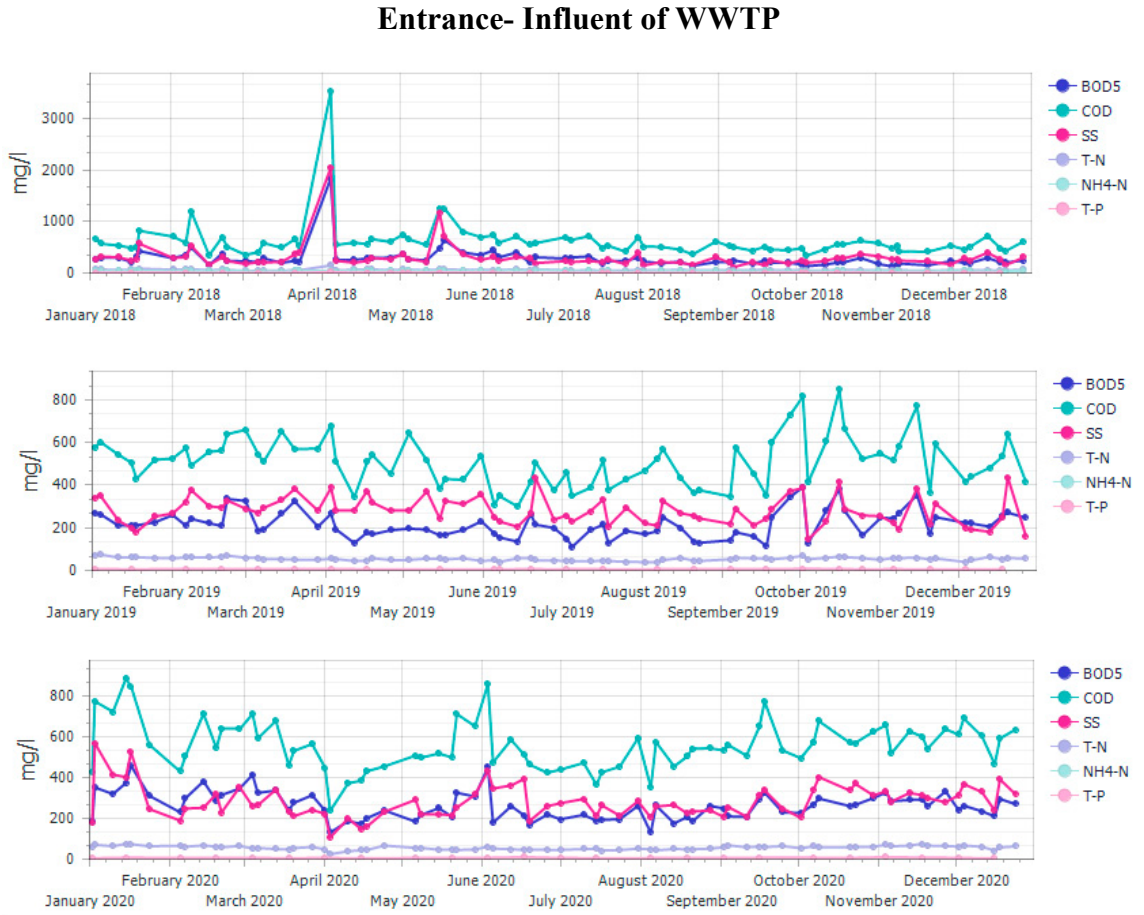


Figure S2 Variation of BOD_5, COD, SS, T-N, NH_4-N, NO_3-N and T-P at the entrance of WWTP for 2018-2020

(Data obtained from http://astikalimata.ypeka.gr/Services/Pages/WtpViewApp.aspx#)

Treated outflow-Effluent of WWTP

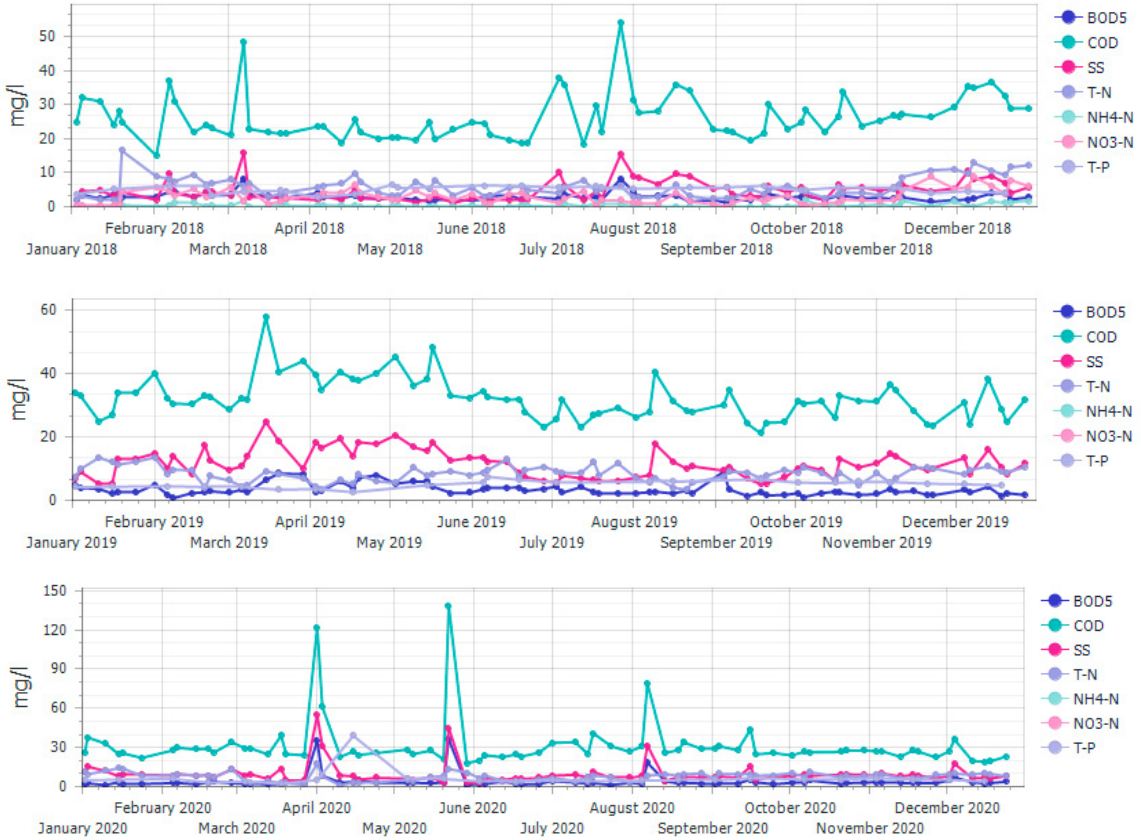


Figure S3 Variation of BOD_5, COD, SS, T-N, NH_4-N, NO_3-N and T-P at the treated outflow of WWTP for 2018-2020

(Data obtained from http://astikalimata.ypeka.gr/Services/Pages/WtpViewApp.aspx#)

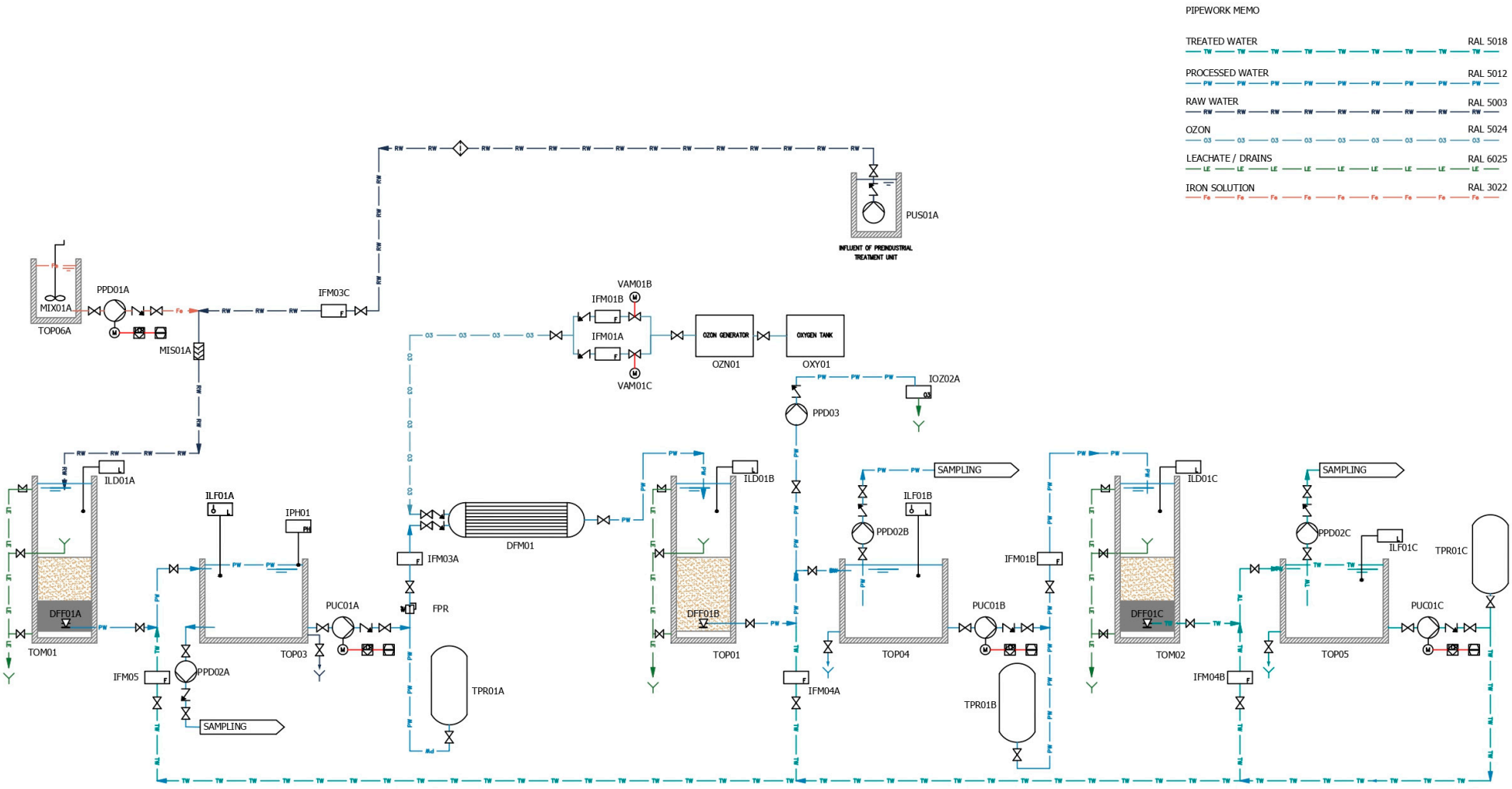


Figure S4 Detailed flowchart of the pre-industrial level unit

Figure S5 Photograph of the pre-industrial level unit