

Supporting information for:

Elimination of micropollutants during post-treatment of hospital wastewater with powdered activated carbon, ozone and UV

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1. Analyzed micropollutants

Table S1. Alphabetical list of analysed micropollutants

Compound	CAS number (supplier)	Description
4-Acetamidoantipyrine	83-15-8 (S-A)	3 rd metabolite of Aminopyrine / Metamizole
4-Aminoantipyrine	83-07-8 (R)	2 nd metabolite of Aminopyrine / Metamizole
4-Dimethylaminoantipyrine (Aminopyrine) ¹	58-15-1 (R)	analgesic / antipyretic
4-Formylaminoantipyrine	1672-58-8 (S-A)	4 th (final) metabolite of Aminopyrine / Metamizole
4-Methylaminoantipyrine	519-98-2 (H)	active substance of Aminopyrine / Metamizole - analgesic, N02BB02
4/5-Methylbenzotriazole (2 isomers) ²	136-85-6, 29878-31-7 (S-A)	corrosion inhibitors
Atenolol	29122-68-7 (S-A)	beta blocking agent
Atenolol acid (Metoprolol acid)	56392-14-4 (TRC)	metabolite of Atenolol / Metoprolol
Azithromycin	83905-01-5 (S-A)	macrolide antibacterial
Benzotriazole	95-14-7 (S-A)	corrosion inhibitor
Bezafibrate	41859-67-0 (S-A)	lipid modifying agent
Carbamazepine	298-46-4 (S-A)	antiepileptic
Cilastatin	82009-34-5 (TRC)	enzyme inhibitor (used with Imipenem - antibacterial, J01DH51)
Ciprofloxacin	85721-33-1 (F)	fluoroquinolone antibacterial
Clarithromycin	81103-11-9 (IDC)	macrolide antibacterial
Clindamycin	18323-44-9 (S-A)	lincosamide antibacterial
Clofibric acid	882-09-7 (S-A)	metabolite of Clofibrate - lipid modifying agent, C10AB01
Cyclophosphamide	50-18-0 (S-A)	cytostatic
D617	34245-14-2 (TRC)	metabolite of Verapamil
Dexamethasone	50-02-2 (S-A)	corticosteroid
Diatrizoate (Amidotrizoic, or diatrizoic acid)	117-96-4 (BS)	iodinated X-ray contrast medium
Diazepam	439-14-5 (Ro)	anxiolytic
Diclofenac	15307-86-5 (S-A)	antiinflammatory / antirheumatic
Erythromycin ³	114-07-8 (S-A)	macrolide antibacterial
Fluconazole	86386-73-4 (E)	antimycotic
Fluoxetine	54910-89-3 (TRC)	antidepressant
Furosemide	54-31-9 (S-A)	diuretic
Gabapentin	60142-96-3 (TRC)	antiepileptic
Hydrochlorothiazide	58-93-5 (S-A)	diuretic
Ifosfamide	3778-73-2 (S-A)	cytostatic
Indometacin	53-86-1 (S-A)	antiinflammatory / antirheumatic
Iohexol	66108-95-0 (F)	iodinated X-ray contrast medium
Iomeprol	78649-41-9 (BG)	iodinated X-ray contrast medium
Iopamidol	62883-00-5 (BG)	iodinated X-ray contrast medium
Iopromide	73334-07-3 (BS)	iodinated X-ray contrast medium
Ioxitalamic acid	28179-44-4 (BG)	iodinated X-ray contrast medium
Levetiracetam	102767-28-2 (TRC)	antiepileptic
Lidocaine	137-58-6 (S-A)	anesthetic, local
Mefenamic acid	61-68-7 (S-A)	antiinflammatory / antirheumatic
Methylprednisolone	83-43-2 (F)	corticosteroid
Metoprolol	37350-58-6 (S-A)	beta blocking agent
Metronidazole	443-48-1 (R)	imidazole antibacterial
Morphine	57-27-2 (L)	analgesic (opioid)
N4-Acetylsulfamethoxazole	21312-10-7 (S-A)	metabolite of Sulfamethoxazole
Naproxen	22204-53-1 (S-A)	antiinflammatory / antirheumatic

¹ 4-Dimethylaminoantipyrine (Aminophenazone, or aminopyrine) is not used in Switzerland due to severe side effects (agranulocytosis)

² Methylbenzotriazole measured in this study is a sum of 4-Methylbenzotriazole and 5-Methylbenzotriazole (mixture called Tolyltriazole)

³ Erythromycin measured in this study is a sum of Erythromycin and Erythromycin-H₂O

table continues

Table S1. Alphabetical list of analyzed micropollutants (*continued*)

Compound	CAS number (supplier)	Description
Norfloxacin	70458-96-7 ^(R)	fluoroquinolone antibacterial
Oseltamivir	196618-13-0 ^(Ro)	antiviral
Oseltamivir carboxylate	187227-45-8 ^(Ro)	active substance of Oseltamivir
Oxazepam	604-75-1 ^(L)	anxiolytic
Paracetamol (Acetaminophen)	103-90-2 ^(S-A)	analgesic / antipyretic
Phenazone (Antipyrine)	60-80-0 ^(E)	analgesic / antipyretic
Primidone	125-33-7 ^(S-A)	antiepileptic (barbiturate)
Propranolol	525-66-6 ^(S-A)	beta blocking agent
Ranitidine	66357-35-5 ^(S-A)	acid disorders - alimentary system
Ritalinic acid	19395-41-6 ^(S-A)	metabolite of Methylphenidate (Ritalin) - psychostimulant, N06BA04
Ritonavir	155213-67-5 ^(TRC)	antiviral
Roxithromycin	80214-83-1 ^(S-A)	macrolide antibacterial
Sotalol	3930-20-9 ^(S-A)	beta blocking agent
Sulfadiazine	68-35-9 ^(S-A)	sulfonamide antibacterial
Sulfamethoxazole	723-46-6 ^(S-A)	sulfonamide antibacterial
Sulfapyridine	144-83-2 ^(R)	sulfonamide antibacterial
Thiopental	76-75-5 ^(TRC)	anesthetic, general (barbiturate)
Tramadol	27203-92-5 ^(F)	analgesic (opioid)
Trimethoprim	738-70-5 ^(S-A)	antibacterial
Valsartan	137862-53-4 ^(TRC)	angiotensin II receptor antagonist
Venlafaxine	93413-69-5 ^(TRC)	antidepressant
Verapamil	152-11-4 ^(S-A)	calcium channel blocker

List of suppliers:

(BG)	courtesy of Byk Gulden, Singen, Germany
(BS)	courtesy of Bayer Schering Pharma, Berlin, Germany
(CDN)	CDN Isotopes INC., Pointe-Claire, Canada
(E)	Dr. Ehrenstorfer GmbH, Augsburg, Germany
(F)	Fluka, Sigma-Aldrich, Buchs, Switzerland
(H)	in-house synthesis (hydrolysis of metamizole)
(IDC)	IDC, Abbott Laboratories, Zug, Switzerland
(L)	Lipomed AG, Arlesheim, Switzerland
(R)	Riedel-de Haen Laborchemikalien GmbH & Co., Seelze, Germany
(Ro)	courtesy of F. Hoffmann-La Roche Ltd., Basel, Switzerland
(S-A)	Sigma-Aldrich, Seelze, Germany
(TRC)	Toronto Research Chemicals, North York, Canada

Table S2. Classification of analyzed pharmaceuticals and industrial chemicals

Compound		ATC code	Description
ANTIINFECTIVES			
<i>Antibacterials</i>	Azithromycin	J01FA10	macrolide antibacterial
	Ciprofloxacin	J01MA02	fluoroquinolone antibacterial
	Clarithromycin	J01FA09	macrolide antibacterial
	Clindamycin	J01FF01	lincosamide antibacterial
	Erythromycin ¹	J01FA01	macrolide antibacterial
	Metronidazole	J01XD01	imidazole antibacterial
	Norfloxacin	J01MA06	fluoroquinolone antibacterial
	Roxithromycin	J01FA06	macrolide antibacterial
	Sulfadiazine	J01EC02	sulfonamide antibacterial
	Sulfamethoxazole	J01EC01	sulfonamide antibacterial
	Sulfapyridine	J01EB04	sulfonamide antibacterial
	Trimethoprim	J01EA01	antibacterial
<i>Antimycotics</i>	Fluconazole	J02AC01	antimycotic
<i>Antivirals</i>	Oseltamivir	J05AH02	antiviral
	Ritonavir	J05AE03	antiviral
<i>Metabolites</i>	N4-Acetylsulfamethoxazole		metabolite of Sulfamethoxazole
	Oseltamivir carboxylate		active substance of Oseltamivir
ANTIINFLAMMATORY PREPARATIONS			
<i>Non-steroidal antiinflammatory</i>	Diclofenac	M01AB05	NSAID / antirheumatic
	Indometacin	M01AB01	NSAID / antirheumatic
	Mefenamic acid	M01AG01	NSAID / antirheumatic
	Naproxen	M01AE02	NSAID / antirheumatic
ANTINEOPLASTICS			
<i>Cytostatics</i>	Cyclophosphamide	L01AA01	cytostatic
	Ifosfamide	L01AA06	cytostatic
CARDIOVASCULAR SYSTEM PREPARATIONS			
<i>Diuretics</i>	Furosemide	C03CA01	diuretic
	Hydrochlorothiazide	C03AA03	diuretic
<i>Beta blocking agents</i>	Atenolol	C07AB03	beta blocking agent
	Metoprolol	C07AB02	beta blocking agent
	Propranolol	C07AA05	beta blocking agent
	Sotalol	C07AA07	beta blocking agent
<i>Calcium channel blocker</i>	Verapamil	C08DA01	calcium channel blocker
<i>Angiotensin II receptor antagonist</i>	Valsartan	C09CA03	angiotensin II receptor antagonist
<i>Lipid modifying agent</i>	Bezafibrate	C10AB02	lipid modifying agent
<i>Metabolites</i>	Atenolol acid (Metoprolol acid)		metabolite of Atenolol / Metoprolol
	Clofibric acid		metabolite of Clofibrate - lipid modifying agent, C10AB01
	D617		metabolite of Verapamil
CONTRAST MEDIA			
<i>X-ray contrast media</i>	Diatrizoate (Diatrizoic acid)	V08AA01	iodinated X-ray contrast medium
	Iohexol	V08AB02	iodinated X-ray contrast medium
	Iomeprol	V08AB10	iodinated X-ray contrast medium
	Iopamidol	V08AB04	iodinated X-ray contrast medium
	Iopromide	V08AB05	iodinated X-ray contrast medium
	Ioxitalamic acid	V08AA05	iodinated X-ray contrast medium

¹ Erythromycin measured in this study is a sum of Erythromycin and Erythromycin-H₂O

table continues

Table S2. Classification of analyzed pharmaceuticals and industrial chemicals (*continued*)

Compound		ATC code	Description
HORMONAL PREPARATIONS			
	Dexamethasone	H02AB02	corticosteroid
	Methylprednisolone	H02AB04	corticosteroid
NERVOUS SYSTEM PREPARATIONS			
<i>Anesthetics</i>	Lidocaine	N01BB02	anesthetic, local
	Thiopental	N01AF03	anesthetic, general (barbiturate)
<i>Analgesics / antipyretics</i>	4-Dimethylaminoantipyrine ²	N02BB03	analgesic / antipyretic
	Morphine	N02AA01	analgesic (opioid)
	Paracetamol (Acetaminophen)	N02BE01	analgesic / antipyretic
	Phenazone (Antipyrine)	N02BB01	analgesic / antipyretic
	Tramadol	N02AX02	analgesic (opioid)
<i>Antiepileptics</i>	Carbamazepine	N03AF01	antiepileptic
	Gabapentin	N03AX12	antiepileptic
	Levetiracetam	N03AX14	antiepileptic
	Primidone	N03AA03	antiepileptic (barbiturate)
<i>Psycholeptics</i>	Diazepam	N05BA01	anxiolytic
	Oxazepam	N05BA04	anxiolytic
<i>Psychoanaleptics</i>	Fluoxetine	N06AB03	antidepressant
	Venlafaxine	N06AX16	antidepressant
<i>Metabolites</i>	4-Acetamidoantipyrine		3 rd metabolite of Aminopyrine / Metamizole
	4-Aminoantipyrine		2 nd metabolite of Aminopyrine / Metamizole
	4-Formylaminoantipyrine		4 th (final) metabolite of Aminopyrine / Metamizole
	4-Methylaminoantipyrine		active substance of Aminopyrine / Metamizole - analgesic, N02BB02
	Ritalinic acid		metabolite of Methylphenidate (Ritalin) - psychostimulant, N06BA04
OTHER PHARMACEUTICALS			
	Cilastatin		enzyme inhibitor (used with Imipenem - antibacterial, J01DH51)
	Ranitidine	A02BA02	acid disorders - alimentary system
INDUSTRIAL CHEMICALS			
	Benzotriazole		corrosion inhibitor
	4/5-Methylbenzotriazole (2 isomers) ³		corrosion inhibitor

² 4-Dimethylaminoantipyrine (Aminophenazone, or aminopyrine) is not used in Switzerland due to severe side effects (agranulocytosis)³ Methylbenzotriazole measured in this study is a sum of 4-Methylbenzotriazole and 5-Methylbenzotriazole (mixture called Tolytriazole)

Table S3. Speciation, pK_a, and Log D_{ow} values of analyzed micropollutants (JChem for Excel, ChemAxon)

Compound	Strongest Basic pK _a	Strongest Acidic pK _a	Speciation at pH 1 - 14														Log D _{ow}						
																	pH 4	pH 5	pH 6	pH 7	pH 8	pH 9	pH 10
4-Acetamidoantipyrine	(-)	12.52	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.15	0.15	0.15	0.15	0.15	0.15	0.15
4-Aminoantipyrine	(-)	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.33	0.33	0.33	0.33	0.33	0.33	0.33
4-Dimethylaminoantipyrine	3.46	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.04	1.14	1.15	1.15	1.15	1.15	1.15
4-Formylaminoantipyrine	(-)	12.66	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.11	0.11	0.11	0.11	0.11	0.11	0.10
4-Methylaminoantipyrine	1.22	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.77	0.77	0.77	0.77	0.77	0.77	0.77
4/5-Methylbenzotriazole	1.01	8.86	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.81	1.81	1.81	1.81	1.76	1.45	0.77
Atenolol	9.67	14.08	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.82	-2.80	-2.68	-2.14	-1.24	-0.33	0.26
Atenolol acid	9.67	3.54	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.59	-3.42	-4.05	-4.17	-3.80	-3.03	-2.46
Azithromycin	9.57	12.43	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-4.54	-4.41	-3.64	-1.99	-0.08	1.55	2.29
Benzotriazole	0.58	8.63	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.30	1.30	1.30	1.29	1.21	0.80	0.11
Bezafibrate	(-)	3.83	1	2	3	4	5	6	7	8	9	10	11	12	13	14	3.59	2.79	1.83	0.97	0.55	0.47	0.46
Carbamazepine	(-)	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	2.77	2.77	2.77	2.77	2.77	2.77	2.77
Cilastatin	9.14	2.53	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.44	-2.00	-2.91	-3.86	-4.58	-4.99	-5.53
Ciprofloxacin	8.68	5.76	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.68	-1.62	-1.46	-1.38	-1.43	-1.68	-1.92
Clarithromycin	8.38	12.46	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.21	0.10	0.89	1.84	2.71	3.15	3.23
Clindamycin	7.55	12.16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.19	-1.47	-0.52	0.38	0.91	1.02	1.03
Clofibric acid	(-)	3.37	1	2	3	4	5	6	7	8	9	10	11	12	13	14	2.18	1.27	0.32	-0.38	-0.60	-0.63	-0.63
Cyclophosphamide	(-)	12.78	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.10	0.10	0.10	0.10	0.10	0.10	0.10
D617	10.54	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.28	-0.28	-0.26	-0.10	0.50	1.42	2.31
Dexamethasone	(-)	12.42	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.68	1.68	1.68	1.68	1.68	1.68	1.68
Diatrizoate	(-)	2.17	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.54	-2.46	-3.06	-3.22	-3.23	-3.24	-3.24
Diazepam	2.92	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	3.04	3.07	3.08	3.08	3.08	3.08	3.08
Diclofenac	(-)	4.00	1	2	3	4	5	6	7	8	9	10	11	12	13	14	3.96	3.21	2.26	1.37	0.85	0.74	0.73
Erythromycin	8.38	12.44	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.85	-0.54	0.25	1.20	2.06	2.50	2.58
Fluconazole	2.56	12.71	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.55	0.56	0.56	0.56	0.56	0.56	0.56
Fluoxetine	9.80	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.93	0.94	1.04	1.50	2.38	3.31	3.96
Furosemide	(-)	4.25	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.56	0.93	0.00	-0.93	-1.58	-1.81	-2.10
Gabapentin	9.91	4.63	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.88	-1.61	-1.52	-1.51	-1.51	-1.55	-1.80
Hydrochlorothiazide	(-)	9.09	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.58	-0.58	-0.58	-0.58	-0.61	-0.82	-1.60
Ifosfamide	(-)	12.39	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.10	0.10	0.10	0.10	0.10	0.10	0.09
Indometacin	(-)	3.80	1	2	3	4	5	6	7	8	9	10	11	12	13	14	3.12	2.31	1.35	0.50	0.08	0.01	0.00
Iohexol	(-)	11.73	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.95	-1.95	-1.95	-1.95	-1.95	-1.95	-1.96
Iomeprol	(-)	11.73	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.45	-1.45	-1.45	-1.45	-1.45	-1.45	-1.45
Iopamidol	(-)	11.00	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.04	-2.04	-2.04	-2.04	-2.04	-2.05	-2.08
Iopromide	(-)	11.09	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.74	-1.74	-1.74	-1.74	-1.75	-1.75	-1.78
Ioxitalamic acid	(-)	2.13	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.12	-2.04	-2.63	-2.77	-2.79	-2.79	-2.79
Levetiracetam	(-)	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.59	-0.59	-0.59	-0.59	-0.59	-0.59	-0.59
Lidocaine	7.75	13.78	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.77	-1.14	-0.21	0.72	1.35	1.52	1.54
Mefenamic acid	(-)	3.89	1	2	3	4	5	6	7	8	9	10	11	12	13	14	5.04	4.25	3.30	2.42	1.97	1.88	1.87
Methylprednisolone	(-)	12.58	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.56	1.56	1.56	1.56	1.56	1.56	1.56
Metoprolol	9.67	14.09	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.48	-1.47	-1.34	-0.81	0.09	1.01	1.59
Metronidazole	3.09	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.51	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46
Morphine	9.12	10.26	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.30	-2.23	-1.83	-0.99	-0.03	0.74	0.89
N4-Acetylsulfamethoxazole	0.38	5.88	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.85	0.81	0.55	0.10	-0.06	-0.08	-0.09
Naproxen	(-)	4.19	1	2	3	4	5	6	7	8	9	10	11	12	13	14	2.77	2.11	1.18	0.25	-0.36	-0.52	-0.54
Norfloxacin	8.68	5.77	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.79	-1.73	-1.56	-1.48	-1.52	-1.78	-2.03

LEGEND:

1 cationic at pH 1

6 zwitterionic at pH 6

4 anionic at pH 14

table continues

Table S3 Speciation, pKa, and Log Dow values of analyzed micropollutants (*continued*)

Compound	Strongest Basic pK _a	Strongest Acidic pK _a	Speciation at pH 1 - 14														Log D _{ow}						
																	pH 4	pH 5	pH 6	pH 7	pH 8	pH 9	pH 10
Oseltamivir	9.31	14.03	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.87	-1.85	-1.69	-1.07	-0.16	0.68	1.08
Oseltamivir carboxylate	9.33	4.38	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.37	-2.13	-2.08	-2.07	-2.09	-2.22	-2.66
Oxazepam	(-)	10.61	1	2	3	4	5	6	7	8	9	10	11	12	13	14	2.92	2.92	2.92	2.92	2.92	2.91	2.83
Paracetamol	(-)	9.46	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.91	0.91	0.91	0.91	0.89	0.78	0.27
Phenazone	(-)	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.22	1.22	1.22	1.22	1.22	1.22	1.22
Primidone	(-)	11.50	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.12	1.12	1.12	1.12	1.12	1.12	1.11
Propranolol	9.67	14.09	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.66	-0.64	-0.52	0.02	0.92	1.83	2.42
Ranitidine	8.08	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-2.46	-1.96	-1.09	-0.13	0.64	0.93	0.98
Ritalinic acid	10.08	3.73	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.63	-0.51	-0.49	-0.49	-0.50	-0.52	-0.71
Ritonavir	2.84	13.68	1	2	3	4	5	6	7	8	9	10	11	12	13	14	5.20	5.22	5.22	5.22	5.22	5.22	5.22
Roxithromycin	9.08	12.45	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.50	-0.40	0.06	0.93	1.89	2.66	2.95
Sotalol	9.43	10.07	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-3.19	-3.18	-3.04	-2.48	-1.58	-0.71	-0.41
Sulfadiazine	2.01	6.99	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.38	0.38	0.35	0.13	-0.33	-0.52	-0.55
Sulfamethoxazole	1.97	6.16	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.78	0.76	0.60	0.14	-0.11	-0.15	-0.15
Sulfapyridine	2.63	8.52	1	2	3	4	5	6	7	8	9	10	11	12	13	14	0.99	1.01	1.01	1.00	0.91	0.53	0.16
Thiopental	(-)	7.85	1	2	3	4	5	6	7	8	9	10	11	12	13	14	2.77	2.77	2.77	2.72	2.43	1.90	1.67
Tramadol	9.23	13.80	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-1.04	-0.98	-0.59	0.24	1.20	2.02	2.38
Trimethoprim	7.16	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.18	-0.11	0.27	0.92	1.23	1.28	1.28
Valsartan	(-)	4.28	1	2	3	4	5	6	7	8	9	10	11	12	13	14	4.31	3.49	1.92	0.46	-0.36	-0.60	-0.63
Venlafaxine	8.91	14.42	1	2	3	4	5	6	7	8	9	10	11	12	13	14	-0.75	-0.62	-0.07	0.84	1.78	2.48	2.70
Verapamil	9.68	(-)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	1.54	1.57	1.76	2.42	3.36	4.28	4.87

LEGEND:

1 cationic at pH 1

6 zwitterionic at pH 6

14 anionic at pH 14

Table S4. Analytical quality control and limits of quantification (for more details on analytics, see ¹⁾)

Expanded uncertainty at 95% confidence interval	Quality control (QC) label	Number of analytes
Uncertainty less than 14%	a (best)	23
Uncertainty 15 – 29%	b (good)	20
Uncertainty 30 – 100%	c (high uncertainty)	20
Uncertainty above 100%	d (semiquantitative)	5

	Matching internal standard	QC label	Estimated limits of quantification – LOQ (ng/L)							
			Nanopure water	Effluent of MBR and UV			PAC effluent		O ₃ effluent	
				no dilution	dilution 1:10	dilution 1:100	no dilution	dilution 1:10	no dilution	dilution 1:10
4-Acetamidoantipyrine	-	c	1	50	220	33	3	17		
4-Aminoantipyrine	-	d	250	1800	18000	3000	140	2400		
4-Dimethylaminoantipyrine	-	c	50	7	200	2900	200	2700	8	290
4-Formylaminoantipyrine	-	c	1	21	200	27	2	15		
4-Methylaminoantipyrine	-	d	500	4100	19000	500	240	2000		
4/5-Methylbenzotriazole (2 isomers)	- *	d	5	1000	480	76		300		
Atenolol	yes	a	10	3	58	770	3	76	2	64
Atenolol acid	yes	a	5		25	300	2	31	1	27
Azithromycin	yes	b	5	9	40	1800	13	190	28	150
Benzotriazole	yes	b	50		630	5800		860		630
Bezafibrate	yes	a	1	2	12	120	1	13	1	13
Carbamazepine	yes	b	1	2	16	160	2	18	2	13
Cilastatin	-	c	25	6	90	1100	8	120	7	110
Ciprofloxacin	yes	c	50		300	3100	18	220	16	150
Clarithromycin	-	a	1	2	24	280	2	33	3	26
Clindamycin	-	c	5		51	690	3	73	2	56
Clofibric acid	yes	b	5	8	46	450	8	56	14	49
Cyclophosphamide	yes	a	5	11	90	930	11	110	9	83
D617	-	b	1	2	27	340	2	33	2	24
Dexamethasone	-	a	5	17	86	840	15	95	13	84
Diatrizoate	yes	c	250		5000			3000		3000
Diazepam	yes	a	1	2	15	160	2	18	2	15
Diclofenac	yes	b	1	3	12	120	3	15	2	15
Erythromycin	yes	c	5	8	160	2000	12	210	8	91
Erythromycin-H2O	-	c	5	28	140	3300	17	220	33	230
Fluconazole	yes	a	5		48	500	6	59		46
Fluoxetine	yes	b	1	2	23	270	3	31	2	21
Furosemide	yes	b	5		43	450	4	48	4	47
Gabapentin	yes	b	250		950	11000	100	1100		2000
Hydrochlorothiazide	yes	a	5		45	400	12	50	13	53
Ifosfamide	-	b	1	3	18	200	3	23	2	16
Indometacin	yes	a	1	3	13	130	3	15	3	17
Iohexol	yes	c	100	170	980	10000	160	1400	150	1200
Iomeprol	yes	d	100		14000	10000		10000		960
Iopamidol	yes +	d	250			10000		2000		2000
Iopromide	yes	c	100		7000	4500		3000		3000
Ioxitalamic acid	yes	c	250		5000			3000		3000
Levetiracetam	yes	a	10	24	180	1800	23	210	42	300
Lidocaine	yes	a	5		64	760	5	82	3	64
Mefenamic acid	yes	a	1	1	9	97	2	11	2	13
Methylprednisolone	yes	a	5	15	79	800	11	88	11	84
Metoprolol	yes	a	25	15	260	3300	18	340	14	260
Metronidazole	-	c	25		190	2000	23	220	30	230
Morphine	yes	b	25	6	140	1600	3000	450	7	180
N4-Acetylsulfamethoxazole	yes	a	1	2	14	140	2	16	1	11
Naproxen	yes +	c	100	680	3400	46000	680	4600	860	5800
Norfloxacin	yes +	c	500		1200	27000	150	1800	150	1200

table continues

Table S4. Analytical quality control and limits of quantification (*continued*)

	Matching internal standard	QC label	Estimated limits of quantification – LOQ (ng/L)							
			Nanopure water	Effluent of MBR and UV			PAC effluent		O ₃ effluent	
				no dilution	dilution 1:10	dilution 1:100	no dilution	dilution 1:10	no dilution	dilution 1:10
Oseltamivir	yes	c	5	3	10	710	3	73	3	57
Oseltamivir carboxylate	-	b	25	1	15	200	1	18	1	19
Oxazepam	yes	a	1	1	10	95	1	11	1	10
Paracetamol	yes	b	50	130	790	7100	220	1000	120	780
Phenazone	yes	c	5	9	66	660	10	86	8	58
Primidone	yes	b	5	9	57	600	10	68	8	54
Propranolol	yes	b	5	8	13	160	10	170	8	130
Ranitidine	yes	b	10	3	49	670	3	61	2	52
Ritalinic acid	yes	b	5	1	16	190	1	20	1	17
Ritonavir	yes	b	1	3	21	230	3	26	3	18
Roxithromycin	-	b	1	1	60	250	2	41	3	33
Sotalol	yes	a	25	7	140	1800	7	190	5	150
Sulfadiazine	yes	a	1	2	16	140	2	20	2	13
Sulfamethoxazole	yes	a	5		77	770		100	8	60
Sulfapyridine	- *	c	5	10	73	730	9	94	7	66
Thiopental	-	c	5	22	67	530	22	84	28	71
Tramadol	yes	a	5	3	47	550	3	58	3	47
Trimethoprim	yes	c	25	14	230	2400	16	290	13	250
Valsartan	yes	b	1	1	11	120	1	13	1	11
Venlafaxin	yes	a	5	7	99	1200	7	120	6	100
Verapamil	yes	a	5	5	16	180	5	15	5	16

LEGEND:

- * internal standard (IS) later during the study available, uncertainty with IS was not determined
- + low intensity of IS, low sensitivity
- black LOQ: dilution factor used for quantification
- grey LOQ: dilution factor rarely used for quantification

Table S5. List of measured analytes not detected in the MBR effluent

	Not detected in the MBR influent /effluent	Removed in the MBR
4-Dimethylaminoantipyrine	not detected	-
Cilastatin	-	yes
Clofibric acid	not detected	-
Dexamethasone	not detected	-
Diazepam	not detected	-
Fluoxetine	not detected	-
Iohexol	not detected	-
Methylprednisolone	not detected	-
Naproxen	not detected	-
Paracetamol	-	yes
Roxithromycin	not detected	-

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity of analyzed micropollutants at pH 8-8.5. Log K_{ow} and pK_a values estimated by JChem for Excel, ChemAxon. O₃ reactivity estimated based on the molecular structure as described by von Sontag and von Gunten.²



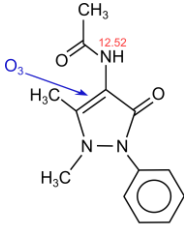
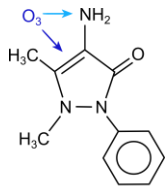
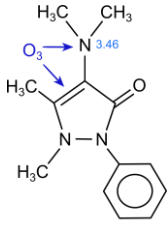
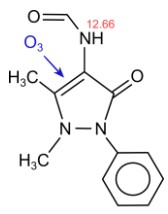
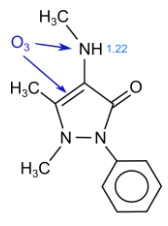
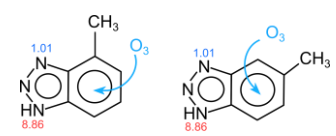
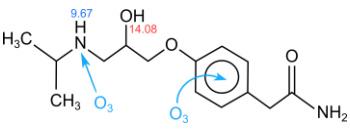
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
4-Acetamidoantipyrine		C13H15N3O2	<chem>CC(=O)NC=NC(=O)N(c1ccccc1)N(C)C=C</chem>	0.15	HIGH (olefin)
4-Aminoantipyrine		C11H13N3O1	<chem>c(ccc1N(N(C=CC)C(=O)C2N)cc1</chem>	0.33	HIGH (olefin, primary amine)
4-Dimethylaminoantipyrine (Aminopyrine)		C13H17N3O	<chem>c(ccc1N(N(C=CC)C(=O)C2N(C)C)cc1</chem>	1.15	HIGH (olefin, tertiary amine)
4-Formylaminoantipyrine		C12H13N3O2	<chem>O=C2C(=NC(=O)C(=O)N(C)N2c1ccccc1</chem>	0.11	HIGH (olefin)
4-Methylaminoantipyrine		C12H15N3O	<chem>CNC1=C(C)N(C)N(C1=O)C2=C(C)C=C2</chem>	0.77	HIGH (olefin, secondary amine)
4-Methylbenzotriazole 5-Methylbenzotriazole		C7H7N3	<chem>Cc1cccc2[nH]nn12</chem> <chem>Cc1ccc2[nH]nnc2c1</chem>	1.81	INTERMEDIATE (benzene derivative)
Atenolol		C14H22N2O3	<chem>CC(C)NCC(O)COc1ccc(cc1)CC(=O)N</chem>	0.43	HIGH (protonated sec. amine, benzene derivative)

table continues

Table S6. Structures, formulas, Log K_{OW}, and estimation of ozone reactivity (*continued*)

Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{OW} (uncharged)	O ₃ reactivity estimation
Atenolol acid (Metoprolol acid)		C ₁₄ H ₂₁ N ₁ O ₄	<chem>CC(C)NCC(O)COc1ccc(cc1)CC(=O)O</chem>	-4.17	HIGH (protonated sec. amine, benzene derivative)
Azithromycin		C ₃₈ H ₇₂ N ₂ O ₁₂	<chem>CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(O)C)[C@H](O)[C@H](C)O2)C(C)[C@H](O)[C@@H]3O[C@H](C)C[C@H]3O)N(C)C[C@H](C)CN(C)[C@H](C)[C@@H](O)[C@]1(C)O</chem>	2.44	HIGH (2x tertiary amine, both protonated)
Benzotriazole		C ₆ H ₅ N ₃	<chem>c12c(nn[nH]1)ccc2</chem>	1.30	INTERMEDIATE (benzene derivative)
Bezafibrate		C ₁₉ H ₂₀ ClNO ₄	<chem>c1(C(NCCc2ccc(OC(C(=O)=O)(C)C)cc2=O)ccc(Cl)cc1</chem>	3.99	INTERMEDIATE (benzene derivative)
Carbamazepine		C ₁₅ H ₁₂ N ₂ O	<chem>N1(c2c(cccc2)C=Cc2c1ccccc2)C(N)=O</chem>	2.77	HIGH (olefin)
Cilastatin		C ₁₆ H ₂₆ N ₂ O ₅ S	<chem>[H][C@](N)(CSCCCC=C/[NC(=O)][C@@]1([H])CC1(C(C)C(O)=O)C(O)=O</chem>	-1.39	HIGH (olefin, thioether)
Ciprofloxacin		C ₁₇ H ₁₈ F ₁ N ₃ O ₃	<chem>C(C1)C1N(C=C(C(=O)C(=O)O)-c(cc(c3F)N(CCN4)CC4)c2c3</chem>	-1.38	HIGH (olefin, protonated secondary amine, aniline type)

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

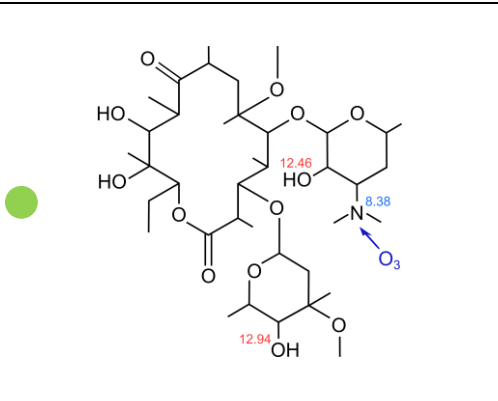
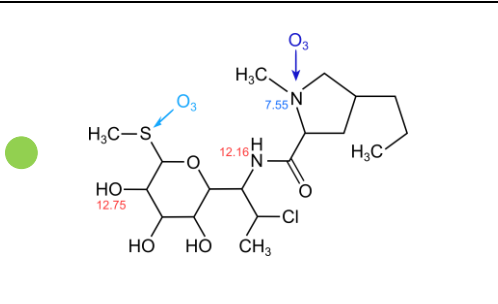
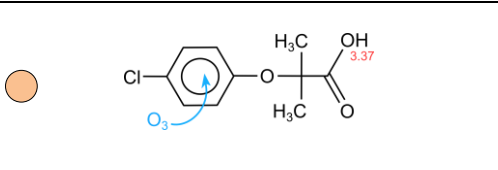
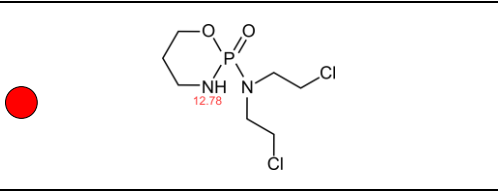
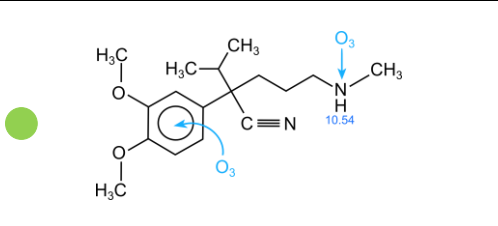
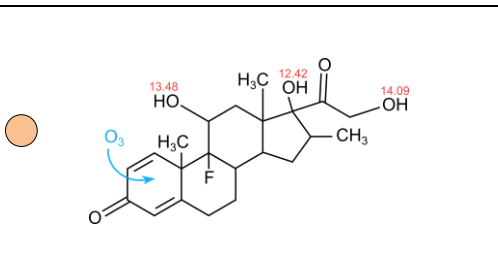
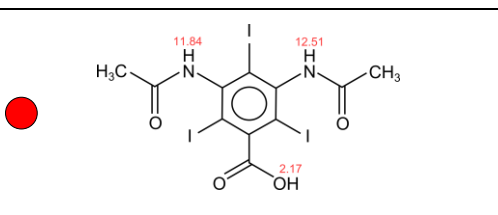
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Clarithromycin		C ₃₈ H ₆₉ NO ₁₃	<chem>CC[C@H]1OC(=O)[C@H](C)[C@@H](OC2CC(C)(OC)C(O)C(C)O2)[C@H](C)[C@@H](OC3OC(C)CC(C3O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC</chem>	3.24	HIGH (tertiary amine)
Clindamycin		C ₁₈ H ₃₃ ClN ₂ O ₅ S ₁	<chem>S(C)C(OC(C1O)C(NC(=O)C(N(C)C2)CC2CCC)C(Cl)C)C(O)C1O</chem>	1.04	HIGH (tertiary amine, thioether)
Clofibric acid		C ₁₀ H ₁₁ ClO ₃	<chem>CC(C)(OC1=CC=C(Cl)C=C1)C(O)=O</chem>	2.90	INTERMEDIATE (deactivated benzene derivative)
Cyclophosphamide		C ₇ H ₁₅ Cl ₂ N ₂ O ₂ P	<chem>C1CCN(CCCl)P1(=O)NCCCC1</chem>	0.10	LOW-NONE
D617		C ₁₇ H ₂₆ N ₂ O ₂	<chem>CNCCC[C@@](C#N)(C(C)C)c1cc(OC)c(OC)c1</chem>	2.96	HIGH (anisole, protonated secondary amine)
Dexamethasone		C ₂₂ H ₂₉ FO ₅	<chem>[H][C@@]12C[C@@H](C)[C@](O)(C(=O)CO)[C@@]1(C)C[C@H](O)[C@@]3(F)[C@@]2([H])C(C4=CC(=O)C=C[C@]34C</chem>	1.68	INTERMEDIATE (quinone type)
Diatrizoate		C ₁₁ H ₉ I ₃ N ₂ O ₄	<chem>CC(=O)NC1=C(I)C(C(O)=O)=C(I)C(NC(C)=O)=C1</chem>	0.29	LOW-NONE

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

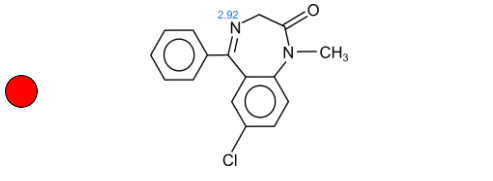
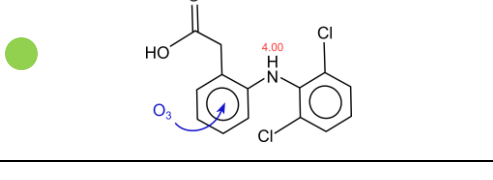
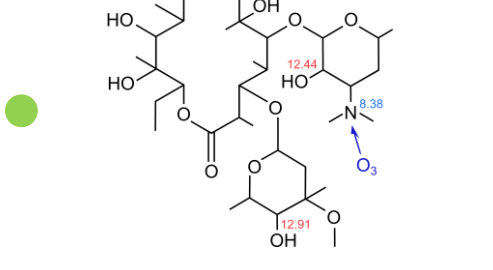
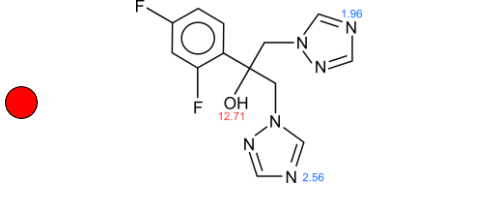
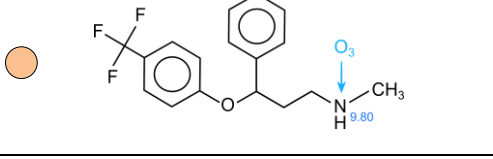
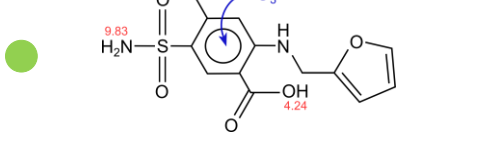
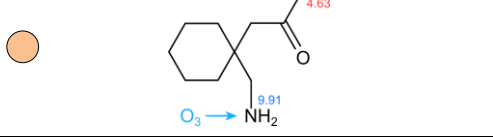
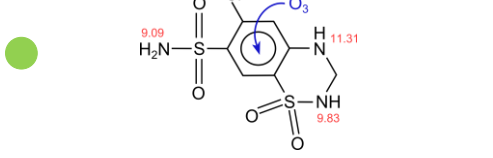
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Diazepam		C ₁₆ H ₁₃ Cl N ₂ O	<chem>CN1C2=C(C=C(Cl)C=C2)C(=NC1=O)C3=CC=CC=C3</chem>	3.08	LOW-NONE
Diclofenac		C ₁₄ H ₁₁ Cl ₂ N ₁ O ₂	<chem>c1c(c(ccc1)Nc1c(cccc1Cl)Cl)CC(=O)O</chem>	4.26	HIGH (aniline type)
Erythromycin ¹		C ₃₇ H ₆₇ N ₁₃	<chem>O(C(C(O)C1(O)C(C)C(C1)OC(C(C(=O)OC(C(O)(C(O)C2C(C)CC)C(C)C(C(C(O)(CC(C2=O)C)C)OC(OC(C3)C)C(O)C3N(C)C</chem>	2.60	HIGH (tertiary amine)
Fluconazole		C ₁₃ H ₁₂ F ₂ N ₆ O	<chem>OC(CN1C=NC=N1)(CN2C=NC=N2)C3=C(F)C=C(F)C=C3</chem>	0.56	LOW-NONE
Fluoxetine		C ₁₇ H ₁₈ F ₃ NO	<chem>c1([C@@H](Oc2ccc(C(F)(F)F)c2)CCNC)ccccc1</chem>	4.17	INTERMEDIATE (protonated secondary amine)
Furosemide		C ₁₂ H ₁₁ Cl N ₂ O ₅ S	<chem>NS(=O)(=O)C1=CC(C(O)=O)=C(NCC2=CC=CO2)C=C1Cl</chem>	1.75	HIGH (aniline type)
Gabapentin		C ₉ H ₁₇ N ₂ O ₂	<chem>NCC1(CC(O)=O)CCCCC1</chem>	-1.51	INTERMEDIATE (protonated primary amine)
Hydrochlorothiazide		C ₇ H ₈ ClN ₃ O ₄ S ₂	<chem>NS(=O)(=O)C1=CC2=C(NCNS2(=O)=O)C=C1Cl</chem>	-0.58	HIGH (aniline type)

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

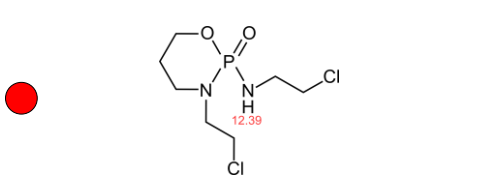
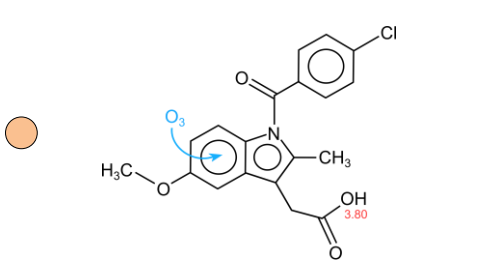
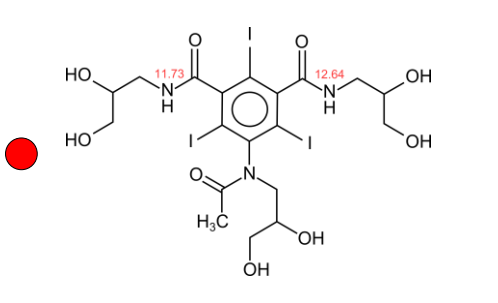
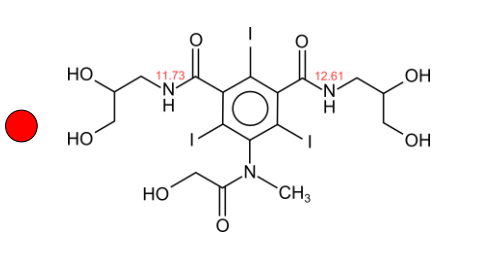
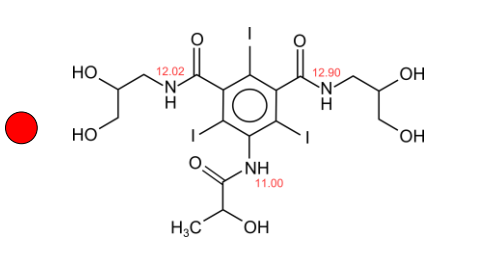
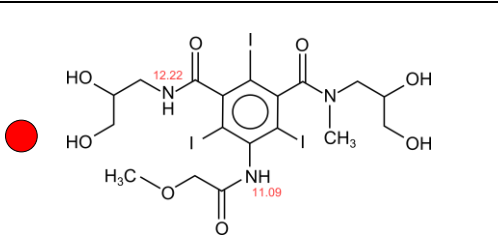
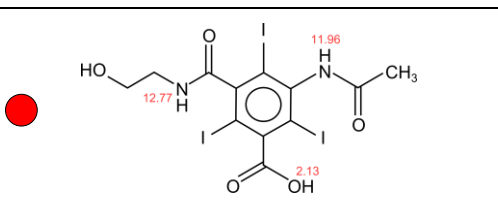
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Ifosfamide		C7H15Cl2 N2O2P	<chem>CICCN(P(OC1)(=O)NCCCl)CC1</chem>	0.10	LOW-NONE
Indometacin		C19H16Cl NO4	<chem>COC1=CC2=C(C=C1)N(C(=O)C3=CC=C(C1)C=C3)C(C)=C2C(=O)O</chem>	3.53	INTERMEDIATE (anisole)
Iohexol		C19H26I3N 3O9	<chem>OCC(O)CNC(=O)c1c(I)c(N(CC(O)CO)C(=O)c(I)c1)C(=O)NCC(O)CO</chem>	-1.95	LOW-NONE
Iomeprol		C17H22I3N 3O8	<chem>Ic1c(c(I)c(c(I)c1N(C)C(=O)CO)C(=O)NCC(O)CO)C(=O)NCC(O)CO</chem>	-1.45	LOW-NONE
Iopamidol		C17H22I3N 3O8	<chem>CC(O)C(=O)NC1=C(I)C(C(=O)N(C(CO)CO)=C(I)C(C(=O)NC(CO)CO)=C1I</chem>	-2.04	LOW-NONE
Iopromide		C18H24I3N 3O8	<chem>c1(c(c(c(I)c(c1)NC(COC)=O)C(NC[C@@H](CO)O)=O)I)C(N(C[C@@H](CO)O)C)=O</chem>	-1.74	LOW-NONE
Ioxitalamic acid		C12H11I3N 2O5	<chem>CC(=O)NC1=C(I)C(C(O)=O)=C(I)C(C(=O)NCCO)=C1I</chem>	0.74	LOW-NONE

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

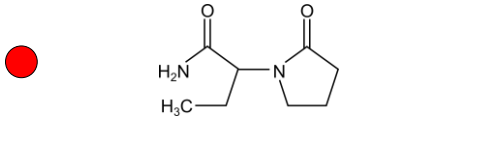
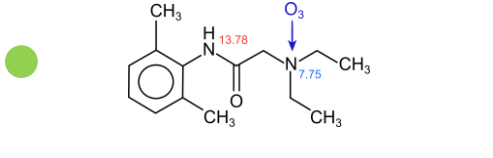
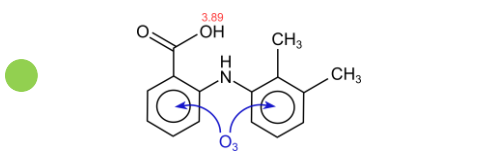
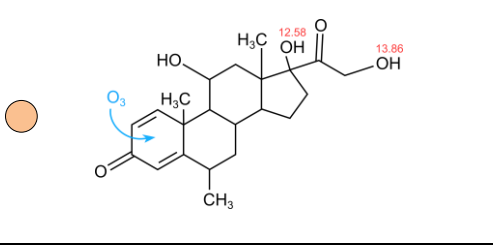
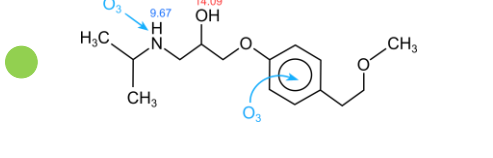
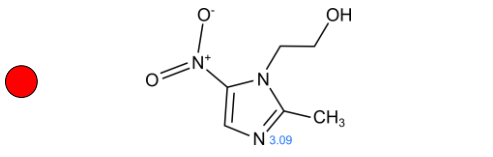
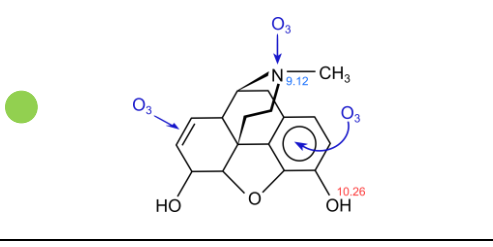
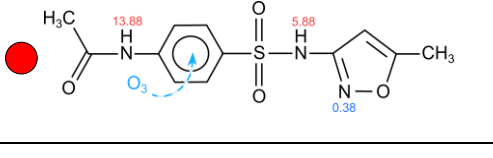
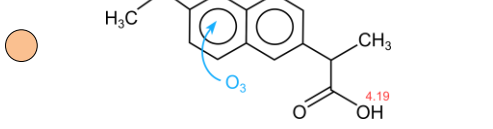
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Levetiracetam		C ₈ H ₁₄ N ₂ O ₂	[H]C(CC)(N1CC(=O)C(N)=O	-0.59	LOW-NONE
Lidocaine		C ₁₄ H ₂₂ N ₂ O	CCN(CC)CC(=O)NC1=C(C)C=C	1.54	HIGH (tertiary amine)
Mefenamic acid		C ₁₅ H ₁₅ N ₁ O ₂	c1(c(cccc1)C(O)=O)Nc1c(c(ccc1)C)C	5.40	HIGH (2x aniline type)
Methylprednisolone		C ₂₂ H ₃₀ O ₅	[H][C@@]12CC[C@](O)(C(=O)C O)[C@@]1(C)C[C@H](O)[C@@]3([H])[C@@]2([H])C[C@]([H])(C)C4=CC(=O)C=C[C@]34C	1.56	INTERMEDIATE (quinone type)
Metoprolol		C ₁₅ H ₂₅ N ₁ O ₃	COCCC1=CC=C(C(OCC(O)CNC(C)C)C=C1	1.76	HIGH (protonated sec. amine, benzene derivative)
Metronidazole		C ₆ H ₉ N ₃ O ₃	CC1=NC=C(N1CCO)[N+](O-)=O	-0.46	LOW-NONE
Morphine		C ₁₇ H ₁₉ N ₁ O ₃	c12[C@]34[C@@H]5[C@H]([N@](C)CC4)Cc2c(cc(c1O[C@H]3[C@@H]4)(O)C=C5)O	0.89	HIGH (olefin, phenol, protonated tertiary amine)
N4-Acetylsulfamethoxazole		C ₁₂ H ₁₃ N ₃ O ₄ S	c1(ccc(cc1)NC(=O)S(Nc1cc(C)on1)(=O)=O	0.86	LOW (N-phenyl amide)
Naproxen		C ₁₄ H ₁₄ O ₃	c12c(cc(OC)cc2)ccc(c1)[C@@H](C(O)=O)C	2.99	INTERMEDIATE (naphthalene)

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

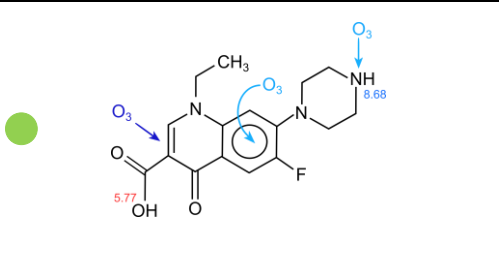
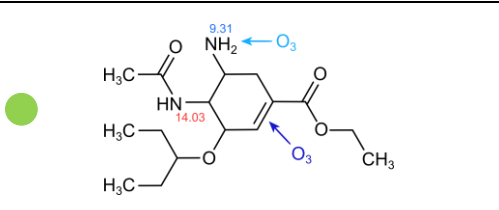
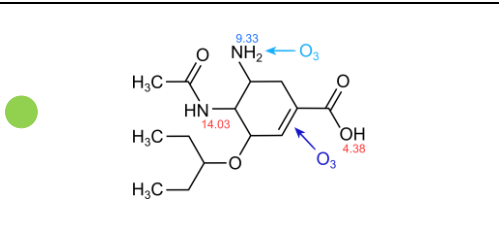
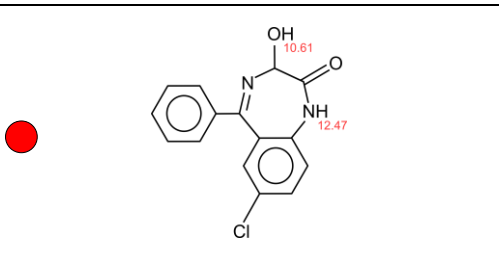
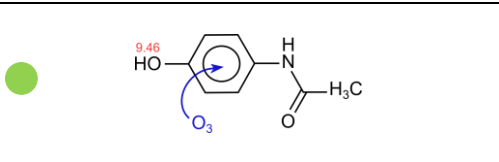
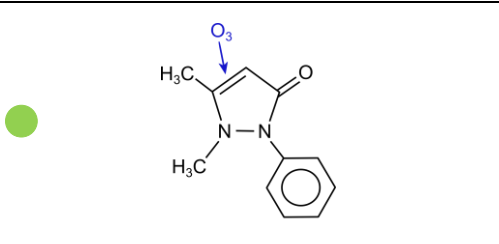
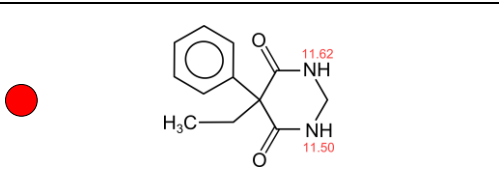
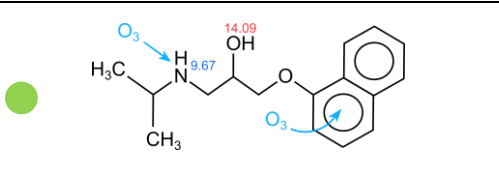
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Norfloxacin		C ₁₆ H ₁₈ F ₁ N ₃ O ₃	<chem>CCN1C=C(C(O)=O)C(=O)C2=C(C(F)=C(C=C12)N3CCNCCC3)</chem>	-1.48	HIGH (olefin, protonated secondary amine, aniline type)
Oseltamivir		C ₁₆ H ₂₈ N ₂ O ₄	<chem>CCOC(=O)C1=CC(OC(CC)CC)C(NC(C)=O)C(N)C1</chem>	1.16	HIGH (olefin, protonated primary amine)
Oseltamivir carboxylate		C ₁₄ H ₂₄ N ₂ O ₄	<chem>CCC(CC)OC1C=C(CC(N)C1NC(C)=O)C(O)=O</chem>	-2.07	HIGH (olefin, protonated primary amine)
Oxazepam		C ₁₅ H ₁₁ ClN ₂ O ₂	<chem>c12C(c3ccccc3)=N[C@@H](O)C(Nc1ccc(c2)Cl)=O</chem>	2.92	LOW-NONE
Paracetamol (Acetaminophen)		C ₈ H ₉ N ₁ O ₂	<chem>CC(=O)NC1=C(C=CC(=O)C1)O</chem>	0.91	HIGH (phenol)
Phenazone (Antipyrine)		C ₁₁ H ₁₂ N ₂ O	<chem>CN1N(C(=O)C=C1C)C2=CC=C(C=C2)C=O</chem>	1.22	HIGH (olefin)
Primidone		C ₁₂ H ₁₄ N ₂ O ₂	<chem>c1(ccccc1)C2(C(=O)NCNC2=O)CC</chem>	1.12	LOW-NONE
Propranolol		C ₁₆ H ₂₁ N ₁ O ₂	<chem>c12c(OC[C@@H](CNC(C)C)O)cccc1cccc2</chem>	2.58	HIGH (protonated sec. amine, naphthalene)

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

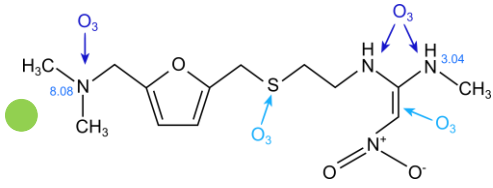
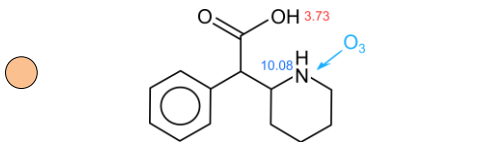
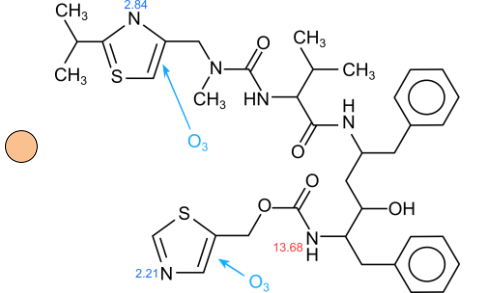
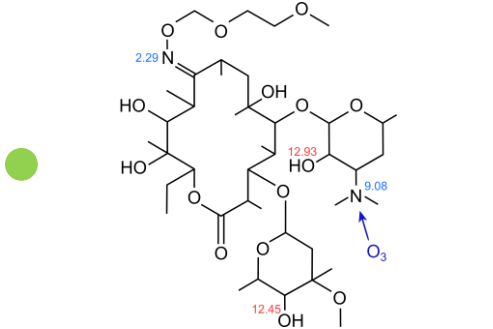
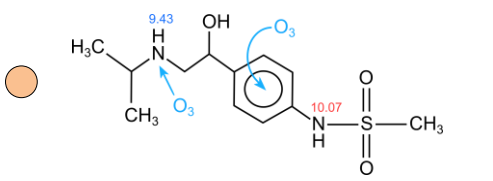
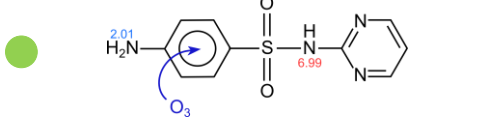
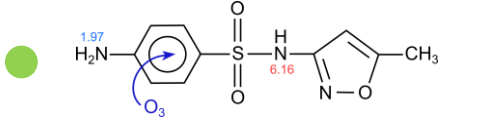
Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Ranitidine		C13H22N4O3S	<chem>CN(C)(NCCSCC1=CC=C(CN(C)C)O1)=C([N+])([O-])=O</chem>	0.98	HIGH (tertiary and secondary amines, thioether, olefin)
Ritalinic acid		C13H17NO2	<chem>c(ccc1C(C(=O)O)C(NCC2)CC2)c1</chem>	-0.49	INTERMEDIATE (protonated secondary amine)
Ritonavir		C37H48N6O5S2	<chem>CC(C)C(NC(=O)N(C)CC1=CSC(=N1)C(C)C)C(=O)N[C@H](CC(O)[C@H](CC2=CC=CC=C2)NC(=O)OCC3=CN=CS3)CC4=CC=CC=C4</chem>	5.22	INTERMEDIATE
Roxithromycin		C41H76N2O15	<chem>CC[C@H]1OC(=O)[C@H](C)[C@H](OC2CC(C)(OC)C(O)C(C)O2)[C@H](C)[C@H](OC2OC(C)CC(C2O)N(C)C)[C@H](C)(O)C[C@@H](C)C(=N/OCOCOC)[C@H](C)[C@H](O)[C@H]1(C)O</chem>	3.00	HIGH (protonated tertiary amine)
Sotalol		C12H20N2O3S	<chem>c1([C@@H](CN(C)C)O)ccc(NS(C)(=O)=O)cc1</chem>	-0.41	INTERMEDIATE (deactivated aniline t., protonated sec. amine)
Sulfadiazine		C10H10N4O2S	<chem>NC1=CC=C(C=C1)S(=O)(=O)N=C2NC=CC=N2</chem>	0.39	HIGH (aniline)
Sulfamethoxazole		C10H11N3O3S1	<chem>c1(S(Nc2cc(C)on2)(=O)=O)ccc(N)cc1</chem>	0.79	HIGH (aniline)
Sulfapyridine		C11H11N3O3S1	<chem>c1(S(Nc2ccccn2)(=O)=O)ccc(N)c1</chem>	1.01	HIGH (aniline)

table continues

Table S6. Structures, formulas, Log K_{ow}, and estimation of ozone reactivity (*continued*)

Compound	Structure / O ₃ reactivity estimation / pK _a (red acidic, blue basic)	Formula	Smile	Log K _{ow} (uncharged)	O ₃ reactivity estimation
Thiopental		C ₁₁ H ₁₈ N ₂ O ₂ S	<chem>C1([C@@](C(N=C(N1)S)=O)([C@@H](CCC)C)CC)=O</chem>	2.77	HIGH (deprotonated thiol)
Tramadol		C ₁₆ H ₂₅ N ₂ O	<chem>COC1=CC=C(C(=C1)[C@@](O)(CCC[C@@H]2CNC(C)C)C2)C</chem>	2.45	HIGH (protonated tertiary amine, anisole)
Trimethoprim		C ₁₄ H ₁₈ N ₄ O ₃	<chem>c1(Cc2c(nc(N)nc2N)cc(c(OC)c1)OC)OC</chem>	1.28	HIGH (aniline type, anisole)
Valsartan		C ₂₄ H ₂₉ N ₅ O ₃	<chem>CCCCC(=O)N(CC1=CC=C(C(C=C1)C2=C(C(C=CC=C2)C3=NN=NN3)[C@@H](C(C)C)C(O)=O)C1)C</chem>	4.51	LOW-NONE
Venlafaxine		C ₁₇ H ₂₇ N ₂ O	<chem>C1CCCC(C1)([C@@H](c1ccc(cc1)OC)CN(C)C)O</chem>	2.74	HIGH (protonated tertiary amine, anisole)
Verapamil		C ₂₇ H ₃₈ N ₂ O ₄	<chem>COC1=CC(OC)=CC(C=C1)C(=CC(C(C)C)C(C#N)C)CCN(CCC2=CC(OC)=C(C(C)C=C2)C)=C1</chem>	5.04	HIGH (protonated tertiary amine, anisoles)

2. Additionally measured gadolinium and platinum

Gadolinium

The main source of gadolinium in hospital wastewater is very likely coming from magnetic resonance imaging (MRI) contrast media from the ATC class V08CA.

V08C MAGNETIC RESONANCE IMAGING CONTRAST MEDIA

V08CA Paramagnetic contrast media

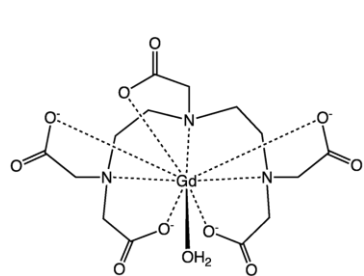
V08CA01	gadopentetic acid	contains Gd
V08CA02	gadoteric acid	contains Gd
V08CA03	gadodiamide	contains Gd
V08CA04	gadoteridol	contains Gd
V08CA05	mangafodipir	
V08CA06	gadoversetamide	contains Gd
V08CA07	ferric ammonium citrate	
V08CA08	gadobenidic acid	contains Gd
V08CA09	gadobutrol	contains Gd
V08CA10	gadoteric acid	contains Gd
V08CA11	gadofosveset	contains Gd

V08CB Superparamagnetic contrast media

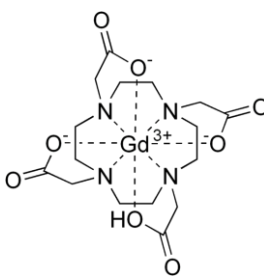
V08CB01	ferumoxsil
V08CB02	ferristene
V08CB03	iron oxide, nanoparticles

V08CX Other magnetic resonance imaging contrast media

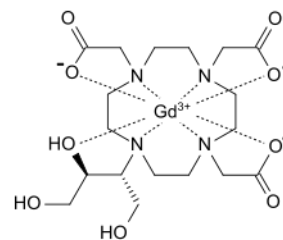
V08CX01	perflubron
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gadopentetic acid



gadoteric acid



gadobutrol

Figure S1. Examples of gadolinium containing MRI contrast media

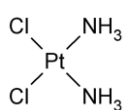
Platinum

The platinum containing cytostatics (antineoplastic agents) from the ATC class L01XA, used for treatment of oncologic patients, are the main source of platinum in hospital wastewater.

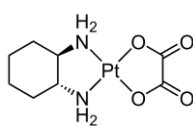
L01X OTHER ANTINEOPLASTIC AGENTS

L01XA Platinum compounds

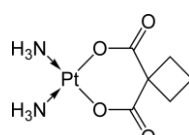
L01XA01	cisplatin	all contain Pt
L01XA02	carboplatin	
L01XA03	oxaliplatin	
L01XA04	satraplatin	
L01XA05	polyplatillen	



cisplatin



oxaliplatin



carboplatin

Figure S2. Examples of platinum containing cytostatics

3. Post-treatment by activated carbon, ozone and UV

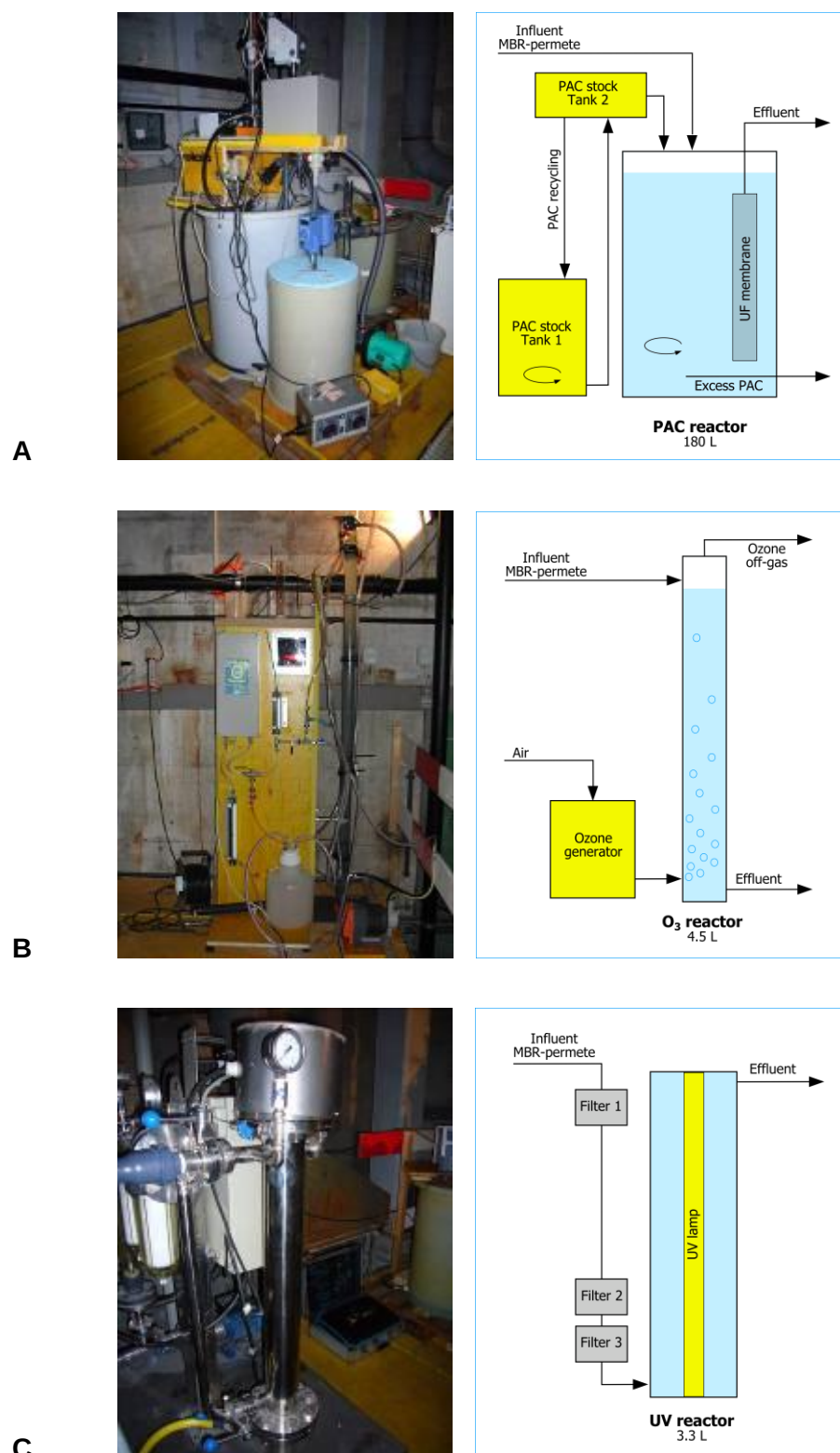


Figure S3. Set-up of the three post-treatments: A adsorption to powdered activated carbon, B oxidation by ozone, and C photolysis by ultraviolet light.

Table S7. Experimental conditions of adsorption experiments with powdered activated carbon (PAC) Norit SAE Super (1300 m²/g, 15µm, pH_{PZC} 9.8)

	Replicate (date)	DOC [mg C/L]		COD _{dis} [mg O/L]		pH		Temp. (PAC-reactor) [°C]
		Infl.	Effl.	Infl.	Effl.	Infl.	Reactor	
8.2±4 mg PAC/ L	A (12.-16.10.2009)	7.2	4.5	18.3	11.3	8.4	8.7	26.8
	B (16.-19.10.2009)	6.8	4.2	19.2	n.a.	8.3	8.8	30.0
23±7 mg PAC/ L	A (2.-6.11.2009)	6.8	n.a.	16.3	7.1	8.4	8.8	31.7
	B (6.-9.11.2009)	8.3	3.7	20.8	8.2	8.2	8.8	33.2
	C (19.-23.11.2009)	7.0	2.7	19.7	7.2	8.3	n.a.	31.5
	D (23.-26.11.2009)	7.5	3.0	21.3	8.5	8.2	8.8	32.9
43±14 mg PAC/ L	A (15.-19.2.2010)	6.7	2.0	13.3	<5.0	8.4	8.9	26.7
	B (19.-22.2.2010)	5.9	1.9	13.0	<5.0	8.8	9.0	28.0

n.a. – data not available

Table S8. Experimental conditions of ozonation experiments

	Replicate	Transferred ozone dose [mg O ₃ /L]	Contact time [min]	DOC [mg C/L]	COD _{dis} [mg O/L]	pH	T [°C]
O ₃ -reactor influent (MBR permeate)	A	-	-	6.7	15.8	8.4	21.4
	B	-		6.4	16.1	8.5	22.4
O ₃ -reactor effluent (dose 0.64 ± 0.01 g O ₃ /g DOC)	A	4.3	12	6.3	13.4	8.7	20.4
	B	4.1		6.2	16.0	8.5	22.8
O ₃ -reactor effluent (dose 0.89 ± 0.03 g O ₃ /g DOC)	A	5.8	17	6.2	12.7	8.6	22.1
	B	5.8		5.8	15.3	8.5	22.4
O ₃ -reactor effluent (dose 1.08 ± 0.05 g O ₃ /g DOC)	A	6.9	23	6.0	15.1	8.6	21.3
	B	7.2		5.6	13.0	8.5	22.3

Table S9. Experimental conditions of UV experiments

	Replicate	DOC [mg C/L]	COD _{dis} [mg O/L]	pH	Temp. [°C]
Influent	A	7.8	20.5	8.1	n.a.
	B	n.a.	22.3	n.a.	n.a.
1 run	A	7.4	20.6	8.2	n.a.
	B	n.a.	24.7	n.a.	n.a.
3 cycles	A	8.8	23.3	8.5	24.7
	B	n.a.	22.8	n.a.	n.a.
9 cycles	A	7.8	22.7	8.6	26.7
	B	n.a.	19.9	n.a.	n.a.

n.a. – data not available

Effective fluence rate calculation

Partial depletion of pharmaceuticals has been shown to occur during the disinfection of drinking water at 400 J/m² with a UV-C (254 nm) lamp.³ Depletion rates (under conditions of negligible optical density) were mostly unaffected by the presence of natural water components. At pH 8, a depletion of 27% for diclofenac and 15% for sulfamethoxazole and iopromide was found at this fluence. The nominal fluence rate of the UV/TiO₂ reactor given by the manufacturer is 10 mW/cm². With a residence time of 20 seconds in the reactor (without fibers), a fluence of 200 mW·sec/cm² = 200 mJ/cm² = 2000 J/m² is calculated.

For a fluence of 2000 J/m², the expected elimination rate of diclofenac can be calculated as follows:

$$R_{2000} = R_{400}^{\left(\frac{2000}{400}\right)} = 0.73^5 = 0.21$$

where R_x is the remaining fraction at a certain fluence (73% for diclofenac at 400 J/m^2 , see Canonica et al. (2008)). Therefore, the expected elimination of diclofenac without the fibers is 79%, which is not reached at all. Obviously, the hospital wastewater has a screening effect and is adsorbing radiation, so the effective fluence rate is smaller than the theoretical nominal fluence rate.

From the observed elimination rates, the effective fluence rate can be calculated.

$$E^0 = \frac{H^0}{t_r} = \frac{H_p^0 \cdot cf}{t_r} = \frac{H_p^0 \cdot 4.71 \cdot 10^5}{t_r} = \frac{-\frac{\ln R}{k_{EP}} \cdot 4.71 \cdot 10^5}{t_r}$$

E^0 (W/m^2): effective fluence rate

t_r (s): residence time in column (20 seconds without fibers)

H_p^0 (einstein/ m^2): photon fluence

H^0 (J/m^2): fluence

cf: conversion factor from photon fluence to fluence: $4.71 \times 10^5 \text{ J/einstein}$ at the wavelength of 254 nm

R: remaining fraction of pharmaceutical in experiment (0.53 for diclofenac, 0.72 for iopromide without fibers)

k_{EP} ($\text{m}^2/\text{einstein}$): photon fluence-based rate constant (Table 1 in Canonica et al. 2008):
376 $\text{m}^2/\text{einstein}$ for diclofenac, 191 $\text{m}^2/\text{einstein}$ for iopromide at pH 7-8.

With this equation, an effective fluence rate of 4.0 mW/cm^2 was calculated for the UV/ TiO_2 reactor with hospital wastewater (39.8 W/m^2 for diclofenac, 40.5 W/m^2 for iopromide). Therefore, the fluence rate is lower by a factor of 2.5 than the nominal value (10 mW/m^2), probably mostly due to the adsorption of light by the wastewater.

With the photocatalytic fibers, we (might) have an additional indirect phototransformation. However, the elimination is smaller than with UV only. Obviously, the screening and sorption of the light by the fibers is higher than the possible indirect phototransformation.

If we assume there is no indirect phototransformation happening for diclofenac and iopromide, we can calculate the fluence rate for the system with the fibers the same way as above ($R=0.79$ for diclofenac and 0.88 for iopromide, $t_r=18$ sec with photocatalytic fibers). The calculated fluence rate with the fiber is only 1.7 mW/cm^2 (16.4 W/m^2 for diclofenac, 17.5 W/m^2 for iopromide), so by a factor 2.4 lower than without the fibers (4.0 mW/cm^2).

Table S10. PAC elimination - comparison with prediction and literature for the micropollutants with: A – high elimination efficiency; B – intermediate and low elimination efficiency; and C – unknown or approximate experimental data. Elimination of micropollutants from an MBR permeate by 23±7 mg/L PAC (Norit SAS Super) from this study (DOC 7.0 ± 0.7 mg/L, pH 8.8, hydraulic residence time 1 day) compared to: adsorbability at pH 8.5 predicted from Log D_{ow} values (Table S3); and results of other studies.

A					B				
CHARGE at pH 8.5	PREDICTION	This study	Literature		CHARGE at pH 8.5	PREDICTION	This study	Literature	
		HIGH removal (>97%)	% Removal	Ref.			INTERMEDIATE and LOW removal	% Removal	% Removal Ref.
+	◦	Azithromycin	-	-		◦	4-Acetamidoantipyrine	73 ± 4	- -
	■	Carbamazepine	100, 98	4, 5		◦	4-Aminoantipyrine	95 ± 2	- -
+/-	■	Ciprofloxacin	69**	6		◦	4-Formylaminoantipyrine	81 ± 5	- -
(+)	■	Clarithromycin	99	5		◦	4-Methylaminoantipyrine	75 ± 4	- -
(+)	◦	Clindamycin	100	4	-	◦	4/5-Methylbenzotriazole	93 ± 2	95** 5
+	◦	D617	-	-	+/-	■	Atenolol acid	94 ± 2	- -
-	◦	Diclofenac	97, 78	4, 7	-	◦	Benzotriazole	84 ± 2	85-98 5
-	■	Furosemide	-	-		◦	Cyclophosphamide	73 ± 7	- -
(-)	■	Hydrochlorothiazide	-	-	-	■	Diazotriazole	14 ± 2	44, 55-70 4, 5
(+)	◦	Lidocaine	-	-		◦	Fluconazole	95 ± 2	- -
-	◦	Mefenamic acid	35**	5	+/-	■	Gabapentin	42 ± 4	- -
+	◦	Metoprolol	98	4		■	Iomeprol	65 ± 10	96, 46 4, 7
+/-	■	Norfloxacin	-	-		■	Iopamidol	69 ± 11	91, 42 4, 7
	■	Oxazepam	98	5		■	Iopromide	85 ± 8	87, 50 4, 7
+	■	Tramadol	-	-	-	■	Ioxitalamic acid	9 ± 12	- -
-	■	Valsartan	-	-		■	Levetiracetam	73 ± 2	- -
+	■	Venlafaxine	90**	5		■	Metronidazole	67 ± 9	90 4
					-	■	N4-Acetylsulfamethoxazole	92 ± 2	45-70 5
					+/-	■	Oseltamivir carboxylat	36 ± 4	- -
						◦	Phenazone	88 ± 11	90* 5
						◦	Primidone	79 ± 10	55-90, 84 5, 7
					+/-	■	Ritalinic acid	40 ± 4	- -
					+/(^c)	■	Sotalol	96 ± 1	96 4
					-	■	Sulfadiazine	40 ± 15	85* 5
					-	■	Sulfamethoxazole	33 ± 9	25-70 5
					-	◦	Sulfapyridine	95 ± 1	- -

C				
CHARGE at pH 8.5	PREDICTION	This study	Literature	
		Absence in PAC influent or concentrations in effluent below LOQ	% Removal	% Removal Ref.
	◦	4-Dimethylaminoantipyrine	absent	- -
+	■	Atenolol	> 88	92, 98* 4, 5
-	◦	Bezafibrate	> 86	99 4
+/-	■	Cilastatin	absent	- -
-	■	Clofibric acid	absent	- -
	◦	Dexamethasone	absent	- -
	■	Diazepam	absent	95-100 5
(+)	■	Erythromycin	> 88	66* 7
+	◦	Fluoxetine	absent	91* 8
-	◦	Ifosfamide	> 60	- -
-	◦	Indometacin	> 91	73 4
	■	Iohexol	absent	20-85 5
	◦	Methylprednisolone	absent	- -
+/(^c)	◦	Morphine	> 63	- -
-	■	Naproxen	absent	75**, 97 4, 5
+	◦	Oseltamivir	> 63	- -
(-)	◦	Paracetamol	absent	78* 8
+	◦	Propranolol	> 94	- -
(+)	◦	Ranitidine	> 96	100** 5
	■	Ritonavir	> 87	- -
+	■	Roxithromycin	absent	98 5
-	◦	Thiopental	> 66	- -
	◦	Trimethoprim	> 83	92 4
+	■	Verapamil	> 88	- -

Legend:

- + positively charged
- negatively charged
- +/- zwitterionic
- (+) or (-) partially charged (less than 50%)

- Log D_{ow} < 0 (low adsorbability)
- 0 < Log D_{ow} < 2 (intermediate ads.)
- Log D_{ow} > 2 (high adsorbability)

Log D_{ow} at pH 8.5 was calculated by JChem for Excel 5.3.3.165 (ChemAxon Ltd.)

- * lower PAC dose: 16 mg/L [Ref. ⁵]; 10 mg/L [Ref. ⁶]; 5 mg/L [Ref. ⁸]
- ** higher PAC dose: 30 [Ref. ⁵]; 50 (15 min t_c) [Ref. ⁶]

Table S11. O₃ elimination - comparison with prediction and literature for the micropollutants with: A – high elimination efficiency; B – intermediate and low elimination efficiency; and C – unknown or approximate experimental data. Elimination by ozonation from this study at 1.08 gO₃/gDOC (pH 8.5, 22°C, hydraulic residence time 23 min.) compared to: prediction from the molecular structure at pH 8-8.5 (see also Table S6); and results of other studies.

A

PREDICTION	This study		Literature				
	HIGH elimination (≥97%)	% Elimination	k'' _{O3} (M ⁻¹ s ⁻¹)			k'' _{O3,app} (M ⁻¹ s ⁻¹)	
			neutral	charged	Ref.	pH 7	pH 8 (or 8.5)
	4-Acetamidoantipyrine	99* ⁹					
	4-Formylaminoantipyrine	-					
	4-Methylaminoantipyrine	-					
°	4/5-Methylbenzotriazole	99 ⁹	1.6×10 ⁻²	(-) 1×10 ⁻⁴	²	1.3×10 ⁻³	(1.7×10 ⁻⁴)
	Atenolol acid	93* ⁹	6.3×10 ⁻⁵	(+) 1.1×10 ⁻²	¹⁰ structure sim.	1.6×10 ⁻³	(5.0×10 ⁻⁴)
	Carbamazepine	100 ⁹	3×10 ⁻⁵		¹¹	3×10 ⁻⁵	3×10 ⁻⁵
	Ciprofloxacin	16* ¹²	7.5×10 ⁻³	(-) 9.0×10 ⁻⁵	¹³	1.4×10 ⁻⁴	1.3×10 ⁻⁵
	Clarithromycin	99 ⁹	1.1×10 ⁻⁷		¹⁴	6.9×10 ⁻⁴	6.5×10 ⁻⁵
	Clindamycin	96** ⁹					
	D617	-					
	Diclofenac	99 ⁹ , 96 ⁸	1×10 ⁻⁶		¹¹	1×10 ⁻⁶	1×10 ⁻⁶
	Furosemide	-		(-) 2.2×10 ⁻⁴	QSAR ¹⁵	2.2×10 ⁻⁴	(2.2×10 ⁻⁵)
	Hydrochlorothiazide	-					
°	Indometacin	50* ¹⁶					
	Lidocaine	98* ⁹	4.4×10 ⁻⁵	(+) 1.1×10 ⁻⁴	QSAR ¹⁵	6.0×10 ⁻⁴	(3.6×10 ⁻⁵)
	Mefenamic acid	97 ⁹		(-) 5.5×10 ⁻⁶	QSAR ¹⁵	5.5×10 ⁻⁶	(5.5×10 ⁻⁶)
	Metoprolol	98 ⁹	8.6×10 ⁻⁵	(+) 3.3×10 ⁻²	¹⁷	2.0×10 ⁻³	1.7×10 ⁻⁴
	Norfloxacin	-					
	Ranitidine	-	1.1×10 ⁻⁶	(+) 3.0×10 ⁻⁵	QSAR ¹⁵	3.7×10 ⁻⁵	(1.0×10 ⁻⁶)
	Sulfamethoxazole	96 ⁹	4.7×10 ⁻⁴	(-) 5.7×10 ⁻⁵	¹³	5.7×10 ⁻⁵	5.7×10 ⁻⁵
	Tramadol	-	1.6×10 ⁻⁶	(+) 7.7×10 ⁻¹	¹⁸	4.0×10 ⁻³	(1.1×10 ⁻⁵)
	Venlafaxine	99* ⁹	8.3×10 ⁻⁵	(+) 3.0×10 ⁻³	QSAR ¹⁵	6.3×10 ⁻³	(9.6×10 ⁻⁴)

B

This study			Literature					
PREDICTION	INTERMEDIATE and LOW elimination	% Elimination	% Elimination	k'' _{O3} (M ⁻¹ s ⁻¹)			k'' _{O3,app} (M ⁻¹ s ⁻¹)	
				neutral	charged	Ref.	pH 7	pH 8 (or 8.5)
o	Benzotriazole	90 ± 0.3	90 ⁹	3.5×10 ⁻¹	(-) 2.7×10 ⁻³	²	2.4×10 ⁻²	1.4×10 ⁻³
o	Bezafibrate ^(spike)	87 ± 3.8	99 ^{*19}		(-) 5.9×10 ⁻²	¹¹	5.9×10 ⁻²	5.9×10 ⁻²
	Cyclophosphamide	57 ± 0.2	>60 ²⁰					
	Diatrizoate	16 ± 1.9	14 ^{*16}		(-) <1	¹¹	<1	<1
	Fluconazole	47 ± 1.7	>91 ^{*9}	<1		QSAR ¹⁵	<1	(<1)
o	Gabapentin	74 ± 0.9	-	2.2×10 ⁻⁵		QSAR ¹⁵	4.4×10 ⁻¹	(1.4×10 ⁻³)
	Ifosfamide	62	-					
	Iomeprol	52 ± 3.4	48 ^{*19}	<1		¹¹	<1	<1
	Iopamidol	55 ± 0.5	47 ^{*19}	<1		¹¹	<1	<1
	Iopromide	60 ± 1.9	49 ^{**9} , 59 ^{*19}	<0.8		¹¹	<0.8	<0.8
	Ioxitalamic acid	25 ± 6.8	1-66 ^{*9}					
	Levetiracetam	54 ± 3.0	12-55 ^{*9}	<1		QSAR ¹⁵	<1	(<1)
	Metronidazole	49 ± 3.7	-					
	N4-AcSMX	80 ± 0.2	85 ^{*19}	2.6×10 ⁻²	(+) 2.0×10 ⁻¹	¹³	2.6×10 ⁻²	2.6×10 ⁻²
	Oxazepam	83 ± 0.6	not removed ^{*21}	<10		QSAR ¹⁵	<10	(<10)
	Primidone	78	91 ^{**9}	<10		QSAR ¹⁵	<10	(<10)
	Valsartan	78 ± 1.5	-		(-) 2.4×10 ⁻¹	QSAR ¹⁵	2.4×10 ⁻¹	(2.4×10 ⁻¹)

table continues

Table S11. O₃ elimination - comparison with prediction and literature (*continued*).

C

PREDICTION	This study		Literature					
	Absence in O ₃ influent or concentrations in effluent below LOQ	% Elimination	% Elimination	k'' _{O3} (M ⁻¹ s ⁻¹)			k'' _{O3,app} (M ⁻¹ s ⁻¹)	
				neutral	charged	Ref.	pH 7	pH 8 (or 8.5)
	4-Aminoantipyrine	> 83	-					
	4-Dimethylaminoantipyrine	absent	99* ⁹					
	Atenolol	> 23	99 ⁹	6.3×10 ⁵	(+) 1.1×10 ²	¹⁰	1.6×10 ³	(5.0×10 ⁴)
	Azithromycin	> 91	100* ¹⁹	6.0×10 ⁶		¹³	1.2×10 ⁵	9.9×10 ⁵
	Cilastatin	absent	-					
°	Clofibric acid	absent	86** ⁹		<20	¹⁹	~6	~6
°	Dexamethasone	absent	-					
	Diazepam	absent	66 ⁸	7.5×10 ⁻¹		¹¹	7.5×10 ⁻¹	7.5×10 ⁻¹
	Erythromycin	> 93	96 ⁸					
°	Fluoxetine	absent	98 ⁸					
	Iohexol	absent	39* ⁹	<0.8		¹¹	<1	<1
°	Methylprednisolone	absent	-					
	Morphine	> 84	-					
°	Naproxen	absent	86-95 ⁸		(-) 2.0×10 ⁵	¹⁹	2.0×10 ⁵	2.0×10 ⁵
	Oseltamivir	> 79	-					
	Oseltamivir carboxylat	> 93	-					
	Paracetamol	absent	90-97 ⁸	1.4×10 ³	(-) 9.9×10 ⁸	²²	1.3×10 ⁶	3.8×10 ⁷
	Phenazone	> 71	100* ⁹					
	Propranolol	> 92	98 ⁹	1×10 ⁵		¹⁰	1×10 ⁵	1×10 ⁵
°	Ritalinic acid	> 93	-					
°	Ritonavir	> 74	-					
	Roxithromycin	absent	100* ¹⁹	1.0×10 ⁷		¹¹	2.8×10 ⁴	5.9×10 ⁵
°	Sotalol	> 94	98 ⁹				4.8×10 ²	(1.4×10 ⁴)
	Sulfadiazine	> 47	86** ⁹	>10 ⁵		¹¹		
	Sulfapyridine	> 96	98 ⁹	>10 ⁵		¹¹	7.1×10 ⁴	(3.6×10 ⁵)
	Thiopental	> 56	-					
	Trimethoprim	absent	94 ⁹ , 100 ⁸	5.2×10 ⁵	(+) 7.4×10 ⁴	¹³	2.7×10 ⁵	4.7×10 ⁵
	Verapamil	> 76	-					

Legend:

* lower ozone dose: 0.6 - 0.8^{9, 19}; 0.3¹², 0.4 - 0.7¹⁶, 0.3²¹ gO₃/gDOC)

** higher ozone dose: 1.16 gO₃/gDOC⁹)

Prediction of reactivity with ozone for pH 8.5 (Tab. S6):

■ low or no reactivity with ozone
(≈ k''_{O3,app} < 10 M⁻¹s⁻¹)

■ intermediate reactivity with ozone
(≈ k''_{O3,app} between 10 and 1×10⁵ M⁻¹s⁻¹)

■ high reactivity with ozone
(≈ k''_{O3,app} > 1×10⁵ M⁻¹s⁻¹)

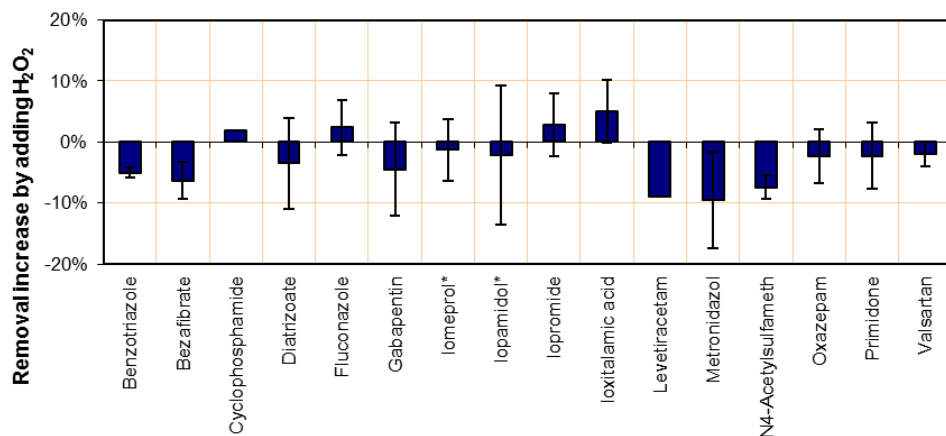


Figure S4. Comparison of ozonation treatment with and without hydrogen peroxide (0.7 gO₃/gDOC, 2.5 mg/L H₂O₂).

Table S12. UV elimination – comparison of UV and UV/TiO₂. Average and deviation from the average of two experiments. All compounds with an elimination >20% after 9 cycles UV treatment are shown.

	% Elimination with UV/TiO ₂		% Elimination with UV	
	3 cycles (918 J/m ²)	9 cycles (2754 J/m ²)	3 cycles (2400 J/m ²)	9 cycles (7200 J/m ²)
4-Acetamidoantipyrine	16 ± 3.0	89 ± 1.6	87 ± 1.1	99 ± 0.3
4-Aminoantipyrine	54 ± 23	78 ± 3.0	41 ± 6.0	55 ± 5.2
4-Formylaminoantipyrine	62 ± 1.0	88 ± 3.8	85 ± 0.3	98 ± 0.9
4-Methylaminoantipyrine	18 ± 1.1	18 ± 8.8	8.5 ± 16	26 ± 10
Azithromycin	5.1 ± 4.6	6.4 ± 6.0	14 ± 3.6	23 ± 5.4
Ciprofloxacin	19 ± 1.5	35 ± 2.4	29 ± 3.5	57 ± 3.1
Diatrizoate	42 ± 4.8	73 ± 3.0	72 ± 2.4	97 ± 0.4
Diclofenac	62 ± 4.5	90 ± 1.2	88 ± 1.3	98 ± 1.0
Furosemide	0.6 ± 4.6	13 ± 1.4	14 ± 3.5	35 ± 5.6
Hydrochlorothiazide	13 ± 3.5	20 ± 1.3	14 ± 2.9	50 ± 1.6
Indomethacin	9.5 ± 0.6	14 ± 3.0	9.0 ± 13	24 ± 5.3
Iomeprol	11 ± 25	21 ± 46	65 ± 0.4	90 ± 2.1
Iopamidol	25 ± 11	41 ± 26	66 ± 0.4	92 ± 0.8
Iopromide	35 ± 0.6	63 ± 1.7	60 ± 3.0	92 ± 0.5
Ioxitalamic acid	34 ± 2.1	69 ± 0.8	52 ± 4.9	92
Mefenamic acid	7.0 ± 2.2	11 ± 2.8	8.3 ± 0.9	21 ± 4.5
Metronidazole	0 ± 24	0 ± 33	0 ± 36	22 ± 7.6
Morphine	54 ± 4.3	74	66 ± 0.4	84
N4-Acetylsulfamethoxazole	3.7 ± 0.5	11 ± 0.2	14 ± 3.6	33 ± 1.1
Norfloxacin	20 ± 1.1	35 ± 0.3	40 ± 1.4	63 ± 2.4
Oseltamivir	7.8 ± 0.7	13 ± 0.2	19 ± 0.6	40 ± 0.4
Phenazone	42 ± 5.1	55 ± 6.7	50 ± 5.7	64 ± 5.3
Propranolol	8.7 ± 3.8	17 ± 11	13 ± 1.2	23 ± 2.5
Ranitidine	24 ± 1.8	41 ± 3.0	41 ± 1.0	71 ± 0.8
Sotalol	53 ± 5.3	87 ± 3.2	79 ± 1.1	>95
Sulfadiazine	0 ± 2.8	5.3 ± 8.3	21 ± 4.1	25 ± 0.5
Sulfamethoxazole	26 ± 1.4	50 ± 5.9	55 ± 1.9	85 ± 3.2
Sulfapyridine	44 ± 17	64 ± 2.4	6.0 ± 12	69 ± 3.3
Thiopental	18	25	35	47
Tramadol	2.6 ± 2.2	11 ± 2.2	15 ± 1.5	26 ± 1.3
Verapamil	14 ± 4.2	28 ± 5.9	19 ± 3.6	40 ± 4.6

Table S13. AOX (adsorbable organic halogen compounds, expressed as Cl-equivalents) after biological treatment in MBR, after PAC and after ozone treatment.

	AOX (mg/L)
After MBR	0.557
After PAC (43 mg/L)	0.157
After ozonation (1.08 g ozone/g DOC)	0.334

4. Cost estimation

The costs of three different treatment concepts were calculated:

1. Decentralized treatment of hospital wastewater: a biological treatment (with a screen, a fine screen, and a membrane bioreactor) and 10 mg/L ozone, followed by a biofilter
2. Decentralized treatment of hospital wastewater: a biological treatment (with a screen, a fine screen, and a membrane bioreactor) and 20 mg/L PAC
3. Source separation by collecting urine with bottles or road bags from patients being treated with contrast media (stationary and out-patients). Part of the urine is already collected by the means of catheters. The collected urine is incinerated with the household waste.

The parameters of the hospital Baden which were taken as a basis of the cost calculations are listed in Table S14. The calculated costs are shown detailed in Table S15 and summarized in Table S16. The investment and annual operating costs were estimated and then calculated to the total annual costs in Swiss Francs, based on an annual interest rate of 4% and an investment period of 15 years. The investment costs included planning and project management, construction and installation costs of the equipment, electromechanical equipment (sieves, containers, aeration), and requirements specific to the different technologies to remove pharmaceuticals (activated carbon, ozonation, etc.). The hospital has the advantage of an already existing building for the wastewater treatment, what reduced the costs. The operating costs were based on estimates for waste disposal (e.g. sewage sludge, urine bags), energy requirements, and replacement of materials such as membranes, costs of activated carbon, and labor costs for extra personnel.

Table S14: Parameters of the analyzed hospital (case study hospital Baden).

Parameter	Units	Value
number of hospital beds ¹	[beds]	371
sewage flow ¹	[m ³ /y]	116'000
urine collected with catheters ²	[m ³ /y]	68
urine in urine bags (stationary) ²	[m ³ /y]	3.75
urine in urine bags (stationary and out-patients) ²	[m ³ /y]	10.4

¹ measured values in 2007

² calculated values based on assumptions

Table S15: Detailed investment and annual operating costs in Swiss Francs.

	screen - fine screen - MBR - ozonation (10mg/l)	screen - fine screen - MBR - PAC (20mg/l)	urine bag - disposal together with municipal waste
Construction of MBR	650'000	650'000	-
containers, screen	80'000	80'000	-
membrane, aeration	300'000	300'000	-
PAC installation	-	400'000	-
ozone installation	120'000	-	-
biofilter as post-treatment	100'000	100'000	-
EMSRL	400'000	400'000	-
planning	248'000	290'000	0
reserve	380'000	444'000	0
Total investment costs	2'278'000	2'664'000	0
waste disposal			166'000
waste in screen	3'000	3'000	
sludge waste	22'000	22'000	4'000
energy MBR	40'000	40'000	-
energy ozonation	8'000	-	-
energy PAC	-	4'000	-
Replacement of MBR	20'000	20'000	-
PAC	-	4'000	-
replacement reserve	10'000	12'000	-
personnel	30'000	30'000	1'000
Total operating costs	133'000	135'000	171'000

Table S16. Costs of different concepts at the hospital in Swiss Francs.

	screen - fine screen - MBR - ozonation (10mg/l)	screen - fine screen - MBR - PAC (20mg/l)	urine bag
investment costs	2'278'000 Fr.	2'664'000 Fr.	0 Fr.
operating costs	133'000 Fr.	135'000 Fr.	171'000 Fr.
annual costs	337'886 Fr.	374'603 Fr.	171'000 Fr.
costs per hospital bed and day	2.50 Fr.	2.77 Fr.	0.46 Fr. ² 1.26 Fr.
Costs per m ³ waste water ¹	2.91 Fr.	3.23 Fr.	1.47 Fr.

¹ The costs per m³ waste water are calculated by dividing the annual costs by the annual waste water amount.² only stationary patients

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