

Prioritization of organic contaminants in a reclaimed water irrigation system using wide-scope LC-HRMS screening

Supporting Information

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Table S1. GPS coordinates for the sampling points

Sampling Point		Latitude	Longitude
A	Influent WRP	41.276142	2.040351
B	Effluent WRP	41.276142	2.040351
C	First surface discharge	41.278750	1.997611
D	Irrigation Point	41.278384	2.009450

Table S2. Calibrants used in the RTI model in the positive ionization mode (ESI+), and corresponding SMILES and experimental retention time (RT).

RTI calibrant	SMILES	Experimental RT (min)
Amitrole	<chem>C1=NNC(=N1)N</chem>	1.17
Guanylurea	<chem>C(=NC(=O)N)(N)N</chem>	1.18
Histamine	<chem>C1=C(NC=N1)CCN</chem>	n.d.
Chlormequat	<chem>C[N+](C)(C)CCCl</chem>	1.25
Methamidophos	<chem>COP(=O)(N)SC</chem>	2.77
Vancomycin	<chem>CC1C(C(CC(O1)OC2C(C(C(OC2OC3=C4C=C5C=C3OC6=C(C=C(C=C6)C(C(C(=O)NC(C(=O)NC5C(=O)NC7C8=CC(=C(C=C8)O)C9=C(C=C(C=C9O)O)C(NC(=O)C(C(C1=CC(=C(O4)C=C1)C)O)NC7=O)C(=O)O)CC(=O)N)NC(=O)C(CC(C)C)NC)O)C)O)C)N)O</chem>	4.34
Trichlorfon	<chem>COP(=O)(C(C(Cl)(Cl)Cl)O)OC</chem>	6.69
Cefoperazone	<chem>CCN1CCN(C(=O)C1=O)C(=O)NC(C2=CC=C(C=C2)O)C(=O)NC3C4N(C3=O)C(=C(CS4)CSC5=NN=NN5C)C(=O)O</chem>	7.35
Butocarboxim	<chem>CC(C(=NOC(=O)NC)C)SC</chem>	8.50
Dichlorvos	<chem>COP(=O)(OC)OC=C(Cl)Cl</chem>	9.69
Tylosin	<chem>CCC1C(C=C(C=CC(=O)C(C(C(C(C(C(=O)O1)O)C)OC2C(C(C(O2)C)OC3CC(C(C(O3)C)O)(C)O)N(C)C)O)CC(=O)C)C)COC4C(C(C(C(O4)C)O)OC)OC</chem>	n.d.
Rifaximin	<chem>CC1C=CC=C(C(=O)NC2=C(C3=C(C4=C(C(=C3O)C)OC(C4=O)OC=CC(C(C(C(C(C1O)C)O)C)OC(=O)C)C)OC)C)C5=C2N6C=CC(=CC6=N5)C)O)C</chem>	12.35
Spinosad_A	<chem>CCC1CCCC(C(C(=O)C2=CC3C4CC(CC4C=CC3C2CC(=O)O1)OC5C(C(C(C(O5)C)OC)OC)OC)OC6CCC(C(O6)C)N(C)C</chem>	12.85
TCMTB	<chem>C1=CC=C2C(=C1)N=C(S2)SCSC#N</chem>	13.57
Emamectin	<chem>CCC(C)C1C(C=CC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)NC)OC)OC)C</chem>	14.28
Avermectin	<chem>CCC(C)C1C(C=CC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)O)OC)OC)C</chem>	17.79
Nigericin	<chem>CC1CCC(OC1C(C)C(=O)O)CC2CC(C(C3(O2)C(CC(O3)(C)C4C(CC(O4)(C)C5C(CC(O5)C6C(CC(C(O6)(CO)O)C)C)C)C)OC</chem>	n.d.
Ivermectin	<chem>CCC(C)C1C(CCC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)O)OC)OC)C</chem>	20.05

n.d.: not detected

Table S3. Calibrants used in the RTI model in the negative ionization mode (ESI-), and corresponding SMILES and experimental retention time (RT).

RTI calibrant	SMILES	Experimental RT (min)
Amitrole	<chem>C1=NNC(=N1)N</chem>	1.27
Benzoic acid	<chem>C1=CC=C(C=C1)C(=O)O</chem>	n.d.
Acephate	<chem>CC(=O)NP(=O)(OC)SC</chem>	3.52
Salicylic acid	<chem>C1=CC=C(C(=C1)C(=O)O)O</chem>	4.39
Tepraloxydim	<chem>CCC(=NOCC=CCl)C1=C(CC(CC1=O)C2CCOCC2)O</chem>	5.26
Simazine-2-Hydroxy	<chem>CCNC1=NC(=NC(=O)N1)NCC</chem>	5.61
Valproic acid	<chem>CCCC(CCC)C(=O)O</chem>	6.41
Bromoxynil	<chem>C1=C(C=C(C(=C1Br)O)Br)C#N</chem>	6.66
MCPA	<chem>CC1=C(C=CC(=C1)Cl)OCC(=O)O</chem>	6.69
Flamprop	<chem>CC(C(=O)O)N(C1=CC(=C(C=C1)F)Cl)C(=O)C2=CC=CC=C2</chem>	7.89
Dinoterb	<chem>CC(C)(C)C1=C(C(=CC(=C1)[N+](=O)[O-])[N+](=O)[O-])O</chem>	9.66
Phenytoin	<chem>C1=CC=C(C=C1)C2(C(=O)NC(=O)N2)C3=CC=CC=C3</chem>	9.70
Inabenfide	<chem>C1=CC=C(C=C1)C(C2=C(C=CC(=C2)Cl)NC(=O)C3=CC=N(C=C3)O</chem>	11.74
Benodanil	<chem>C1=CC=C(C=C1)NC(=O)C2=CC=CC=C2I</chem>	12.23
Coumaphos	<chem>CCOP(=S)(OCC)OC1=CC2=C(C=C1)C(=C(C(=O)O2)Cl)C</chem>	15.32
Triclosan	<chem>C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl</chem>	15.48
Abamectin	<chem>CCC(C)C1C(C=CC2(O1)CC3CC(O2)CC=C(C(C(C=CC=C4COC5C4(C(C=C(C5O)C)C(=O)O3)O)C)OC6CC(C(C(O6)C)OC7CC(C(C(O7)C)O)OC)OC)C.CC1C=CC=C2COC3C2(C(C=C(C3O)C)C(=O)OC4CC(CC=C(C1OC5CC(C(C(O5)C)OC6CC(C(C(O6)C)O)OC)OC)OC)OC7(C4)C=CC(C(O7)C(C)C)O</chem>	17.76
Salinomycin	<chem>CCC(C1CCC(C(O1)C(C)C(C(C)C(=O)C(CC)C2C(CC(C3(O2)C=CC(C4(O3)CCC(O4)(C)C5CCC(C(O5)C)(CC)O)O)C)O)C)C(=O)O</chem>	18.18

n.d.: not detected

Table S4. Calibrants used to harmonize the analyte ionization efficiency in the semi-quantification process, and their corresponding SMILES and internal standard (imidacloprid-*d4*) calibration slopes.

Compound	SMILES	Slope
Acetaminophen	<chem>CC(=O)NC1=CC=C(C=C1)O</chem>	13.39
Acetamiprid	<chem>CC(=NC#N)N(C)CC1=CN=C(C=C1)Cl</chem>	21.91
2-Amino-benzothiazole	<chem>C1=CC=C2C(=C1)N=C(S2)N</chem>	75.13
Atrazine	<chem>CCNC1=NC(=NC(=N1)Cl)NC(C)C</chem>	147.98
Caffeine	<chem>CN1C=NC2=C1C(=O)N(C(=O)N2C)C</chem>	16.21
Carbamazepine	<chem>C1=CC=C2C(=C1)C=CC3=CC=CC=C3N2C(=O)N</chem>	41.48
Cefoperazone	<chem>CCN1CCN(C(=O)C1=O)C(=O)NC(C2=CC=C(C=C2)O)C(=O)NC3C4N(C3=O)C=C(CS4)CSC5=NN=NN5C)C(=O)O</chem>	0.38
Desethyl atrazine (DEA)	<chem>CC(C)NC1=NC(=NC(=N1)N)Cl</chem>	65.41
N, N-Diethyl-meta-toluamide (DEET)	<chem>CCN(CC)C(=O)C1=CC=CC(=C1)C</chem>	151.15
Dichlorvos	<chem>COP(=O)(OC)OC=C(Cl)Cl</chem>	11.77
Imidacloprid	<chem>C1CN(C(=N[N+](=O)[O-])N1)CC2=CN=C(C=C2)Cl</chem>	12.06
Rifaximin	<chem>CC1C=CC=C(C(=O)NC2=C(C3=C(C4=C(C(=C3O)C)OC(C4=O)(OC=CC(C(C(C(C(C1O)C)O)C)OC(=O)C)C)OC)C)C5=C2N6C=CC(=CC6=N5)C)O)C</chem>	8.66
Simazine	<chem>CCNC1=NC(=NC(=N1)Cl)NCC</chem>	111.27
Sulfamethoxazole	<chem>CC1=CC(=NO1)NS(=O)(=O)C2=CC=C(C=C2)N</chem>	20.88
Spinosad A	<chem>CCC1CCCC(C(C(=O)C2=CC3C4CC(CC4C=CC3C2CC(=O)O1)OC5C(C(C(C(O5)C)OC)OC)OC)C)OC6CCC(C(O6)C)N(C)C</chem>	29.73
Theophylline	<chem>CN1C2=C(C(=O)N(C1=O)C)NC=N2</chem>	10.61
Thiacloprid	<chem>C1CSC(=NC#N)N1CC2=CN=C(C=C2)Cl</chem>	13.73
Trichlorfon	<chem>COP(=O)(C(C(Cl)(Cl)Cl)O)OC</chem>	2.734
Tylosin	<chem>CCC1C(C=C(C=CC(=O)C(CC(C(C(C(C(=O)O1)O)C)OC2C(C(C(C(O2)C)OC3CC(C(C(O3)C)O)(C)O)N(C)C)O)CC(=O)C)C)COC4C(C(C(C(O4)C)O)OC)OC</chem>	7.02

Table S5. Individual and mixture ecotoxicological risk ranking categories based on the value of the risk quotient (RQ)

Risk Quotient (RQ)	Categories	Acronym
RQ < 0.1	No risk	NR
0.1 < RQ < 1	Low risk	LR
1 < RQ < 10	Moderate risk	MR
RQ > 10	High risk	HR

Table S6. Compounds tentatively identified in the waters collected in the winter campaign and their area in each water sample.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
10,11-Dihydro-10,11-dihydroxycarbamazepine		28,802,236	33,566,120	51,333,621	23,935,101
10,11-Dihydro-10-Hydroxycarbamazepine		24,933,483	52,809,579	63,229,838	43,776,113
2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile		4,381,333	10,502,821	9,906,463	5,485,307
2-Ethyl-1,5-dimethyl-3,3-diphenylpyrrolinium (EDDP)		9,985,065	23,913,163	31,454,033	26,287,915
2-Mercaptobenzothiazole	871,480	3,177,200	3,890,011	5,165,838	2,070,890
3,3,5,5-Tetramethyl-1-pyrroline N-oxide		26,859,935	38,645,652	323,515,205	551,028,316
3-Hydroxycotinine		1,877,722	2,752,381	2,621,400	17,236,118
4'-Hydroxydiclofenac					6,089,163
4-Androstene-3,17-dione		-	-	-	77,110,913
4-Formylaminoantipyrine		175,584,323	299,236,807	511,525,481	153,697,176
4-Indolecarbaldehyde	222,304	2,123,078	9,221,892	5,701,027	28,412,659
4-Phenylbutyric acid		-	-	-	33,847,981
5-Hydroxyomeprazole		-	2,231,351	3,688,848	6,931,047
8-Hydroxyquinoline	69,096	1,981,849	1,239,311	1,365,183	42,933,129
Acephylline		1,626,513	1,699,435	3,363,678	150,188
Acetaminophen		-	-	-	3,606,214,471
Acetaminophen sulfate					181,938,708
Acetyl sulfamethoxazole					19,571,136
Amisulpride		27,028,566	32,515,543	61,171,839	16,402,012
Amitriptyline		3,412,679	22,633,319	13,044,835	16,783,038
Ampyrone/ 4-aminoantipyrine		1,834,271	4,672,515	26,193,761	59,818,639
Atenolol		6,113,266	11,091,006	18,422,944	57,699,520
Azithromycin				909,560.00	
Azoxystrobin		6,755,362	205,953	314,829	374,328
Azoxystrobin acid		5,501,093	-	-	-
Benzoyllecgonine		10,332,351	-	-	129,574,213
Bezafibrate		291,604	454,797	491,114	5,013,108
Bisoprolol		12,978,670	19,432,304	23,736,639	33,176,998
Boldenone		-	-	-	60,154,066
Boscalid		5,790,429	66,974	105,456	-

Table S6. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
Bupropion		2,840,306	4,841,521	3,813,620	1,481,301
Butyrophenone	1,580,852	39,887,861	26,614,913	47,605,092	6,533,394
Caffeine		34,632,858	1,029,111	1,266,623	1,233,948,117
Caprolactam	28,197,270	2,631,402,710	236,750,939	234,777,778	195,242,444
Carbamazepine	298,001	18,439,369	44,572,422	31,713,778	16,487,527
Carbamazepine-10,11-epoxide		1,089,705	4,460,027	41,018,817	15,025,874
Carbendazim		10,085,701	1,610,915	1,819,522	5,519,371
Carboxy-ibuprofen					7,944,030
Cetirizine		9,286,820	39,569,660	27,748,873	32,211,946
Chlorpheniramine		399,516	4,122,959	4,748,106	-
Ciprofloxacin		-	296,886	7,139,247	14,214,891
Citalopram		10,412,011	56,933,934	41,440,923	41,766,110
Clopidogrel		1,225,882	7,063,010	7,164,165	2,889,293
Clopidogrel carboxylic acid		12,734,076	15,282,108	21,677,900	7,680,546
Cocaine	110,787	2,106,619	-	1,012,461	112,417,140
Cotinine	69,293	6,101,028	1,195,333	1,031,565	64,595,751
Coumarin		-	414,870	-	36,008,492
Cyprodinil		-	-	76,515	46,151,878
DEET (N, N-Diethyl-meta-toluamide)	8,485,815	30,734,296	32,267,346	43,034,198	265,149,494
Desacetyl diltiazem		2,582,415	8,018,496	9,630,096	2,852,343
Desmethylocitalopram		7,316,943	27,924,962	21,894,533	17,904,849
Desmethyldiazepam		3,827,689	10,027,743	7,218,687	4,974,750
Dextromethorphan		4,557,018	16,534,719	10,769,300	6,059,018
dextrorphan/levorphanol		34,690,035	42,548,985	107,405,045	37,456,824
Diazepam		1,068,872	1,707,557	2,376,854	1,168,373
Diazinon		333,316	475,452	1,349,985	1,318,161
Dibutyl phthalate	18,042,016	44,817,763	41,446,794	87,899,239	35,302,504
Diclofenac		2,317,957	12,278,978	23,368,196	13,550,597
Diethyl phthalate	8,556,187	29,607,075	29,173,902	36,165,725	77,487,160
Diltiazem		1,370,584	4,125,310	4,386,467	5,622,543
Diphenhydramine		1,143,231	8,788,560	6,907,068	4,765,788
Diuron				4,530,668.00	

Table S6. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
Ecgonine methyl ester		3,378,260	5,423,467	5,384,177	7,481,055
Emtricitabine		1,732,701	839,195	4,596,483	5,495,139
Ephedrine		4,272,290	12,502,940	16,822,804	48,894,748
Epoxiconazole		-	3,460,534	4,281,339	122,307
Fenofibric acid		160,665	2,221,117	2,191,615	43,589,568
Flecainide		51,695,391	111,976,548	73,739,033	78,249,003
Fluconazole		3,489,715	4,649,614	8,178,337	2,758,996
Flufenamic acid		1,932,496	5,980,904	15,507,235	4,621,538
Gabapentin		39,346,796	37,901,862	72,850,065	457,100,720
Galaxolidone	1,278,044	148,815,289	217,463,268	257,869,604	101,497,021
Hydroxy-bupropion					3,939,358
Ibuprofen		-	-	-	2,466,589
Imidacloprid				4,090,139.00	
Isoproturon		5,881,582	6,051,649	6,640,211	7,559,292
Ketamine		11,177,334	15,730,056	24,722,700	6,296,912
Ketoprofen		433,119	6,891,024	8,424,571	42,790,663
Lamotrigine	40,662	36,078,747	47,214,397	67,600,595	11,329,320
Lamotrigine 2-N-glucuronide					1,003,666
Lauryl diethanolamide	8,785,485	15,204,060	11,964,749	11,552,279	2,670,872,257
Levamisole		10,583,716	23,467,684	38,985,559	7,579,722
Levofloxacin/ofloxacin		674,276	4,580,973	12,114,013	10,143,758
Lidocaine		66,526,748	66,544,115	90,657,902	33,252,288
MDMA		12,243,616	11,946,960	18,088,081	5,898,410
Mebendazole		230,739	1,044,795	932,917	9,423,980
Memantine		12,005,828	21,577,450	20,771,071	18,283,092
Metformin		198,713,057	13,107,946	15,242,462	1,128,019,508
Methadone		8,418,179	20,092,707	20,179,267	8,945,427
Metoclopramide		-	2,779,834	7,282,234	1,482,540
Metoprolol		2,487,618	2,875,558	4,319,653	2,065,162
Metoprolol acid		38,524,508	39,131,354	58,080,433	13,820,458
Mirtazapine		520,239	3,428,278	6,393,503	2,302,115
Mycophenolic acid		-	-	-	54,097,106

Table S6. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
N,N'-Diphenylguanidine	337,666	147,344,113	38,551,527	77,911,650	40,636,189
N-Acetyl-5-aminosalicylic acid		-	-	-	59,411,235
N-Acetylaminoantipyrine		121,008,666	156,205,169	268,655,500	502,486,674
Naproxen		-	-	-	2,381,368
Nicotine		-	-	-	90,319,120
N-Phenyl-1-naphthylamine	10,110,039	57,321,224	56,063,410	117,208,575	4,869,026
O-Desmethyl Venlafaxine		280,376,328	265,772,408	534,563,953	167,066,027
O-desmethyltramadol		184,847,728	161,948,712	373,755,687	94,706,883
Omeprazole sulfone		-	1,570,559	2,816,011	1,255,802
Oxazepam		4,432,088	7,715,176	8,059,645	6,236,707
Oxybenzone	89,267,904	423,078,174	78,864,335	115,773,003	17,894,347
Pentaethylene glycol (PEG)	7,958,492	82,843,782	26,003,007	59,434,458	1,420,018,883
Perfluorobutanesulfonic acid (PFBS)	411,539	5,119,992	3,710,469	6,772,305	1,360,360
Perfluorobutanoic acid (PFBA)	81,903	1,148,274	624,487	1,052,114	718,794
Perfluoroheptanoic acid (PFHpA)	127,467	1,226,857	633,071	1,356,920	176,094
Perfluorohexanoic acid (PFHxA)	1,356,104	1,356,104	1,991,227	6,259,050	1,522,888
Perfluorooctanoic acid (PFOA)	68,074	2,115,278	841,397	967,575	520,828
Perfluoropentanoic acid (PFPeA)		1,379,211	1,027,568	1,964,029	205,337
Pregabalin		3,278,291	1,424,433	3,027,276	148,874,629
Propranolol		4,834,741	19,393,365	17,066,150	7,241,523
Quetiapine		-	-	-	3,590,722
R-Methyl-benzotriazole (R=1, 4, 5)			340,406,757	360,541,484	125,863,115
R-Methyl-benzotriazole (R=1, 4, 5)				323,956,720	
Ritalinic acid		6,432,319	4,397,258	7,416,885	14,982,791
Secbumeton		2,576,470	8,010,429	4,162,586	88,215
Sertraline		313,098	1,651,038	1,986,788	8,905,255
Sitagliptin		39,352,462	67,541,917	114,218,139	56,483,851
Sotalol		4,156,110	5,862,502	9,996,212	3,346,857
Sulfamethoxazole		5,206,590	5,772,014	10,380,316	16,441,035
Sulpiride		57,801,159	53,558,905	81,264,144	13,119,337
Tapentadol		100,940,372	111,568,461	270,317,932	98,090,255
Tebuconazole		531,948	614,900	868,677	-

Table S6. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
Temazepam		4,651,440	9,226,487	8,763,810	5,293,719
Terbutryn	146,627	21,702,033	30,713,604	47,394,253	53,749,219
Testosterone propionate		-	-	-	37,607,007
Tetradecylamine	7,636,971	20,571,457	17,854,000	21,926,063	14,619,996,349
Tetrakis(2-hydroxypropyl)ethylenediamine		-	-	-	21,982,019
Theobromine		12,001,253	3,147,484	6,900,279	378,510,747
Theophylline/ Paraxanthine		13,738,154	1,777,135	-	326,542,019
Tramadol		309,180,190	381,509,621	560,585,832	157,888,451
Tri(chloropropyl) phosphate	2,520,094	18,971,233	20,657,976	31,809,710	85,956,630
Tributyl phosphate	15,890,995	63,944,436	65,512,766	75,424,227	29,316,906
Triethanolamine	1,573,674	8,977,992	2,227,076	2,824,968	298,674,507
Triethylene glycol monobutyl ether	1,042,465	2,336,948	1,001,677	2,061,741	437,488,081
Triisobutyl phosphate	4,953,077	51,714,297	12,165,553	18,384,292	6,217,829
Trimethoprim	44,780	1,011,207	3,792,529	8,493,457	11,843,418
Triphenyl phosphate	956,138	2,479,712	1,509,219	2,929,440	10,768,324
Tris(2-butoxyethyl) phosphate	224,981	11,002,007	10,611,995	7,740,892	216,715,060
Venlafaxine	221,857	123,110,873	260,409,983	232,418,941	119,510,457
Vildagliptin		7,036,946	9,118,227	14,785,127	4,899,123
Imidacloprid- <i>d4</i>	186,326,480	13,236,126	10,676,844	14,378,600	5,787,204

Table S7. Compounds tentatively identified in the water samples collected in the summer campaign and their area in each water sample.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
1,2-Benzisothiazol-3(2H)-one		704,246	3,545,607	5,217,069	99,157,476
1,5-Naphthalenediamine		-	-	-	7,262,825
10,11-Dihydro-10,11-dihydroxycarbamazepine		136,189,705	121,576,004	133,233,311	47,103,354
10,11-Dihydro-10-Hydroxycarbamazepine		78,736,372	125,718,413	122,662,927	81,524,615
2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile		980,702	3,325,804	32,580,821	13,111,395
2(3H)-Benzothiazolone		51,977,226	28,114,643	10,278,039	73,216,345
2-(Methylthio)benzothiazole	3,036,258	66,770,897	77,869,422	7,544,591	17,177,678
2-Ethylhexyl diphenyl phosphate	11,618,981	103,943,268	7,771,437	5,706,774	189,432
2-Mercaptobenzothiazole		-	-	-	66,034,497
3-Hydroxycotinine		-	-	-	169,753,693
4-Androstene-3,17-dione		-	-	-	142,929,816
4-Formylaminoantipyrine		1,145,860,802	1,191,591,497	1,488,014,498	454,837,010
4'-Hydroxydiclofenac/5-Hydroxydiclofenac		-	23,333,243	17,629,507	15,017,990
4-Phenylbutyric acid		-	-	-	88,250,015
6-Methylthioguanine		-	-	9,105,063	20,083,174
8-Hydroxy Mirtazapine		-	-	1,314,019	6,679,767
8-Hydroxyquinoline		90,276,617	-	6,616,901	484,577,393
Acetaminophen		-	-	-	8,332,637,735
Acetaminophen sulfate		-	-	-	69,669,379
Acetyl sulfamethoxazole		-	-	236,280	24,366,860
Amisulpiride		-	201,442,592	239,647,655	76,790,775
Amitriptyline		-	71,328,179	53,404,581	23,962,951
Ampyrone/ 4-aminoantipyrine		-	38,749,862	59,909,524	277,139,574
Atenolol		-	-	32,935,878	180,079,727
Azithromycin		-	5,324,438	4,472,447	-
Azoxystrobin		12,797,978	6,913,954	7,601,419	4,539,617
Benzothiazole	17,157,905	25,354,727	23,231,145	252,285,850	55,231,119
Benzoyllecgonine		-	-	-	553,014,848
Bezafibrate		-	968,451	1,609,895	11,308,149
Bisoprolol		-	53,389,871	62,272,462	69,542,141
Boldenone		-	-	-	82,641,226
Caffeine		-	-	-	4,192,368,457
Caprolactam	691,330,512	704,713,517	2,978,548,464	516,134,058	1,156,643,965
Carbamazepine		96,308,554	130,569,553	126,862,957	47,831,638

Table S7. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
Carbamazepine-10,11-epoxide		-	91,105,243	85,626,038	398,856,756
Cetirizine		24,853,418	50,919,639	70,653,265	22,978,273
Ciprofloxacin		4,592,809	953,486	32,335,623	49,507,096
Citalopram		1,922,927	158,613,548	169,277,156	80,015,579
Clopidogrel carboxylic acid		16,689,100	56,247,348	74,596,220	23,071,005
Cocaine		-	-	-	392,572,728
Cotinine		-	-	-	319,768,193
DEET (N, N-Diethyl-meta-toluamide)	83,485,122	464,493,357	1,138,242,141	688,838,202	4,580,483,685
Desacetyl diltiazem		-	36,698,748	39,108,738	10,616,105
Desmethyl-citalopram		-	66,701,670	77,637,767	29,066,695
Desmethyldiazepam		18,239,787	25,961,091	28,991,441	8,034,835
Dextromethorphan		-	19,707,844	16,683,602	3,426,631
Dextrorphan		10,766,046	44,380,180	61,720,642	19,005,426
Diazepam		7,250,467	10,453,862	11,305,512	2,208,866
Diazinon		1,427,457	3,135,782	5,031,091	-
Diclofenac		-	70,581,364	66,804,866	25,587,729
Dicyclohexylamine	10,583,688	205,177,872	242,890,624	77,645,484	129,230,358
Dicyclohexylurea	1,702,039	63,585,647	111,113,240	106,352,974	496,994,326
Diltiazem		-	29,950,505	33,141,965	30,582,732
Diphenhydramine		-	35,733,344	33,668,864	-
Diphenylamine		127,885,222	235,113,027	22,694,209	29,150,408
Diuron		27,151,237	75,945,061	63,429,446	12,064,084
Ecgonine methyl ester		-	-	-	56,914,466
Emtricitabine		6,479,965	7,517,833	10,026,286	17,743,407
Fenofibric acid		-	9,781,715	7,468,368	54,672,236
Flecainide		130,718,339	512,372,618	477,465,644	181,176,759
Fluconazole		30,126,100	19,575,304	25,559,883	9,401,484
Flufenamic acid		814,649	75,165,673	82,440,437	5,123,015
Gabapentin		76,346,190	237,595,680	261,276,676	1,201,211,545
Galaxolidone	22,551,886	93,837,255	2,143,333,231	1,957,618,908	160,827,836
Hydroxy-bupropion		4,702,311	5,646,123	34,333,988	8,823,470
Isoproturon		17,125,234	49,493,681	43,858,862	18,232,609
Ketamine		20,565,183	30,140,369	42,808,973	10,246,345
Ketoprofen		-	17,525,207	16,950,062	67,926,058
Lamotrigine		181,268,490	154,059,137	159,227,803	28,333,355
Lamotrigine 2-N-glucuronide		-	-	241,743	3,501,092
Lauryl diethanolamide	30,185,464	20,438,615	18,117,515	18,824,597	2,102,788,546

Table S7. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
Levamisole		5,408,098	56,287,716	77,119,993	14,538,148
Levofloxacin/ofloxacin		1,940,291	20,841,698	23,088,832	16,377,390
Lidocaine		86,993,060	282,460,679	326,429,343	125,558,123
MDMA		-	60,415,654	56,125,387	30,085,837
Mebendazole		-	4,935,073	5,161,978	9,086,032
Memantine		25,193,965	43,912,192	41,556,054	9,525,650
Metformin	1,252,183	30,613,164	434,378,392	597,964,284	4,731,065,645
Methadone		1,772,911	76,323,622	65,294,813	22,427,236
Metoclopramide		-	13,226,941	17,562,221	6,500,771
Metoprolol		-	8,359,143	11,511,432	5,433,326
Metoprolol acid		91,662,578	186,616,061	210,219,213	43,270,304
Metribuzin-desamino		22,688,523	738,323	696,812	-
Mycophenolic acid		-	-	-	47,336,661
N,N'-Diphenylguanidine	647,989	3,098,197	67,372,702	184,521,388	168,107,447
N-Acetyl-5-aminosalicylic acid		-	-	-	78,997,186
N-Acetylaminoantipyrine		408,373,817	299,846,763	375,737,292	1,254,883,869
Naproxen		-	1,756,495	1,229,059	12,748,751
Nicotine		-	-	-	563,684,919
N-Phenyl-1-naphthylamine	2,003,929	242,277,493	16,167,278	2,304,658	5,204,983
O-Desmethyl Venlafaxine		133,642,119	1,202,096,879	1,535,081,093	561,323,005
O-Desmethyltramadol		123,773,298	679,456,713	1,032,712,812	206,222,094
Oxazepam		8,653,874	28,568,948	30,398,013	10,842,116
Oxybenzone	25,180,952	169,725,868	151,796,906	5,376,206	23,977,678
Pentaethylene glycol (PEG)	209,293,814	28,673,469	100,984,159	33,310,584	3,721,047,990
Perfluorobutanesulfonic acid (PFBS)	845,554	116,627,211	69,417,414	56,321,320	26,000,550
Perfluorobutanoic acid (PFBA)	-	13,404,718	7,606,668	4,920,534	2,417,047
Perfluorooctanoic acid (PFOA)	2,685,822	41,864,582	16,572,818	8,628,298	3,790,582
Perfluoropentanoic acid (PFPeA)	162,182	33,147,293	17,061,039	11,678,099	2,411,174
Pregabalin		18,777,672	16,423,049	16,398,326	313,591,229
Propranolol		-	53,524,909	52,588,968	15,392,764
R-Methyl-benzotriazole (R = 1, 4, 5)	1,600,427	-	329,378,879	574,494,598	556,676,311
Ritalinic acid		-	-	-	30,173,631
Rosuvastatin		-	-	-	14,785,224
Secbumeton		3,354,509	58,404,039	10,083,790	-
Sertraline		-	9,637,472	18,324,202	-
Sitagliptin		25,203,221	206,749,882	242,182,707	157,247,661
Sotalol		-	19,971,959	24,192,917	11,852,352

Table S7. Continued.

Compound	Blank	Water used for irrigation	Reclaimed water discharge	WRP effluent	WRP influent
Sulfamethoxazole		7,548,802	17,443,696	12,035,469	33,402,309
Sulpiride		39,277,469	190,700,686	245,106,954	94,966,466
Tapentadol		54,083,495	576,773,782	815,701,883	281,334,608
Temazepam		19,773,671	32,814,438	37,026,134	10,556,989
Terbutryn		130,363,394	126,316,583	135,069,915	56,513,841
Testosterone propionate		-	-	-	22,001,843
Tetradecylamine	313,533,485	130,660,744	120,493,636	95,773,432	16,976,077,798
Tetrakis(2-hydroxypropyl)ethylenediamine		-	28,091,742	36,635,444	152,795,591
Theobromine		-	-	-	833,782,289
Theophylline/ Paraxanthine		-	-	-	868,649,990
Tramadol		133,642,119	1,202,096,879	1,535,081,093	561,323,005
Tri(chloropropyl) phosphate		134,058,966	224,482,952	162,444,404	201,778,582
Tributyl citrate	1,701,878	2,108,156	1,549,308	2,531,716	33,543,227
Tributyl phosphate	45,518,968	132,693,070	214,062,622	136,244,557	26,542,521
Triethanolamine		-	3,396,025	8,755,350	1,043,183,529
Triethylene glycol monobutyl ether		-	-	-	683,827,002
Trimethoprim		-	3,747,854	5,576,792	22,214,798
Tris(2-butoxyethyl) phosphate	2,740,762	48,237,538	383,925,225	135,976,808	805,793,003
Venlafaxine		46,535,508	790,273,016	819,910,795	237,922,829
Vildagliptin		14,665,719	28,443,872	39,845,515	19,918,909
Imidacloprid- <i>d4</i>	129,880,185	77,157,443	55,603,714	59,279,036	24,700,435

Table S8. MS/MS fragments observed in the MS² spectra of the compounds tentatively identified in the waters corresponding to the winter campaign.

Compound	MS ² fragments
10,11-Dihydro-10,11-dihydroxycarbamazepine	271.1088/180.0805/210.0910/254.0808/208.0755/192.0810/182.0962/167.0723
10,11-Dihydro-10-Hydroxycarbazepine	194.0963/192.0807/193.0872/195.0997
2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile	291.2065/260.1643/248.1516/218.1174/233.1534/177.0908/165.0909/151.0753/142.1590/122.0963/96.0807/70.0651
2-Ethyl-1,5-dimethyl-3,3-diphenylpyrrolinium (EDDP)	278.1903/249.1510/234.1274/186.1270/201.1501/172.1116/200.1429
2-Mercaptobenzothiazole	167.9935/136.0215/135.0137/124.0215/109.0106/104.0495/92.0495
3,3,5,5-Tetramethyl-1-pyrroline N-oxide	142.1226/86.0599/68.0495
3-Hydroxycotinine	134.0600/80.0495/149.0709/162.0555
4'-Hydroxydiclofenac/5-OH-DCF	266.0130/231.0442/230.0367/196.0760
4-Androstene-3,17-dione	287.2003/269.1902/251.1792/241.2356/211.1480/185.1326/159.1173/123.0804/109.0648/97.0648
4-Formylaminoantipyrine	232.1094/214.0973/204.1131/187.0864/173.0709/159.0916/146.0600/104.0494/83.0603/56.0495
4-Indolecarbaldehyde	146.0599/118.0649/117.0571/91.0542/65.0386
4-Phenylbutyric acid	165.0909/147.0804/137.0961/123.0804/119.0855/105.0699/93.0699/91.0542/81.0698/67.0544
5-Hydroxyomeprazole	362.1172/214.0529/196.0426/184.0967/168.0479/152.0705/149.0708/106.0653
8-Hydroxyquinoline	146.0600/128.0493/118.0650/91.0542
Acephylline	237.0620/193.0732/179.0579/136.0516/108.0563
Acetaminophen	152.0705/110.0599/134.0601/109.0524/93.0334
Acetaminophen sulfate	152.0706/134.0598/110.0600/93.0334/74.0601
Acetyl sulfamethoxazole	232.0273/198.0220/188.0819/162.0662/160.0869/136.0757/134.0600/108.0443/93.0573
Amisulpride	370.1791/242.0478/196.0058/214.0171/155.1178/112.1119
Amitriptyline	278.1903/233.1323/218.1089/205.1012/193.1012/191.0854/179.0853/155.0855/117.0698/105.0698/91.0542/84.0807/58.0654
Ampyrone/ 4-aminoantipyrine	204.1129/189.0899/187.0865/173.0714/159.0918/146.0601/130.0653/118.0652/111.0552/94.0651/83.0604/56.0498
Atenolol	267.1700/249.1594/225.1231/208.0966/190.0861/178.0861/164.0703/162.0912/152.0704/145.0647/133.0648/121.0646/116.1068/98.0963/74.0600/72.0808
Azithromycin	573.4109/158.1175/116.1069/83.0491/72.0808
Azoxystrobin	372.0975/344.1026/329.0790/316.1083/216.0657/172.0387/134.0600
Azoxystrobin acid	372.0976/344.1030/329.0794/216.0654/134.0600/143.0607
Benzoyllecgonine	290.1387/272.1277/168.1017/150.0913/140.1067/124.1120/105.0334/100.0757/82.0651
Bezafibrate	318.2998/276.0779/161.0960/138.9944/121.0646
Bisoprolol	326.2324/222.1482/204.1381/162.0912/147.0804/133.0646/116.1069/107.0490/98.0964/91.0541/74.0600/56.0498
Boldenone	287.2004/203.0700/173.0959/135.1167/121.0646/93.0699
Boscalid	343.0392/307.0633/271.0865/272.0944/139.9897/112.0397/96.0444
Bupropion	184.0523/166.0416/133.0759/139.0305/131.0729/57.0701/167.0256
Butyrophenone	149.0959/131.0854/129.0697/131.0854/107.0489/93.0698/91.0541/79.0542/71.0492/57.0334

Table S8. Continued.

Compound	MS ² fragments
Caffeine	195.0875/138.0661/110.0711/69.0448
Caprolactam	114.0912/55.0546/69.0699/79.0541/96.0886/97.0646
Carbamazepine	237.1019/194.0963/192.0806/220.0752/193.0868
Carbamazepine-10,11-epoxide	208.0754/210.0910/180.0804/182.0963/236.0703/192.0808/181.0857
Carbendazim	192.0772/160.0504/133.0643/132.0556/105.0447/92.0494
Carboxy-ibuprofen	235.0982/191.1081/73.0296/117.0195
Cetirizine	201.0465/193.0758/187.1076/183.0807/166.0777/165.0695/111.0910
Chlorpheniramine	167.0729/230.0729/232.0701/202.0417
Ciprofloxacin	332.1395/288.1503/268.1440/245.1082/231.0924/205.0768/204.0687/203.0609/70.0651/58.0652
Citalopram	325.1709/307.1602/280.1133/262.1026/247.0792/234.0712/221.0631/184.0762/166.065/156.0809/116.0494/109.0448
Clopidogrel	184.0524/212.0473/152.0262/155.0258/125.0153
Clopidogrel carboxylic acid	308.0514/198.0315/170.0367/169.0049/152.0260/141.0100/125.0151
Cocaine	304.1548/272.1282/182.1174/150.0912/105.0334/91.0541/82.0651/108.0807/154.0867
Cotinine	177.1020/146.0598/98.0599/80.0494/81.0527
Coumarin	147.0439/103.0541/91.0541/105.0697
Cyprodinil	226.1336/209.1071/210.1020/185.1073/133.0759/108.0808/93.0572
DEET (N, N-Diethyl-meta-toluamide)	192.1382/119.0492/109.0646/100.0757/72.0444/91.0542
Desacetyl diltiazem	178.0321/223.0902/72.0808/328.0994/197.1107/150.0372
Desmethylcitalopram	311.1545/293.1445/262.1024/247.0792/234.0711/221.0632/166.0649/156.0805/116.0495/109.0447/69.0448
Desmethyldiazepam	271.0630/243.0682/208.0991/165.0214/140.0260/226.0413/
Dextromethorphan	272.2007/215.1430/147.0803/213.1272/159.0801/171.0802/121.0646
Dextrorphan/levorphanol	258.1850/201.1272/199.1116/157.0646/145.0647/133.0647
Diazepam	228.0574/154.0418/257.0839/222.1151/193.0886
Diazinon	169.0795/153.1024/114.9613/84.0444
Dibutyl phthalate	149.0233/57.0702/121.0284/167.0336/150.0266
Diclofenac	215.0493/250.0182/214.0418/180.0800/179.0730
Diethyl phthalate	149.0231/150.0264/177.0543/178.0580/167.0336
Diltiazem	178.0320/371.2054/310.0890/191.0402/150.0371/72.0808/137.0597
Diphenhydramine	167.0854/165.0696/152.0618
Diuron	233.0238/187.9671/159.9719/72.0444
Ecgonine methyl ester	200.1279/182.1174/82.0651/108.0807/150.0913/168.1014
Emtricitabine	130.0411/113.0144/101.0055/73.0105
Ephedrine	166.1225/149.1154/148.1119/133.0885/117.0698/70.0651/56.0497
Epoxiconazole	121.0448/123.0241/141.0100/70.0400
Fenofibric acid	233.0361/138.9944/121.0830
Flecainide	415.1445/315.1070/301.0291/287.0486/232.0968/178.0317/98.0964/81.0699

Table S8. Continued.

Compound	MS ² fragments
Fluconazole	307.1127/238.0784/220.0679/169.0458/141.0510/127.0353/70.0400
Flufenamic acid	264.0631/244.0568/195.0679/167.0729
Gabapentin	172.1329/154.1224/137.0960/119.0854/109.1011/95.0854/55.0181/67.0543/156.1097
Galaxolidone	273.1846/255.1742/240.1508/227.1790/203.1063/175.1118/157.1014
Hydroxy-bupropion	238.0990/167.0494/184.0523/139.0307/131.0728/166.0416
Ibuprofen	161.1325/119.0855/105.0698/91.0543/133.1011
Imidacloprid	256.0616/209.0588/175.0978/128.0261/84.0556
Isoproturon	207.1494/165.1022/134.0964/72.0444
Ketamine	238.0991/220.0884/207.0570/189.0463/179.0619/163.0306/152.0259/125.0153/67.0543
Ketoprofen	255.1008/209.0958/194.0724/177.0543/131.0490/109.1010/105.0334/95.0490
Lamotrigine	256.0148/229.0041/210.9821/186.9824/185.9871/166.9871/165.0211/158.9760
Lamotrigine 2-N-glucuronide	256.0151
Lauryl diethanolamide	288.2536/227.2003/106.0861/88.0756/70.0652/57.0701
Levamisole	205.0793/178.0683/146.0964/88.0215/118.0649/188.0523
Levofloxacin/ofloxacin	362.1511/318.1611/344.1431/261.1033/221.0712/247.0878/233.0711/58.0654/72.0808
Lidocaine	235.1803/86.0964/87.0997/58.0654
3,4-Methylenedioxyamphetamine (MDMA)	194.1171/163.0751/151.0753/135.0439/133.0648/105.0697/58.0653
Mebendazole	296.1031/264.0767/159.0436/105.0335/95.0491
Memantine	180.1746/163.1479/107.0853/121.1010
Metformin	130.1087/113.0822/88.0869/85.0508/71.0604/60.0558
Methadone	310.2164/265.1583/223.1114/219.1166/195.1167/159.1167/129.0698/117.0696/105.0333/91.0541/57.0337
Metoclopramide	227.0581/184.0159/222.0347
Metoprolol	268.1905/250.01426/226.1434/218.1538/191.1064/176.1064/159.0804/133.0647/121.0648/116.1069/98.0964/74.0600/56.0497
Metoprolol acid	268.1540/226.1070/191.0700/165.0543/145.0646/116.1068/98.0963/74.0600/72.0807/56.0497
Mirtazapine	266.1650/235.1225/209.1071/195.0916/110.0600/72.0808
Mycophenolic acid	321.1330/275.1275/285.1119/207.0651/159.0437/177.0545/195.0651
N,N'-Diphenylguanidine	212.1180/195.0914/119.0602/94.0650/95.0683/92.0493
N-Acetyl-5-aminosalicylic acid	196.0603/178.0499/152.0706/136.0392/108.0442/110.0600/80.0493
N-Acetylaminoantipyrine	246.1238/228.1128/204.1131/104.0494/83.0603/187.0864/159.0916/146.0600/94.0650/56.0498
Naproxen	170.0742/158.0378/185.0977
Nicotine	163.1228/132.0807/130.0651/120.0807/116.0527/106.0560/84.0808/80.0494
N-Phenyl-1-naphthylamine	220.1118/205.0886/143.0729/142.0651/128.0619/115.0540/92.0494/65.0388
O-Desmethyl Venlafaxine	264.1960/246.1852/201.1273/173.0957/159.0804/133.0647/107.0491/58.0654
O-desmethyiltramadol	250.1815/58.0651/232.1690

Table S8. Continued.

Compound	MS ² fragments
Omeprazole sulfone	214.0532/195.0226/184.0971/168.1019/166.0863/149.0710/150.0913/120.0807/93.0698
Oxazepam	287.0579/269.0476/241.0526/231.0683/216.0994/166.0055/128.0262/104.0495
Oxybenzone	229.0860/151.0388/105.0334/95.0491/152.0421
Pentaethylene glycol (PEG)	89.0596/107.0702/133.0858/151.0964/177.1127
Perfluorobutanesulfonic acid (PFBS)	298.9435/168.9897/118.9927/98.9562/82.9612/79.9576
Perfluorobutanoic acid (PFBA)	168.9894
Perfluoroheptanoic acid (PFHpA)	168.9897/118.9930
Perfluorohexanoic acid (PFHxA)	3112.9728/268.9830/118.9925
Perfluorooctanoic acid (PFOA)	168.9897/118.9930
Perfluoropentanoic acid (PFPeA)	218.9862
Pregabalin	160.1330/143.1066/142.1225/125.0961/124.1119/107.0854/97.1011/83.0854/69.0698/55.0545
Propranolol	260.1643/218.1174/183.0804/157.0647/155.0853/116.1068/98.0963/74.0600
Quetiapine	384.1739/253.0791/279.0950/221.1072/247.1225/210.0370/158.1175
R-Methyl-benzotriazole (R=1, 4, 5)	134.0711/106.0650/79.0542/77.0382
R-Methyl-benzotriazole (R=1, 4, 5)	134.0711/106.0650/79.0542/77.0382
Ritalinic acid	220.1330/174.1275/84.0807
Secbumeton	226.1662/170.1035/142.0723/114.0660/100.0502/86.0345/85.0757/57.0703
Sertraline	275.0389/240.0707/196.9918/158.9763/129.0698/91.0542
Sitagliptin	408.1234/391.0984/235.0798/193.0694/174.0523/127.0353
Sotalol	255.1158/213.0690/176.1308/133.0759/106.0649
Sulfamethoxazole	254.0593/156.0112/108.0442/92.0494/68.0495/110.0599/188.0817/99.0552
Sulpiride	342.1479/214.0164/112.1119/98.0963/84.0807/58.0653
Tapentadol	222.1852/135.0804/121.0647/107.0490/177.1272
Tebuconazole	70.0399/125.0153
Temazepam	301.0747/283.0632/255.0680/228.0570/216.0572/193.0883/180.0211/107.0853
Terbutryn	242.1432/186.0808/158.0492/171.0573/138.0774/116.0275/102.0377/91.0324
Testosterone propionate	345.2430/97.0648/109.0648/271.2054/253.1947/175.1481/123.0804/213.1633/79.0541/81.0698/83.0491
Tetradecylamine	214.2529/141.0003/85.1011/71.0856/57.0701
Tetrakis(2-hydroxypropyl)ethylenediamine	293.2433/160.1330/142.1226/102.0913/84.0807
Theobromine	181.0718/137.0821/138.0661/110.0712
Theophylline/ Paraxanthine	181.0717/142.0610/124.0504/96.0554/69.0447
Tramadol	264.1964/246.1850/58.0654
Tri(chloropropyl) phosphate	98.9841/174.9920/116.9946/77.0152
Tributyl phosphate	116.9945/98.9841/57.0701/155.0471
Triethanolamine	150.1124/132.1018/114.0912/88.0756/70.0652
Triethylene glycol monobutyl ether	133.0858/101.0960/89.0596/73.0648/57.0701
Triisobutyl phosphate	98.9842/116.9971/57.0698
Trimethoprim	291.1451/275.1139/261.0980/245.1034/230.1160/181.0859/123.0664

Table S8. Continued.

Compound	MS ² fragments
Triphenyl phosphate	327.0776/309.0676/251.0465/233.0359/228.0930/215.0253/202.0777/171.0802/153.0698/152.0621/105.0446/95.0490/77.0382
Tris(2-butoxyethyl) phosphate	199.0729/143.0105/124.9997/101.0690/83.0854/57.0701
Venlafaxine	278.2124/260.2007/215.1430/187.1118/173.0962/159.0802/147.0803/121.0646/107.0854/58.0654
Vildagliptin	304.2016/154.0973/151.1117/97.0760/70.0652/93.0698/107.0854/133.1012

Table S9. MS/MS fragments observed in the experimental MS2 spectra of the compounds tentatively identified in the waters corresponding to the summer campaign..

Compound	Fragments
1,2-Benzisothiazol-3(2H)-one	152.0162/134.0060/109.0105
1,5-Naphthalenediamine	143.0729/130.0651/115.0542
10,11-Dihydro-10,11-dihydroxycarbamazepine	180.0804/182.0960/210.0908/236.0697/254.0805
10,11-Dihydro-10-Hydroxycarbazepine	194.0964/237.1021/192.0806/196.1391
2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile	260.1642/248.1514/218.1170/177.0907/165.0907/151.0751/122.0961/96.0806/70.0651
2(3H)-Benzothiazolone	124.0214/109.0106/92.0493
2-(Methylthio)benzothiazole	182.0089/166.9855/135.0132/109.0106
2-Ethylhexyl diphenyl phosphate	251.0454/153.0690/233.0350/175.0145/95.0486
2-Mercaptobenzothiazole	135.0130/109.0101/136.0208/124.0209
3-Hydroxycotinine	193.0970/134.0599/80.0494
4-Androstene-3,17-dione	287.2004/251.1792/229.1582/211.1481/185.1325/173.1325/159.1167/123.0803/109.0647/97.0647
4-Formylaminoantipyrine	204.1127/159.0913/146.0599/130.0651/128.0494/104.0491/83.06032
4'-Hydroxydiclofenac/5-Hydroxydiclofenac	266.0133/230.0355/231.0433/224.0715/196.0754
4-Phenylbutyric acid	165.0909/147.0801/137.0960/122.0724/119.0851/109.1010/95.0854/91.0542/67.0543
6-Methylthioguanine	134.0464/167.0252/80.0238/107.0347
8-Hydroxy Mirtazapine	282.1586/211.0855/72.0808
8-Hydroxyquinoline	128.0490/129.0441/95.0486/117.0567
Acetaminophen	152.0703/110.0594/92.0489/93.0329
Acetaminophen sulfate	152.0706/134.0598/110.0600/93.0334/74.0601
Acetyl sulfamethoxazole	198.0220/188.0819/162.0662/160.0869/136.0757/134.0600/108.0443/93.0573
Amisulpiride	242.0478/340.1790/112.1119/196.0058
Amitriptyline	233.1320/278.1898/91.0540/105.0696/117.0696/191.0851/155.0852/205.1008/218.1084
Ampyrone/ 4-aminoantipyrine	204.1144/189.0896/187.0863/173.0707/159.0915/146.0600/111.0550/94.0650/85.0759/83.0603/56.0497
Atenolol	267.1699/190.0860/145.0646/116.1068/74.0600/72.0808/225.1230/208.0966/178.0860/162.0912/98.0963/56.0497
Azithromycin	591.4185/158.1167/116.1063/83.0487
Azoxystrobin	372.0960/344.1013/316.1065
Benzothiazole	65.0388/95.0489/105.0443/109.0100
Benzoylcegonine	168.1017/105.0333/82.0650/150.0911/119.0490
Bezafibrate	69.0336/87.0439/121.0648/138.9943/161.0958/189.0911/207.1015/276.0786/316.1099
Bisoprolol	56.0498/58.0654/72.0808/74.0600/91.0542/98.0964/116.1069/133.0647/147.0803/162.0911/204.1385/222.1491/326.2325
Boldenone	121.0647/135.1167/147.0804/149.1324/161.1324/173.0961/179.1430/187.1116/269.1895/
Caffeine	138.0654/110.0707/83.0599/123.0421/69.0444
Caprolactam	55.0546/69.0699/79.0541/96.0886/97.0646/
Carbamazepine	237.1020/194.0962/192.0806
Carbamazepine-10,11-epoxide	208.0755/210.0911/236.0704/180.0806/182.0964/253.0972
Cetirizine	165.0696/166.0776/187.1073/201.0464

Table S9. Continued.

Compound	MS ² fragments
Ciprofloxacin	288.1507/268.1440/245.1081/224.0693/191.0612/170.0651
Citalopram	58.0653/109.0446/116.0492/156.0806/166.0648/234.0708/247.0786/262.1021/325.1703
Clopidogrel carboxylic acid	198.0305/170.0360/169.0047/152.0257/141.0100/140.0257/125.0152/113.0149/111.0262/
Cocaine	182.1174/82.0650/105.0334/150.0912/122.0961
Cotinine	177.1020/80.0494/98.0599/146.0597
DEET (N, N-Diethyl-meta-toluamide)	72.0443/91.0539/100.0754/119.0488/192.1378
Desacetyl diltiazem	373.1566/328.1001/223.0899/197.1107/178.0319/150.0372/72.0807
Desmethyl-citalopram	311.1542/293.1446/280.1127/262.1024/234.0711/221.0631/166.0651/116.0493/109.0447
Desmethyldiazepam	243.0682/208.0991/165.0214/140.0260
Dextromethorphan	272.2004/241.1581/215.1427/213.1273/171.0799/159.0801/147.0803/121.0644
Dextrorphan/levorphanol	258.1852/199.1117/201.1273/157.0647/133.0647/145.0647
Diazepam	257.0827/222.1140/193.0876/154.0410
Diazinon	169.0786/153.1014/114.9607/96.9502
Diclofenac	278.0124/250.0175/215.0175
Dicyclohexylamine	55.0544/83.0854/100.1119/182.1901
Dicyclohexylurea	225.1956/143.1176/100.1118/83.0854/61.0398
Diltiazem	178.0318/150.0370/137.00595/72.0807/174.0370/310.0891/191.0398
Diphenhydramine	167.0847/152.0612/167.0847/165.0690
Diphenylamine	93.0568/92.0493/153.0702/170.0961
Diuron	187.9667/159.9715/72.0444
Ecgonine methyl ester	200.1278/182.1174/168.1016/156.1015/150.0912/108.0805/100.0755/82.0650
Emtricitabine	130.0410/113.0143/101.0055/73.0106/61.0110
Fenofibric acid	233.0361/138.9944/121.0830
Flecainide	415.1447/398.1180/315.1074/301.0290/232.0966/98.0963/81.0698
Fluconazole	238.0774/220.0774/169.0451/139.0347/70.0400
Flufenamic acid	244.0566/216.0623/195.0678/167.0733/57.0701
Gabapentin	172.1329/155.1258/154.1224/137.0959/119.0855/109.1009/95.0854/93.0698/67.0543/55.0181
Galaxolidone	256.1777/255.1735/245.1536/240.1505/227.1791/225.1275/212.1555/211.1116/210.1038/203.1064/197.1317/185.0963/183.1168/182.1090/175.1111/171.1166/170.1090/169.1005/168.0935/157.1010/156.0938/155.0855/142.0778/141.0693/16.361/3876107/129.0696/128.0616/117.0696/115.0540/255.1737/240.1507/227.1792/225.1274/197.1318/185.0962/183.1168/171.1166/169.1007/157.1010/156.0936/143.0856/142.0778/129.0697/128.0617/117.0696
Hydroxy-bupropion	238.0990/220.0884/167.0494/184.0523/139.0307/131.0728/166.0416
Isoproterenol	165.1022/134.0964/72.0444
Ketamine	238.0991/220.0884/207.0568/189.0463/179.0619/165.0098/163.0306/152.0259/141.0104/125.0153/67.0542

Table S9. Continued.

Compound	MS ² fragments
Ketoprofen	255.1015/210.0990/209.0957/194.0724/177.0542/131.0490/105.0333/95.0490
Lamotrigine	256.0143/210.9813/166.0284/212.9784
Lamotrigine 2-N-glucuronide	256.0151
Lauryl diethanolamide	106.0861/88.0756/227.2003/70.0652/270.2422/288.2520
Levamisole	205.0792/178.0683/188.0516/146.0962/88.0214/118.0646
Levofloxacin/ofloxacin	362.1511/319.1645/318.1609/261.1030/247.0874/233.0711/221.0719/205.0404/70.0651/58.0651
Lidocaine	235.1805/87.0996/86.0963/58.0654
3,4-Methylenedioxyamphetamine (MDMA)	194.1173/163.0751/135.1165/133.0646/105.0697/58.0653
Mebendazole	264.0767/159.0436/105.0335
Memantine	180.1744/163.1479/121.1010/107.0852/97.9911/93.0696/81.0697/67.0541
Metformin	130.1080/113.0716/88.0865/85.0505/71.0599
Methadone	105.0333/265.1582/223.1114/219.1164/159.1165/195.1166/187.1116
Metoclopramide	227.0570/184.0150/212.0336/183.0310
Metoprolol	268.1902/250.1435/226.1432/191.1067/159.0804/121.0645/116.1067/98.0963/86.0962/74.0600/72.0807/56.0497
Metoprolol acid	268.1536/226.1069/191.0700/165.0544/145.0645/116.1067/98.0963/74.06/72.0807/56.0497
Metribuzin-desamino	200.0848/172.0899/106.9917/89.0164/57.0701/116.0274
Mycophenolic acid	191.0349/275.1288/319.1183/179.0349/287.0924/192.0425/205.0504/203.0347/207.0660
N,N'-Diphenylguanidine	92.0495/94.0650/95.0489/119.0602/195.0915/212.1178
N-Acetyl-5-aminosalicylic acid	178.0499/152.0706/136.0392/108.0442/110.0600/80.0493
N-Acetylaminoantipyrine	228.1127/204.1128/159.0915/104.0493
Naproxen	171.0774/170.0683/169.0650/158.0372
Nicotine	132.0806/130.0650/120.0806/106.0649/84.0804/80.0494
N-Phenyl-1-naphthylamine	143.0722/128.0614/115.0536/92.0489
O-Desmethyl Venlafaxine	58.0653/107.0490/201.1270/246.1850/264.1957
O-Desmethyltramadol	58.0653/232.1684
Oxazepam	241.0522/269.0471/231.0680/287.0576/104.0492/128.0260/166.0052
Oxybenzone	229.0859/151.0389/105.0334/77.0386
Pentaethylene glycol (PEG)	89.0596/133.0857/151.0964/107.0701
Perfluorobutanesulfonic acid (PFBS)	79.9574/82.9609/84.9906/98.9559/118.9926/168.9892
Perfluorobutanoic acid (PFBA)	168.9892
Perfluorooctanoic acid (PFOA)	218.9859/168.9894
Perfluoropentanoic acid (PFPeA)	218.9859/196.9848
Pregabalin	143.1066/142.1225/125.0959/124.1119/107.0854/97.1010/83.0854/69.0699/59.0494/55.0545
Propranolol	260.1640/218.1176/183.0802/157.0645/155.0852/129.0692/116.1067/98.0962/86.0962/74.0600/58.0651/56.0497

Table S9. Continued.

Compound	MS ² fragments
R-Methyl-benzotriazole (R = 1, 4, 5)	134.071/79.0541/106.49/121.9663
Ritalinic acid	174.1275/84.0807
Rosuvastatin	258.1391/300.1495/272.1547/270.1389
Secbumeton	170.1039/198.1350/152.118/142.0723/128.0818/114.0661/100.0504/96.0556
Sertraline	91.0542/129.0698/158.9754/196.9918/275.0375
Sitagliptin	174.0524/193.0695/235.0799/391.0984/408.1237
Sotalol	255.1156/213.0688/176.1305/134.0838/133.0760/106.0649
Sulfamethoxazole	254.0589/188.0815/160.0867/156.0111/147.0789/108.0442/99.0551/92.0493/68.0495
Sulpiride	342.1480/214.0166/112.1119/98.0964/84.0807/58.0654
Tapentadol	222.1850/177.1270/135.0802/121.0646/107.0490
Temazepam	255.0670/177.0205/180.0201
Terbutryn	186.0806/242.1430/171.057/158.0496/144.0591/138.0774/116.0278
Testosterone propionate	345.2425/271.2054/213.1640/189.1638/175.1480/145.1010/123.0803/109.0647/97.0647/83.0491/69.0701
Tetradecylamine	214.2525/85.1012/71.0855/57.0676
Tetrakis(2-hydroxypropyl)ethylenediamine	160.1324/142.1219/102.0908/84.0803/98.0959
Theobromine	163.0606/122.0581/108.0551/69.0444
Theophylline/ Paraxanthine	142.0611/124.0499/69.0444/96.0551
Tramadol	246.1850/58.0653
Tri(chloropropyl) phosphate	98.9841/174.9920/116.9946/77.0152
Tributyl citrate	129.0180/185.0807/157.0130/139.0025/111.0072/89.0595/68.9971/57.0701
Tributyl phosphate	116.9945/98.9841/57.0701/155.0471
Triethanolamine	150.1124/132.1018/114.0912/106.0860/88.0756/70.0652
Triethylene glycol monobutyl ether	89.0596/73.0648/83.0854/90.0631/101.0959/107.0699/133.0561
Trimethoprim	291.1475/275.1137/261.0982/245.1033/230.1162/123.0664
Tris(2-butoxyethyl) phosphate	55.0544 /57.0701 / 98.9840 /101.0959/83.0854/124.9995/ 143.0102/ 59.0493
Venlafaxine	58.0654/121.0647/147.0804/159.0802/173.0962/183.1183/193.1850/215.1430
Vildagliptin	304.2010/154.0972/151.1116/127.0863/107.0853/97.0759/93.0697/70.0651/59.0494

Table S10. Scoring system for the alternative prioritization procedure based on chromatographic peak areas, frequency of detection and PNEC values.

Occurrence					Toxicity		
Chromatographic peak area			Ubiquity		PNEC		
Percentile	Area threshold	Score	Frequency of detection	Score	Percentile	PNEC value threshold (µg/L)	Score
20 th	2,181,764	0.8	1sampling campaign	0.5	20 th	0.21	5
40 th	7,433,214	1.6			40 th	0.99	4
60 th	24,420,439	2.4			60 th	3.56	3
80 th	91,927,261	3.2	2sampling campaigns	1	80 th	14.92	2
100 th	2,603,205,440	4			100 th	6,840	1

Table S11. Prioritization of the CECs tentatively identified in water used for irrigation using the alternative scoring system proposed based on chromatographic peak area and frequency of detection to assess CEC occurrence.

Compound	Areas	Score Areas	Score campaigns	PNEC (µg/L)	Score PNEC	Total Score
1,2-benzisothiazol-3(2H)-one	704,246	0.8	0.5	379	1	2.3
10,11-Dihydro-10,11-dihydroxycarbamazepine	136,189,705	4	1	1.91	3	8
10,11-Dihydro-10-Hydroxycarbazepine	78,736,372	3.2	1	4.03	2	6.2
2-(3,4-dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile	4,381,333	1.6	1	1.57	3	5.6
2(3H)-Benzothiazolone	51,977,226	3.2	0.5	14	2	5.7
2-(Methylthio)benzothiazole	63,734,639	3.2	0.5	1.14	3	6.7
2-ethyl-1,5-dimethyl-3,3-diphenylpyrrolinium (EDDP)	9,985,065	2.4	0.5	0.085	5	7.9
2-Ethylhexyl diphenyl phosphate	92,324,287	3.2	0.5	0.018	5	8.7
2-Mercaptobenzothiazole	2,305,720	0.8	0.5	0.76	4	5.3
3,3,5,5-Tetramethyl-1-pyrroline N-oxide	26,859,935	3.2	0.5	13.8	2	5.7
3-Hydroxycotinine	1,877,722	0.8	0.5	20.6	1	2.3
4-Formylaminoantipyrine	1,145,860,802	4	1	1000	1	6
4-indolecarbaldehyde	1,900,774	0.8	0.5	6.08	2	3.3
8-Hydroxyquinoline	90,276,617	3.2	1	1.99	3	7.2
Acephylline	1,626,513	0.8	0.5	13.2	2	3.3
Amisulpride	27,028,566	3.2	0.5	1.43	3	6.7
Amitriptyline	3,412,679	1.6	0.5	0.14	5	7.1
Ampyrone/ 4-aminoantipyrine	1,834,271	0.8	0.5	32.5	1	2.3
Atenolol	6,113,266	1.6	0.5	150	1	3.1
Azoxystrobin	12,797,978	2.4	1	0.2	5	8.4
Azoxystrobin acid	5,501,093	1.6	0.5	0.21	4	6.1
Benzoyllecgonine	10,332,351	2.4	0.5	6840	1	3.9
Bezafibrate	291,604	0.8	0.5	2.3	3	4.3

Table S11 (cont).

Compound	Areas	Score Areas	Score campaigns	PNEC (µg/L)	Score PNEC	Total Score
Bisoprolol	12,978,670	2.4	0.5	3.18	3	5.9
Boscalid	5,790,429	1.6	0.5	11.6	2	4.1
Bupropion	2,840,306	1.6	0.5	4.4	2	4.1
Butyrophenone	38,307,009	3.2	0.5	1.75	3	6.7
Caffeine	34,632,858	3.2	0.5	1.2	3	6.7
Caprolactam	2,603,205,440	4	1	67.40	1	6
Carbamazepine	96,308,554	4	1	0.05	5	10
Carbamazepine-10,11-epoxide	1,089,705	0.8	0.5	2.57	3	4.3
Carbendazim	10,085,701	2.4	0.5	0.15	5	7.9
Cetirizine	24,853,418	2.4	1	0.41	4	7.4
Chlorpheniramine	399,516	0.8	0.5	1.56	3	4.3
Ciprofloxacin	4,592,809	1.6	0.5	0.089	5	7.1
Citalopram	10,412,011	2.4	1	16	1	4.4
Clopidogrel	1,225,882	0.8	0.5	3.21	3	4.3
Clopidogrel carboxylic acid	16,689,100	2.4	1	0.65	4	7.4
Cocaine	1,995,832	0.8	0.5	2.28	3	4.3
Cotinine	6,031,735	1.6	0.5	10	2	4.1
DEET (N, N-Diethyl-meta-toluamide)	381,008,235	4	0.5	88	1	5.5
Desacetyl diltiazem	2,582,415	1.6	0.5	0.36	4	6.1
desmethylcitalopram	7,316,943	1.6	0.5	0.5	4	6.1
Desmethyldiazepam	18,239,787	2.4	1	0.43	4	7.4
Dextromethorphan	4,557,018	1.6	0.5	3.32	3	5.1
Dextrorphan/levorphanol	10,766,046	2.4	0.5	1.36	3	5.9

Table S11 (cont).

Compound	Areas	Score Areas	Score campaigns	PNEC (µg/L)	Score PNEC	Total Score
Diazepam	7,250,467	1.6	1	0.29	4	6.6
Diazinon	1,427,457	0.8	1	0.01	5	6.8
Diclofenac	2,317,957	1.6	0.5	0.05	5	7.1
Dicyclohexylamine	194,594,184	4	0.5	1.60	3	7.5
Dicyclohexylurea	61,883,608	3.2	0.5	5.91	2	5.7
Diethyl phthalate	21,050,888	2.4	0.5	16	1	3.9
Diltiazem	1,370,584	0.8	0.5	0.23	4	5.3
Diphenhydramine	1,143,231	0.8	0.5	0.99	3	4.3
Diphenylamine	127,885,222	4	0.5	1.2	3	7.5
Diuron	27,151,237	3.2	0.5	0.07	5	8.7
Ecgonine methyl ester	3,378,260	1.6	0.5	88.8	1	3.1
Emtricitabine	6,479,965	1.6	1	23.8	1	3.6
Ephedrine	4,272,290	1.6	0.5	3.62	2	4.1
Fenofibric acid	160,665	0.8	0.5	2.35	3	4.3
Flecainide	130,718,339	4	1	0.64	4	9
Fluconazole	30,126,100	3.2	1	0.25	4	8.2
Flufenamic acid	1,932,496	0.8	1	0.4	4	5.8
Gabapentin	76,346,190	3.2	1	10	2	6.2
Galaxolidone	147,537,245	4	1	0.1	5	10
Hydroxy-bupropion	4,702,311	1.6	0.5	11.8	2	4.1
Isoproturon	17,125,234	2.4	1	0.32	4	7.4
Ketamine	20,565,183	2.4	0.5	5.71	2	4.9
Ketoprofen	433,119	0.8	0.5	2.1	3	4.3
Lamotrigine	181,268,490	4	1	10	2	7

Table S11 (cont).

Compound	Areas	Score Areas	Score campaigns	PNEC (µg/L)	Score PNEC	Total Score
Levamisole	10,583,716	2.4	1	1.81	3	6.4
Lidocaine	86,993,060	3.2	1	4.67	2	6.2
3,4-Methylenedioxyamphetamine (MDMA)	12,243,616	2.4	0.5	0.216	4	6.9
Mebendazole	230,739	0.8	0.5	0.16	5	6.3
Memantine	25,193,965	3.2	1	1.84	3	7.2
Metformin	198,713,057	4	1	156	1	6
Methadone	8,418,179	2.4	1	0.84	4	7.4
Metoprolol	2,487,618	1.6	0.5	8.6	2	4.1
Metoprolol acid	91,662,578	3.2	1	49.9	1	5.2
Metribuzin-desamino	22,688,523	2.4	0.5	46.8	1	3.9
Mirtazapine	520,239	0.8	0.5	1	3	4.3
N,N'-Diphenylguanidine	147,006,447	4	1	0.86	4	9
N-Acetylaminoantipyrine	408,373,817	4	1	100	1	6
N-Phenyl-1-naphthylamine	240,273,564	4	0.5	0.06	5	9.5
O-Desmethyl Venlafaxine	280,376,328	4	1	0.0061	5	10
O-desmethyltramadol	184,847,728	4	1	9.12	2	7
Ofloxacin/levofloxacin	1,940,291	0.8	1	0.021	5	6.8
Oxazepam	8,653,874	2.4	1	0.37	4	7.4
Oxybenzone	333,810,270	4	1	0.67	4	9
Pentaethylene glycol (PEG)	74,885,290	3.2	0.5	202	1	4.7
Perfluorobutanesulfonic acid	115,781,657	4	1	4.08	2	7
Perfluorobutanoic acid (PFBA)	13,404,718	2.4	1	27.80	1	4.4
Perfluoroheptanoic acid (PFHpA)	1,099,390	0.8	0.5	0.50	4	5.3
Perfluorohexanoic acid (PFHxA)	25,876,100	3.2	0.5	140.00	1	4.7

Table S11 (cont).

Compound	Areas	Score Areas	Score campaigns	PNEC (µg/L)	Score PNEC	Total Score
Perfluorooctanoic acid (PFOA)	39,178,760	3.2	1	0.18	5	9.2
Perfluoropentanoic acid (PFPeA)	32,985,111	3.2	1	3.91	2	6.2
Pregabalin	18,777,672	2.4	1	66.1	1	4.4
Propranolol	4,834,741	1.6	0.5	0.41	4	6.1
Ritalinic acid	6,432,319	1.6	0.5	14.2	1	3.1
Secbumeton	3,354,509	1.6	1	0.048	5	7.6
Sertraline	313,098	0.8	0.5	0.091	5	6.3
Sitagliptin	39,352,462	3.2	1	0.92	4	8.2
Sotalol	4,156,110	1.6	0.5	6.52	2	4.1
Sulfamethoxazole	7,548,802	1.6	1	0.1	5	7.6
Sulpiride	57,801,159	3.2	1	4.09	2	6.2
Tapentadol	100,940,372	4	1	2.47	3	8
Tebuconazole	531,948	0.8	0.5	0.24	4	5.3
Temazepam	19,773,671	2.4	1	0.071	5	8.4
Terbutryn	130,363,394	4	1	0.065	5	10
Theobromine	12,001,253	2.4	0.5	100	1	3.9
Theophylline/ Paraxanthine	13,738,154	2.4	0.5	0.1	5	7.9
Tramadol	309,180,190	4	1	8.65	2	7
Tri(chloropropyl) phosphate	134,058,966	4	0.5	7.39	2	6.5
Tributyl phosphate	132,693,070	4	0.5	66	1	5.5
Triethanolamine	7,404,318	1.6	0.5	93.7	1	3.1
Trimethoprim	966,427	0.8	0.5	0.5	4	5.3
Tris(2-butoxyethyl) phosphate	45,496,776	3.2	1	0.14	5	9.2
Venlafaxine	122,889,016	4	1	0.0061	5	10
Vildagliptin	14,665,719	2.4	1	9.75	2	5.4

Table S12. Comparison of the 50 top-ranked CECs with both prioritization methods.

Order	Priority CECs using chromatographic peak areas	Priority CECs using semi-quantified concentrations
1	Carbamazepine*	O-Desmethyl Venlafaxine
2	Galaxolidone	Venlafaxine
3	O-Desmethyl Venlafaxine	Galaxolidone
4	Terbutryn	Theophylline/ Paraxanthine
5	Venlafaxine	Oxybenzone
6	N-Phenyl-1-naphthylamine	N-Phenyl-1-naphthylamine
7	Perfluorooctanoic acid (PFOA)	2-Ethylhexyl diphenyl phosphate
8	Tris(2-butoxyethyl) phosphate	Terbutryn
9	Flecainide	Carbamazepine
10	N,N'-Diphenylguanidine	N,N'-Diphenylguanidine
11	Oxybenzone	Caprolactam
12	2-Ethylhexyl diphenyl phosphate	Caffeine
13	Diuron	Sulfamethoxazole
14	Azoxystrobin	Temazepam
15	Temazepam	Tris(2-butoxyethyl) phosphate
16	Fluconazole	3,4-Methylenedioxymethamphetamine (MDMA)
17	Sitagliptin	Secbumeton
18	10,11-Dihydro-10,11-dihydroxycarbamazepine	Flecainide
19	Tapentadol	Ofloxacin/levofloxacin
20	2-ethyl-1,5-dimethyl-3,3-diphenylpyrrolinium (EDDP)	Sitagliptin
21	Carbendazim	Butyrophenone
22	Theophylline/ Paraxanthine	Diuron
23	Secbumeton	Carbendazim
24	Sulfamethoxazole	2-ethyl-1,5-dimethyl-3,3-diphenylpyrrolinium (EDDP)
25	Dicyclohexylamine	Sulpiride
26	Diphenylamine	10,11-Dihydro-10,11-dihydroxycarbamazepine
27	Cetirizine	Clopidogrel carboxylic acid
28	Clopidogrel carboxylic acid	Diclofenac
29	Desmethyldiazepam	Lidocaine
30	Isoproturon	Oxazepam
31	Methadone	Amisulpride
32	Oxazepam	Azoxystrobin
33	8-Hydroxyquinoline	Perfluorooctanoic acid (PFOA)
34	Memantine	Azoxystrobin acid
35	Amitriptyline	Diazinon
36	Ciprofloxacin	Propranolol
37	Diclofenac	Tapentadol
38	Lamotrigine	Tramadol
39	O-desmethyltramadol	Diltiazem
40	Perfluorobutanesulfonic acid (PFBS)	Amitriptyline
41	Tramadol	Diphenylamine
42	3,4-Methylenedioxymethamphetamine (MDMA)	Isoproturon
43	Diazinon	Fluconazole
44	Ofloxacin/levofloxacin	Cetirizine
45	2-(Methylthio)benzothiazole	Desacetyl diltiazem
46	Amisulpride	O-desmethyltramadol
47	Butyrophenone	Dextrorphan/levorphanol
48	Caffeine	Gabapentin
49	Diazepam	Desmethylcitalopram
50	Tri(chloropropyl) phosphate	Perfluorobutanesulfonic acid (PFBS)

*Compounds in bold are present in both lists.

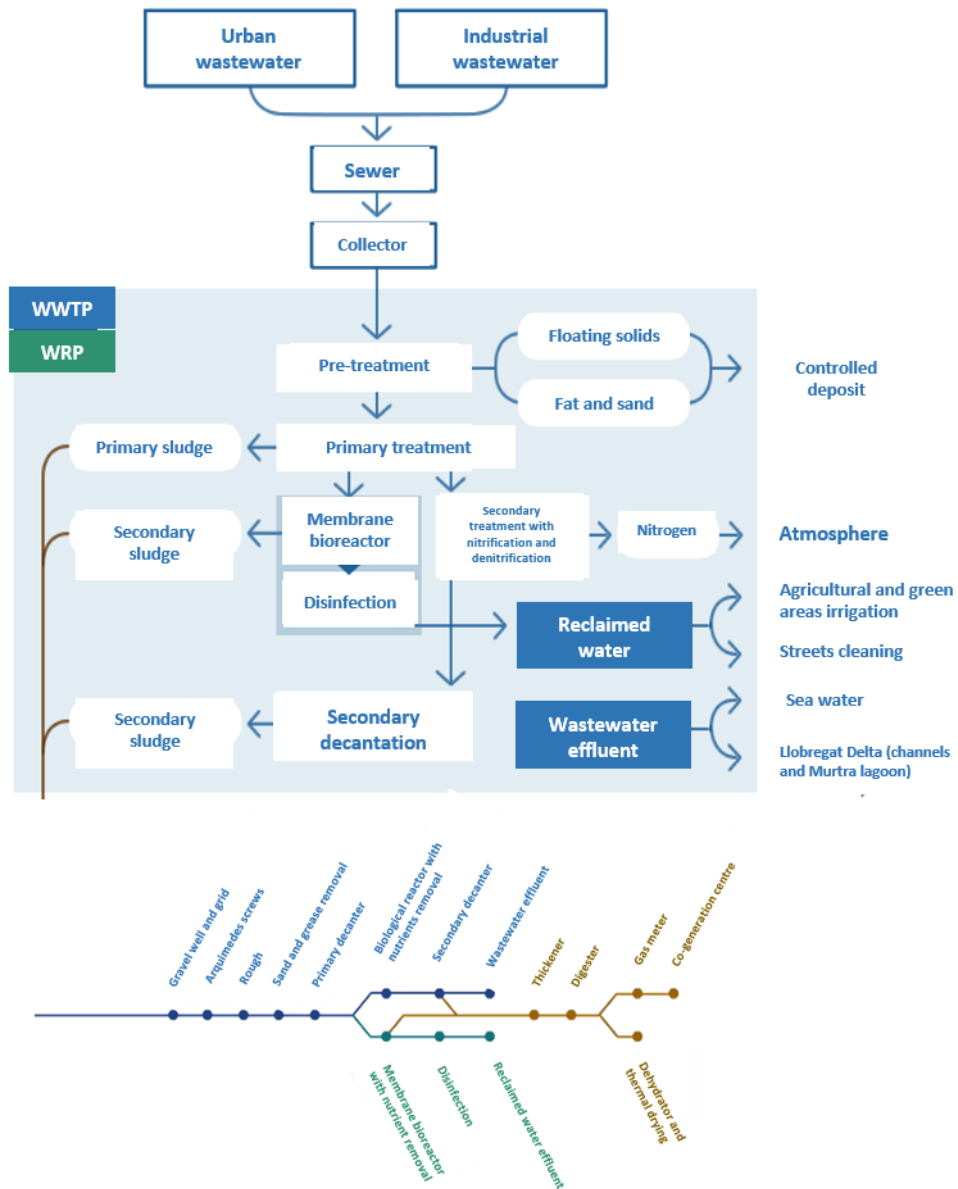


Figure S1. Scheme of the water treatment process at the water regeneration plant.

(Modified from <https://www.amb.cat/es/web/ecologia/aigua/instalacions-i-equipaments/detall/-/equipament/edar-de-gava-i-viladecans/269712/11818>)

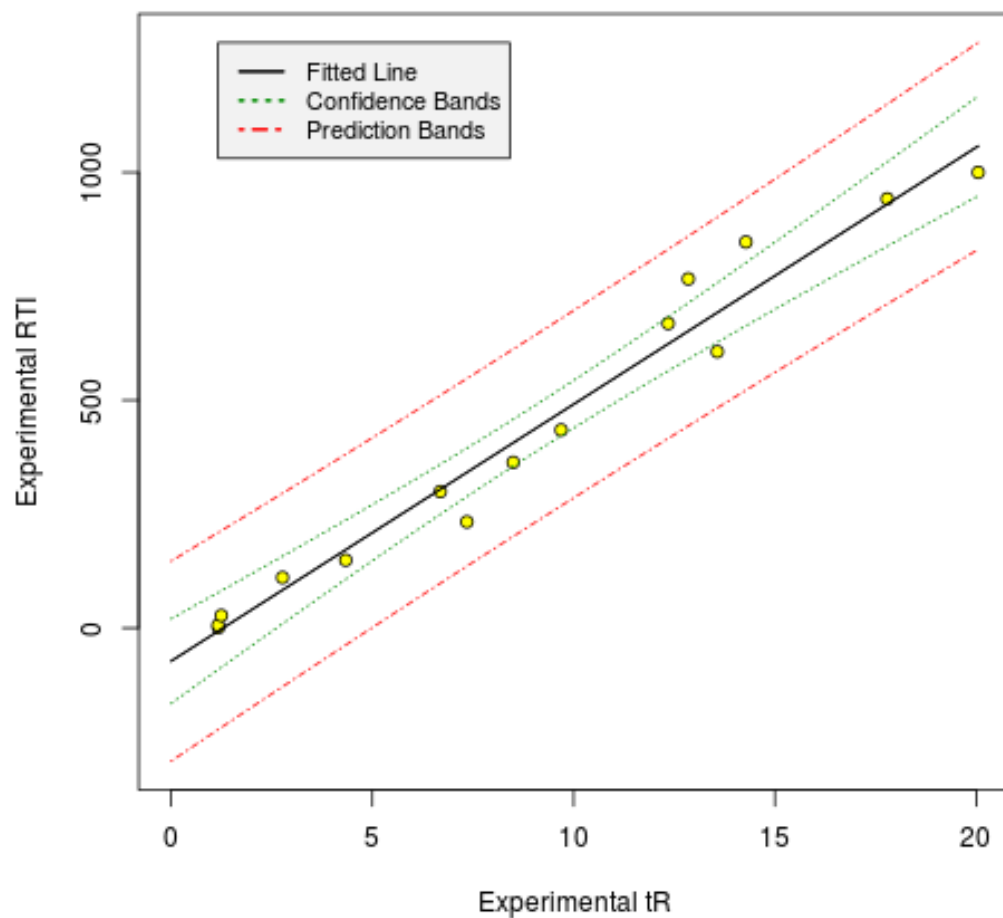


Figure S2. RTI (ESI+) calibration curve obtained through the RTI platform developed by the University of Athens (<http://rti.chem.uoa.gr/>). RTI calibrants are provided in Table S3.

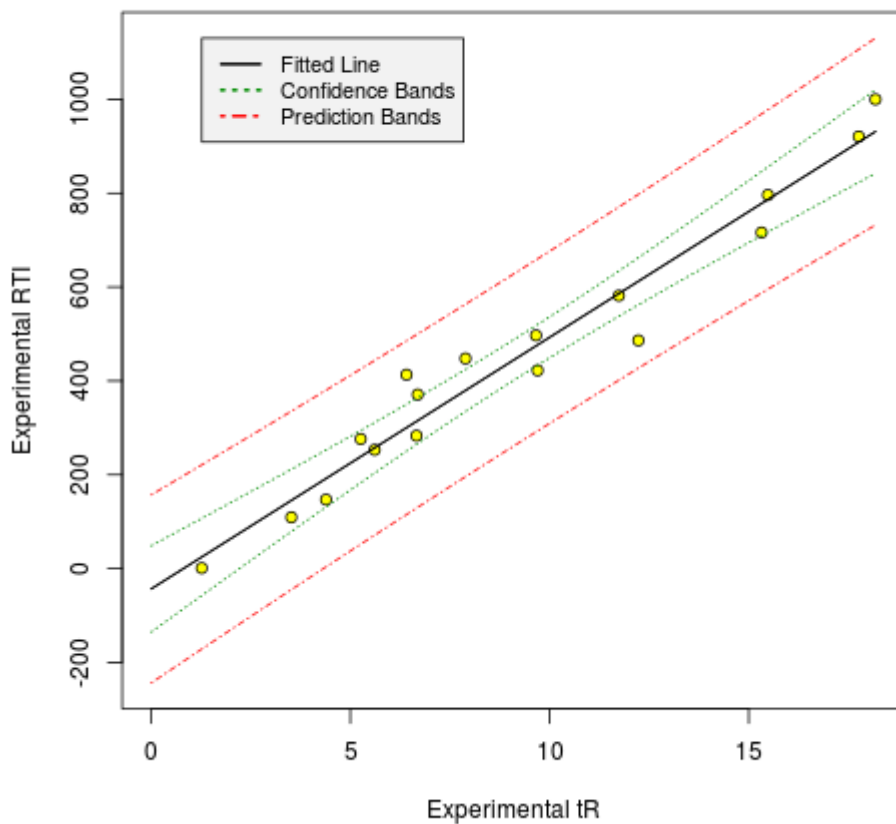


Figure S3. RTI (ESI-) calibration curve obtained through the RTI platform developed by the University of Athens (<http://rti.chem.uoa.gr/>). RTI calibrants are provided in Table S4.

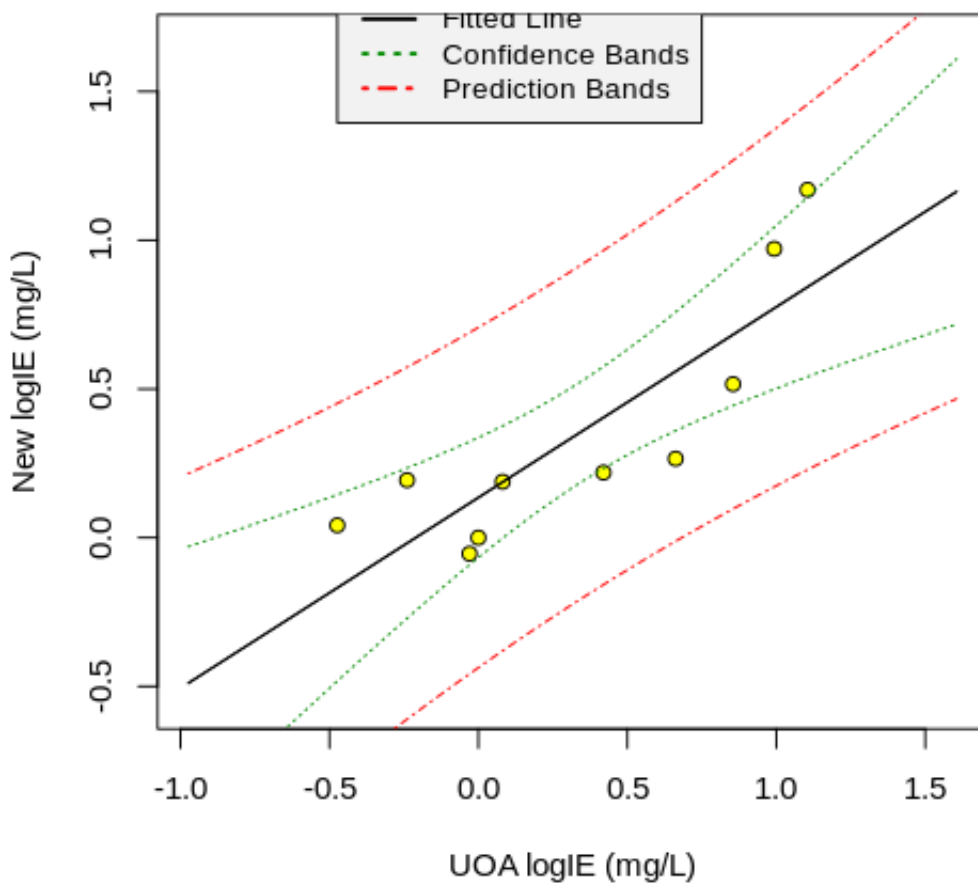


Figure S4. Harmonization of logIE after obtaining the slopes for each calibrant of the semi-quantification process (Table S5). Calculations and graphical report were obtained through the online application developed by the University of Athens (UoA) (<http://trams.chem.uoa.gr/semi quantification/>)