Supplementary material

Combining monitoring and modeling of emerging contaminants in rivers: application of a simple advection-reaction model to assess river basin water quality

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Table 1. Occurrence of emerging contaminants in the Llobregat River basin during 2010 - 2011. Mean and max concentration values and detection frequencies correspond to the 14 sites monitored in the basin (see main text, Fig 1)

				C1: 2010			C2: 2011		
Class	**Compound**	**CAS #**	**LoD ($ng L^{-1}$)**	**Frequency %**	**Mean conc. ($ng \cdot L^{-1}$)**	**Max. conc. ($ng \cdot L^{-1}$)**	**Frequency %**	**Mean conc. ($ng \cdot L^{-1}$)**	**Max. conc. ($ng \cdot L^{-1}$)**
	Acetaminophen	103-90-2	0.040	78.6%	45.213	142.890	64.3%	0.846	3.750
	Acridone	578-95-0	0.030	71.4%	2.013	6.450	100.0%	6.089	42.730
	Alprazolam	28981-97-7	0.020	21.4%	0.482	4.980	50.0%	0.189	1.040
	Amlodipine	88150-42-9	0.080	85.7%	2.480	23.520	21.4%	1.160	7.820
	Atenolol	29122-68-7	0.020	71.4%	37.709	331.580	50.0%	0.515	5.010
	Atorvastatin	134523-00-5	0.010	21.4%	0.193	2.260	35.7%	0.038	0.210
	Azithromycin	83905-01-5	0.050	78.6%	3.230	8.410	85.7%	1.511	12.200
	Bezafibrate	41859-67-0	0.020	71.4%	5.223	24.550	57.1%	0.272	1.320
	Carbamazepin	298-46-4	0.010	71.4%	13.296	64.040	71.4%	1.058	4.800
	Citalopram	59729-33-8	0.020	35.7%	3.240	31.830	71.4%	2.550	19.650
	Clopidogrel	90055-48-4	0.010	64.3%	0.580	3.580	78.6%	1.669	14.490
	Codeine	76-57-3	0.020	92.9%	7.070	44.070	28.6%	0.193	1.530
	Diazepam	439-14-5	0.050	21.4%	2.765	35.510	64.3%	1.604	9.100
	Diclofenac	15307-86-5	0.610	64.3%	22.366	129.050	64.3%	35.855	280.000
	Diltiazem	34933-06-7	0.020	100.0%	6.284	31.800	50.0%	2.098	9.920
	Furosemide	54-31-9	0.450	50.0%	27.173	205.880	71.4%	41.402	296.470
	Gemfibrozil	25812-30-0	0.050	85.7%	72.832	302.670	100.0%	70.266	301.000
	Hydrochlorothiazide	58-93-5	0.050	85.7%	209.665	793.330	100.0%	46.897	304.670
Pharmaceuticals	Ibuprofen	15687-27-1	1.170	64.3%	60.546	179.310	21.4%	2.751	7.460
	Indomethacin	53-86-1	0.090	64.3%	5.112	33.020	64.3%	8.358	63.720
	Irbesartan	138402-11-6	0.020	57.1%	30.301	141.100	71.4%	0.718	3.340
	Ketoprofen	22071-15-4	0.760	92.9%	28.781	153.090	100.0%	38.405	102.350
	Levamisol	14769-73-4	0.010	85.7%	7.619	37.850	64.3%	0.498	3.790
	Lorazepam	846-49-1	0.270	71.4%	36.130	187.870	42.9%	0.976	3.280
	Losartan	114798-26-4	0.100	78.6%	31.295	126.880	78.6%	1.891	6.500
	Meloxicam	71125-38-7	0.010	100.0%	28.781	153.090	100.0%	38.405	102.350
	Metoprolol	37350-58-6	0.110	35.7%	8.059	102.440	21.4%	21.301	291.670
	Metronidazole-OH	4812-40-2	0.400	71.4%	36.130	187.870	21.4%	0.976	3.280
	Naproxen	26159-31-9	0.190	64.3%	19.226	50.880	78.6%	21.700	90.530
	Paroxetine	61869-08-7	0.160	21.4%	0.496	3.410	21.4%	0.496	3.410
	Salbutamol	18559-94-9	0.010	57.1%	1.570	16.090	28.6%	0.084	0.490
	Sertraline	79617-96-2	0.630	14.3%	11.062	144.870	21.4%	3.765	42.920
	Thiabendazole	148-79-8	0.020	50.0%	1.252	12.920	100.0%	3.456	7.840
	Torasemide	56211-40-6	0.020	71.4%	1.881	9.430	64.3%	0.209	0.600
	Trimethoprim	738-70-5	0.100	57.1%	15.747	150.430	100.0%	8.025	60.220
	Valsartan	137862-53-4	0.050	100.0%	123.073	698.900	85.7%	2.914	20.000
	Venlafaxine	93413-69-5	0.020	78.6%	21.208	127.620	100.0%	3.901	26.290
	Chlorpyriphos	2921-88-2	0.200	100.0%	3.950	6.230	78.6%	5.322	13.650
	Diazinon	333-41-5	0.040	100.0%	4.994	13.610	64.3%	6.458	35.770
Pesticides	Diuron	330-54-1	1.000	35.7%	6.128	23.860	21.4%	23.684	159.530
	Imazalil	35554-44-0	0.300	92.9%	2.246	4.800	28.6%	1.052	6.330
	Imidacloprid	138261-41-3	0.040	78.6%	2.135	5.390	64.3%	15.953	66.530

	Isoproturon	34123-59-6	0.300	57.1%	1.541	3.550	28.6%	1.705	9.600
	PFBA	375-22-4	0.040	85.7%	19.479	111.170	50.0%	0.846	6.208
	PFBS	375-73-5	0.020	14.3%	0.330	4.100	71.4%	5.322	25.692
Perfluorinated	PFHxS	355-46-4	0.004	28.6%	6.667	33.175	28.6%	0.758	5.068
	PFOA	335-67-1	0.040	71.4%	20.334	146.400	50.0%	1.880	8.208
	PFOS	1763-23-1	0.004	50.0%	233.900	#######	50.0%	1.502	16.500
	PFPeA	2706-90-3	0.040	21.4%	0.408	2.500	21.4%	0.656	5.256
	1H-Benzotriazole	95-14-7	0.072	92.9%	227.049	#######	100.0%	428.281	1261.419
	Benzylparaben	94-18-8	0.031	21.4%	0.069	0.408	42.9%	1.924	6.690
	Bisphenol A	80-05-7	0.110	78.6%	89.358	530.296	100.0%	95.244	649.352
	Caffeine	58-08-2	0.021	100.0%	181.936	572.195	100.0%	251.259	1220.902
	Estrone	53-16-7	0.050	42.9%	0.758	3.801	50.0%	1.102	6.206
	Ethylparaben	120-47-8	0.270	64.3%	4.739	40.691	50.0%	3.745	12.588
	Methylparaben	99-76-3	0.200	100.0%	8.746	50.937	42.9%	2.720	9.464
	Nonylphenol	104-40-5	0.013	92.9%	18.808	41.660	28.6%	13.514	116.338
Endocrine_disr.	NP2EO	20427-84-3	0.013	100.0%	65.800	287.669	100.0%	18.359	62.839
	NP1EC	-	0.034	92.9%	256.464	989.526	85.7%	175.672	851.653
	Octylphenol	1806-26-4	0.140	100.0%	7.111	16.322	28.6%	7.279	84.725
	OP2EO	2315-61-9	0.011	100.0%	10.433	29.334	85.7%	5.000	32.842
	Propylparaben	94-13-3	0.021	78.6%	2.414	20.209	85.7%	4.756	13.154
	Tolyltriazol	29385-43-1	0.013	100.0%	223.623	749.840	85.7%	862.171	7017.670
	Tris(2-chloroethyl) phosphate	115-96-8	0.034	100.0%	51.599	232.397	92.9%	11.288	39.387
	Tris(butoxyethyl) phosphate	78-51-3	0.002	100.0%	106.938	315.079	100.0%	55.955	216.141
	Tris(chloroisopropyl) phosphate	13674-84-5	0.003	100.0%	221.861	964.283	71.4%	216.010	1117.266
	EDDP	30223-73-5	0.010	92.9%	4.126	13.900	64.3%	8.632	49.500
	MDMA	42542-10-9	0.100	92.9%	2.073	7.580	50.0%	8.775	56.800
Drugs_of_abuse	Methadone hydrochl.	76-99-3	0.060	100.0%	2.590	9.640	85.7%	3.516	20.000
	Ephedrine	299-42-3	0.160	71.4%	7.821	18.800	64.3%	12.789	88.600
	Cocaine	50-36-2	0.020	92.9%	4.805	23.800	92.9%	2.444	7.140

Note: all the analytical determinations were done by HPLC-MS. Experimental details can be found in the references[32-37] provided in the main text (*Section 2.3 Monitoring of emerging contaminants*).