SUPPORTING INFORMATION

Human footprint on the water quality from the northern Antarctic Peninsula region

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ID	Latitude	Longitude
1_D	617815	3014149
2_D	617926	3014032
3_D	623646	3014467
4_D	623625	3014392
5_D	623536	3014552
6_D	623808	3014359
7_D	623168	3012284
8_D	622579	3012300
9_D	617714	3014856
10_D	617800	3014884
11_L	633745	3049248
12_L	633888	3048945
13_L	633729	3049196
14_L	633752	3049308
15_L	633774	3049333
16_L	633580	3049347
17_L	633813	3049306
18_L	632655	3048312
19_L	634701	3049082
20_L	634258	3049340
21_L	632095	3045197
22_L	631914	3045307
23_L	633813	3048903
24_L	633810	3048900
25_B	597523	3050086
26_B	597234	3049566
27_B	597365	3049879
28_B	597584	3050092
29_B	597356	3050454
30_B	597355	3050356
31_B	597076	3050376
32_B	598212	3050426
33_B	598236	3050641
34_B	597812	3050335
35_B	597746	3050411
36_B	597882	3050866
37_B	597078	3050888
38_B	598050	3051245

Text S1. Performance of the online SPE-HPLC-ESI-MS/MS method used to analyze the target organic contaminants.

The performance of the online solid phase extraction-high performance liquid chromatography-electrospray-tandem mass spectrometry (SPE-HPLC-ESI-MS/MS) methodology used for the analysis of the selected organic contaminants in surface water and seawater was evaluated in terms of linearity, accuracy (analyte absolute and relative recoveries), precision (measurement repeatability), and sensitivity.

The linearity was evaluated with the analysis of high-performance liquid chromatography (HPLC)-grade water solutions fortified with the mixture of the target analytes at concentrations between 0.1 and 2000 ng/L and a fixed concentration of the surrogate standard mixture (40 ng/L). Internal standard-based calibration curves were constructed for each analyte with a minimum of 7 points using a least-square linear regression model and a weighting factor of 1/x. The latter contributes to minimizing the error originated by the unequal variance (i.e, higher at higher concentrations) that exists along a wide calibration range. The surrogate standards used in the quantification process are indicated in Table S2. The lowest linearity range was established above the analyte signal, if present, in HPLC-grade water blanks (HPLC-grade water fortified with the surrogate standard mixture, n=3). Moreover, only calibration points that presented deviations below 20% between calculated and theoretical concentrations were used to construct the calibration model. Coefficients of determination (r^2) above 0.99 were obtained for all analytes. Bezafibrate and clarithromycin showed the largest linearity range (0.1-2000 ng/L), while the shortest ones were observed for caffeine (10-2000 ng/L – due to carryover) and ibuprofen (50-2000 ng/L – due to poor instrumental sensitivity). The analyte signal in the HPLC-grade water blanks, if present, was taken into consideration when reporting the final concentration in the water samples ($C_{sample} = C_{quantified} - C_{blank}$, where C stands for concentration in ng/L).

The method accuracy and precision were assessed at three concentration levels (5 ng/L, 50 ng/L, and 500 ng/L). Method accuracy was examined from the analyte absolute and relative recoveries. The absolute recovery was calculated by comparing the average peak area obtained in the online SPE-HPLC-ESI-MS/MS analysis of fortified surface (n=6) or seawater (n=6) aliquots with that obtained in the HPLC-ESI-MS/MS analysis of a pure standard solution (n=3) at equivalent concentrations. The relative recovery was obtained by comparing the absolute recoveries (n=6) of the analyte and the isotopically labeled compound used for

quantification in each matrix at each concentration level. The relative standard deviation (RSD) of the analyte relative recoveries (n=6) was used to express the method precision.

The average absolute recoveries of the target analytes in both matrices at the three concentration levels investigated were in good agreement (RSD of the average values below 26 % and 30 % in surface water and seawater, respectively). The lowest absolute recovery values were obtained for acetaminophen (11 % on average in surface water and not recovered in seawater). This could be attributed to its polar nature and its poor affinity for the extraction sorbent because it is completely washed out from the SPE cartridge when it is thoroughly rinsed with water to remove the salt in the analysis of seawater samples. In contrast, unexpectedly high absolute recoveries were observed in the case of bezafibrate (176 % on average in surface water and 144 % in seawater). This is associated with a different ionization efficiency of this analyte during the offline HPLC-ESI-MS/MS analysis of a pure standard solution and its elution from the SPE cartridge with the aid of the mobile phase in the online HPLC-ESI-MS/MS approach. The average absolute recoveries for the remaining compounds ranged between 31 % and 113 % in surface water and 34 and 85% in seawater.

The average relative recoveries were between 80 % and 125 % for most analytes in both matrices at the three concentration levels tested. Exceptions were found for benzophenone 1 (BP1) (105-138 % in surface water and 126-163 % in seawater), and ibuprofen (60-133 % in seawater). In the case of BP1, the deviations found can be attributed to the use of a related substance (benzophenone-d_{10}) instead of its isotopically labeled analog as a surrogate standard. In the case of ibuprofen, this could be associated with both its poor instrumental sensitivity and the low specificity of the SRM transitions of the analyte and its deuterated analog. These SRM transitions result from the loss of the carboxylic acid group, and therefore, they may be affected to a different extent by the matrix components. This is supported by the high variability observed in the relative recoveries of ibuprofen at the tested levels (RSD values between 16 % and 38 %). For the remaining analytes, RSD values below 9 % were obtained in both matrices at the three investigated levels, except in the case of tolytriazole (11 %), hydrochlorothiazide (15 %), diclofenac (16 %), and nicotine (19 %) at 5 ng/L in seawater.

The method sensitivity was judged from the limits of detection (LOD) and quantification (LOQ). Average values in each matrix were estimated from the signal-to-noise (S/N) ratio observed in the samples where the analyte was positively detected. Otherwise, water samples fortified at the lowest concentration level (5 ng/L) were used. The LOD corresponds with the concentration that would result from an S/N of 3 and the LOQ corresponds with the concentration that would result from an S/N of 10 or the lowest limit of the linearity range (if

this value is higher than the calculated value). The concentration values provided that are below the analyte average LOQ are explained by the slightly lower LOQ of that specific sample as compared to the average LOQ or the subtraction of the average signal present in the HPLC-grade water blanks (e.g., caffeine).

Table S2. Parameters for the online SPE-HPLC-ESI-MS/MS determination of the target organic chemicals.

	Abbrev.	Rt [min]	Ionization type	Precursor ion [m/z] (CV) [V]	Product ions [m/z] (CE) [eV]	Ratio Q/q
Acetaminophen	ACET	4.63 ± 0.01	+	152 (40)	**110 (15)** 93 (20)	6.2
Acetaminophen-d_4	ACET-d		+	156 (40)	114 (15)	-
Benzophenone-1	BP1	11.67±0.17	+	215 (40)	**137 (15)** 105 (15)	4.3
Benzophenone-d_{10}	BP-d		+	193 (10)	110 (15)	-
Bezafibrate	BEZF	7.82±0.03	-	360 (40)	**274 (20)** 154 (30)	2.2
Bezafibrate-d_4	BEZF-d		-	364 (30)	278 (15)	-
Caffeine	CAF	5.54 ± 0.02	+	195 (40)	**138 (20)** 110 (25)	5.3
Caffeine-d_3	CAF-d		+	198 (10)	141 (20)	-
Citalopram	CTPM	9.53 ± 0.07	+	325 (10)	**109 (25)** 262 (15)	4.5
Citalopram-d_6	CTPM-d		+	331 (10)	109 (30)	-
Clarithromycin	CLAR	10.18 ± 0.07	+	748 (40)	**158 (30)** 590 (20)	4.4
Clarithromycin-N-methyl-^{13}C-d_3	CLAR-M-d		+	752 (10)	162 (30)	-
Diclofenac	DCF	9.39 ± 0.05	-	294 (10)	**250 (10)** 214 (20)	28.4
Diclofenac-d_4	DCF-d		-	298 (10)	254 (15)	-
Hydrochlorothiazide	HCTZ	6.11 ± 0.09	-	296 (30)	**269 (20)** 205 (25)	1.6
Hydrochlorothiazide-d_2	HCTZ-d		-	298 (10)	270 (20)	-
Ibuprofen	IBU	10.47 ± 0.07	-	205 (10)	**161 (5)**	-
Ibuprofen-d_3	IBU-d		-	208 (4)	**164 (5)**	-
Nicotine	NIC	5.63 ± 0.09	+	163 (10)	117 (25) **130 (25)**	1.0
Nicotine-d_4	NIC-d		+	167 (10)	134 (25)	-
Tolytriazole*	TTA	7.42 ± 0.03	+	134 (10)	**79 (15)** 77 (25)	1.7
Benzotriazole (ring-d_4)	BTA-d		+	124 (10)	69 (20)	-
Venlafaxine	VFX	8.05 ± 0.04	+	278 (10)	**58 (25)** 260 (10)	1.8
Venlafaxine-d_6	VFX-d		+	284 (10)	64 (25)	-

**Venalfaxine-d6* was used as the surrogate standard for the quantification of seawater samples.

CV: cone voltage; CE: collision energy.

The product ion of the SRM transition used for quantification (Q) is highlighted in bold.

Q/q: the ratio between the areas of the quantification SRM and the confirmation SRM transition.

Table S3. Data and criteria to evaluate the persistence (P) potential of organic CECs.

	P prediction (reliability) (VEGA[a])	Pscore (VEGA[a])	ECHA[b] Biodegradability assessment	BIOWIN Readily biodegradable assessment (EPISuite[c])*	BIOWIN (Ultimate survey model) (EPISuite[c])	STPWIN (Total biodeg. (%) in a CAS STP using data from BIOWIN models) (EPISuite[c])	P1**	P2**	Final SCORE**
Acetaminophen (103-90-2) CC(=O)NC1=CC=C(O)C=C1	nP/P (0.5)	0.571	readily biodegradable	No	weeks	75	0.5		0.5
Benzophenone-1 (131-56-6) Oc1ccc(C(=O)c2ccccc2)c(O)c1	nP (0.7)	0.333	inherently biodegradable	No	weeks	78	0	0	0
Bezafibrate (41859-67-0) c1(C(NCCc2ccc(OC(C(O)=O)(C)C)cc2)=O)ccc(Cl)cc1	P/vP (0.5)	0.712	*n.a.*	No	months	24	1	1	2.0
Caffeine (58-08-2) O=C2c1c(ncn1C)N(C(=O)N2C)C	vP (0.5)	0.854	readily biodegradable	No	weeks	75	0.5	0	0.5
Citalopram (59729-33-8) CN(C)CCCC1(OCC2=C1C=CC(=C2)C#N)C1=CC=C(F)C=C1	nP (0.7)	0.333	*n.a.*	No	recalcitrant	0.24	0.5	1.5	2.0
Clarithromycin (8103-11-9) CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC	nP (0.5)	0.359	not readily biodegradable	No	recalcitrant	0.14	0.5	1.5	2.0
Diclofenac (15307-86-5) c1c(c(ccc1)Nc1c(cccc1Cl)Cl)CC(=O)O	nP/P (0.5)	0.571	not readily biodegradable	No	weeks-months	47	0.5	0.5	1.0
Hydrochlorothiazide (58-93-5) NS(=O)(=O)C1=CC2=C(NCNS2(=O)=O)C=C1Cl	P/vP (0.5)	0.712	*n.a.*	No	months	7	1	1.5	2.5
Ibuprofen (15687-27-1) CC(C)CC1=CC=C(C=C1)C(C)C(O)=O	nP (0.7)	0.333	moderately biodegradable	No	weeks	80	0	0	0
Nicotine (54-11-5) CN1CCC[C@H]1C2=CN=CC=C2	nP/P (0.5)	0.571	readily biodegradable	No	weeks-months	21	0.5	1	1.5

Table S3. (cont)

	P prediction (reliability) (VEGA[a])	Pscore (VEGA[a])	ECHA[b] Biodegradability assessment	BIOWIN Readily biodegradable assessment (EPISuite[c])*	BIOWIN (Ultimate survey model) (EPISuite[c])	STPWIN (Total biodeg. (%) in a CAS STP using data from BIOWIN models) (EPISuite[c])	P1**	P2**	Final SCORE**
Tolytriazole:			not readily biodegradable						
5-Methyl-1H-benzotriazole (136-85-6) Cc1ccc2[nH]nnc2c1	P/vP (0.5)	0.712	n.a.	No	weeks	75	0.5	0	0.5
5-Methyl-1H-benzotriazole (29878-31-7) CC1=CC=CC2=NNN=C12	P/vP (0.5)	0.712	n.a.	No	weeks	75	0.5	0	0.5
Venlafaxine (93413-69-5) CN(C)CC(c1ccc(cc1)OC)C2(CCCCC2)O	nP/P (0.7)	0.584	n.a.	No	months	11	0.5	1	1.5

P: persistent; vP: very persistent; nP: not persistent; n.a.: information not available.

* Conservative statement as described in EPISuite – YES if the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. days, days to weeks, or weeks) AND the Biowin5 (MITI linear model) probability is >= 0.5. If this condition is not satisfied, the prediction is NO (not readily biodegradable).

**Final SCORE for persistence potential is the sum of P1 and P2, where P1 is the assessment of the Pscore and BIOWIN ultimate survey model results and P2 is the assessment of the STPWIN results, as follows:

**P1 = 0 if Pscore is <0.5 and BIOWIN ultimate survey model is *weeks*
0.5 if Pscore is >0.5 and ≤0.7 or
0.7 AND BIOWIN ultimate survey model is *weeks* or
<0.5 and BIOWIN ultimate survey model is *longer than weeks*
1.0 if Pscore is >0.7 and ≤0.8 and BIOWIN ultimate survey model is *months*
1.5 if Pscore is >0.8 and BIOWIN ultimate survey model is longer than *months*

**P2 = 0 if biodegradation in CAS STP is ≥ 75 %
0.5 if biodegradation in CAS STP is > 40 and <75 %
1.0 if biodegradation in CAS STP is >10 and ≤ 40 %
1.5 if biodegradation in CAS STP is ≤ 10 %

[a] Benfenati, E., Cappelli C.I., Petoumenou, M.I. et al. PROMETHEUS – Prioritization Of chemicals: a METHodology Embracing PBT parameters into a Unified Strategy. Texte 28/2016. Umweltbundesamt report, https://www.vegahub.eu/download/prometheus-download/, 2022.
[b] European chemicals agency- information on chemicals. https://echa.europa.eu/information-on-chemicals, 2022.
[c] US EPA. (2022). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US Environmental Protection Agency, Washington, DC, USA.

Table S4. Data and criteria to evaluate the bioaccumulation potential of organic CECs.

	Octanol-water partition coefficient, Log Kow					Bioconcentration factor, Log BCF					
	Exp. (EPISuite[a])	KOWIN (EPISuite[a])	Average predicted (CompTox[b])	Log P Predicted Consensus (ChemAxon[c])	Average	Exp. (CompTox[b]) (Log (median value))	B prediction (reliability) (VEGA[d])	B score (VEGA[d])	K_{ow} score	BCF score	Final SCORE*
Acetaminophen (103-90-2) CC(=O)NC1=CC=C(O)C=C1	0.46	0.27	0.369	0.91	0.50	n.a.	0.39 (0.8)	0.102	0	0	0
Benzophenone-1 (131-56-6) Oc1ccc(C(=O)c2ccccc2)c(O)c1	n.a.	2.96	3.03	3.48	3.16	n.a.	1.3 (0.8)	0.182	1	0	1
Bezafibrate (41859-67-0) c1(C(NCCc2ccc(OC(C(O)=O)(C)C)cc2)=O)ccc(Cl)cc1	n.a.	4.25	3.74	3.99	3.99	n.a.	1.45 (0.8)	0.201	1	0	1
Caffeine (58-08-2) O=C2c1c(ncn1C)N(C(=O)N2C)C	-0.07	0.16		-0.55	-0.11	n.a.	0.77 (0.8)	0.128	0	0	0
Citalopram (59729-33-8) CN(C)CCCC1(OCC2=C1C=CC(=C2)C#N)C1=CC=C(F)C=C1	n.a.	3.74	3.04	3.76	3.51	n.a.	1.63 (0.8)	0.226	1	0	1
Clarithromycin (8103-11-9) CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC	3.16	3.18	3.15	3.24	3.18	0.59	0.66 (0.4)	0.239	1	0	1
Diclofenac (15307-86-5) c1c(c(ccc1)Nc1c(cccc1Cl)Cl)CC(=O)O	4.51	4.02	4.27	4.26	4.27	2.6	2.57 (0.8)	0.403	1.5	0.5	2
Hydrochlorothiazide (58-93-5) NS(=O)(=O)C1=CC2=C(NCNS2(=O)=O)C=C1Cl	-0.07	-0.10	0.058	-0.67	-0.20	n.a.	0.42 (0.4)	0.228	0	0	0
Ibuprofen (15687-27-1) CC(C)CC1=CC=C(C=C1)C(C)C(O)=O	3.97	3.79	3.65	3.84	3.81	0	0.43 (0.8)	0.104	1	0	1
Nicotine (54-11-5) CN1CCC[C@H]1C2=CN=CC=C2	1.17	1	0.928	1.16	1.06	n.a.	0.17 (0.8)	0.09	0	0	0

Table S4. (cont)

	Octanol-water partition coefficient, Log Kow					Bioconcentration factor, Log BCF					
	Exp. (EPISuite[a])	**KOWIN (EPISuite[a])**	**Average predicted (CompTox[b])**	**Log P Predicted Consensus (ChemAxon[c])**	**Average**	**Exp. (CompTox[b]) (Log (median value))**	**B prediction (reliability) (VEGA[d])**	**B score (VEGA[d])**	**K_{ow} score**	**BCF score**	**Final SCORE***
Tolytriazole:											
5-Methyl-1H-benzotriazole (136-85-6) Cc1ccc2[nH]nnc2c1	n.a.	1.71	1.56	1.81	1.69	n.a.	0.6 (0.4)	0.236	0	0	0
5-Methyl-1H-benzotriazole (29878-31-7) CC1=CC=CC2=NNN=C12	n.a.	1.71	1.53	1.81	1.68	n.a.	0.53 (0.4)	0.233	0	0	0
Venlafaxine (93413-69-5) CN(C)CC(c1ccc(cc1)OC)C2(CCCCC2)O	3.2	3.28	3.12	2.74	3.09	1.1	1.53 (0.4)	0.302	1	0	1

n.a., information not available; Exp., experimental

*Final SCORE for bioaccumulation potential results is Kow score + BCF score,

where K_{ow} score is 0 if average Log Kow < 3; 1 if average Log Kow >3 y ≤4; 1.5 if average Log Kow >4

and BCF score is 0 if predicted/experimental log BCF < 2.3; 0.5 if predicted/experimental log BCF > 2.3 y ≤3.3; 1.0 if predicted/experimental log BCF >3.3 y ≤3.7; 1.5 if predicted/experimental log BCF >3.7

[a] US EPA. (2022). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. United States Environmental Protection Agency, Washington, DC, USA

[b] Williams, A.J., Grulke, C.M., Edwards, J. *et al.* The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *J Cheminform* **9,** 61 (2017). https://doi.org/10.1186/s13321-017-0247-6

[c] MarvinSketch (version 22.13, calculation module developed by ChemAxon Ltd, http://www.chemaxon.com/products/marvin/marvinsketch/, 2022.

[d] Benfenati, E., Cappelli C.I., Petoumenou, M.I. et al. PROMETHEUS – Prioritization Of chemicals: a METHodology Embracing PBT parameters into a Unified Strategy. Texte 28/2016. Umweltbundesamt report, https://www.vegahub.eu/download/prometheus-download/, 2022.

Table S5. Data and criteria to evaluate the aquatic ecotoxicity potential of organic CECs.

	FISH (LC50, 96 h, mg/L)			DAPHNIA (LC50 48 h, mg/L)			ALGAE (IG50 48 h, mg/L)			Final SCORE *
	Exp. ECOTOX [a]	Pred TEST [b] ECOSAR [c]	Exp ECHA [d]	Exp. ECOTOX [a]	Pred TEST [b] ECOSAR [c]	Exp ECHA [d]	Exp. ECOTOX [a]	Pred TEST [b] ECOSAR [c]	Exp ECHA [d]	
Acetaminophen (103-90-2) CC(=O)NC1=CC=C(O)C=C1	814	87 30-4458	160	9.2	27 1.6-2157	136	999	344 14-829	134	0.7
Benzophenone-1 (131-56-6) Oc1ccc(C(=O)c2ccccc2)c(O)c1		7.0 3.1-24	3.7		5.7 15-16	7.9	9.1	16 2.1-16	2.1	2.0
Bezafibrate (41859-67-0) c1(C(NCCc2ccc(OC(C(O)=O)(C)C)cc2)=O)ccc(Cl)cc1		0.78 2.8-26			16 1.4-3.5			4.1 1.4-3.5		2.3
Caffeine (58-08-2) O=C2c1c(ncn1C)N(C(=O)N2C)C		503 112-7221	87	182	182 12-3458	182	192	323 0.8-1274	>100	0.3
Citalopram (59729-33-8) CN(C)CCCC1(OCC2=C1C=CC(=C2)C#N)C1=CC=C(F)C=C1		1.2 4.5-7.3		3.9	0.77 0.7-4.9			8.0 0.4-7.0		2.3
Clarithromycin (8103-11-9) CC[C@H]1OC(=O)[C@H](C)[C@@H](O[C@H]2C[C@@](C)(OC)[C@@H](O)[C@H](C)O2)[C@H](C)[C@@H](O[C@@H]2O[C@H](C)C[C@@H]([C@H]2O)N(C)C)[C@@](C)(C[C@@H](C)C(=O)[C@H](C)[C@@H](O)[C@]1(C)O)OC		n/a 17-54			n/a 3.3-38			n/a 2.1-40		1.7
Diclofenac (15307-86-5) c1c(c(ccc1)Nc1c(cccc1Cl)Cl)CC(=O)O		0.40 38		22	5.1 25	68		2.0 41	72	1.7
Hydrochlorothiazide (58-93-5) NS(=O)(=O)C1=CC2=C(NCNS2(=O)=O)C=C1Cl		n/a 2808-18684			n/a 8125-8741			n/a 56-2924		0.3
Ibuprofen (15687-27-1) CC(C)CC1=CC=C(C=C1)C(C)C(O)=O		5.5 42	173	9.1	4.1 28	37		21 41	342	0.7
Nicotine (54-11-5) CN1CCC[C@H]1C2=CN=CC=C2		173 4.9-1058	>3	3.0	25 0.2-547	0.2		246 16-278	11	2.0

Table S5. (cont)

	FISH (LC50, 96 h, mg/L)			DAPHNIA (LC50 48 h, mg/L)			ALGAE (IG50 48 h, mg/L)			Final SCORE
	Exp. ECOTOX [a]	Pred TEST [b] ECOSAR [c]	Exp ECHA [d]	Exp. ECOTOX [a]	Pred TEST [b] ECOSAR [c]	Exp ECHA [d]	Exp. ECOTOX [a]	Pred TEST [b] ECOSAR [c]	Exp ECHA [d]	
Tolytriazole:						15.8-100			53-75	
5-Methyl-1H-benzotriazole (136-85-6) Cc1ccc2[nH]nnc2c1		n/a 16-198			n/a 36-109			n/a 3.9-73		1.0
5-Methyl-1H-benzotriazole (29878-31-7) CC1=CC=CC2=NNN=C12		n/a 16-198			n/a 36-109			n/a 3.9-73		1.0
Venlafaxine (93413-69-5) CN(C)CC(c1ccc(cc1)OC)C2(CCCCC2)O		6.3 7.7-16			8.2 1.1-10			9.0 0.7-13		2.3

* Final SCORE for ecotoxicity potential is the weighted addition of the individual scores obtained at each trophic level:

Final score = $score_{fish}$*0.33 + $score_{daphnia}$*0.33 + $score_{algae}$*0.33

Individual score assignment:
0 if LC/IG > 100 mg/L (low toxicity)
1 if LC/IG ≤ 100 mg/L and >10 mg/L (moderate toxicity)
2 if LC/IG ≤ 10 mg/L and >1 mg/L (high toxicity)
3 if LC/IG < 1 mg/L (very high toxicity)

Experimental values over predicted values will be used for individual score assessment. The lowest limit of the range will be selected to assign the individual score.

[a] Olker, J.,Elonen, C., Pilli, A., Anderson, A. *et al.* The ECOTOXicology Knowledgebase: A Curated Database of Ecologically Relevant Toxicity Tests to Support Environmental Research and Risk Assessment. *Environ Toxicol Chem* **41,** 1520 (2022). https://doi.org/10.1002/etc.5324

[b] Martin, T. Toxicity Estimation Software Tool (TEST). U.S. Environmental Protection Agency, Washington, DC, 2016. https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test

[c] US EPA. (2022). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11. US Environmental Protection Agency, Washington, DC, USA

[d] European chemicals agency- information on chemicals. https://echa.europa.eu/information-on-chemicals, 2022.

Text S2. Statistical analysis – descriptive statistics and pairwise correlations.

Statistics were run only with variables that presented quantifiable concentrations in more than 30 % of the samples, i.e., 5 out of the 9 investigated organic contaminants, and 26 inorganic constituents and water parameters. A substitution method was used to deal with censored data: LOD/2 and LOQ/2 were assigned to non-detected and non-quantifiable cases, respectively. All variables except pH presented positive asymmetry coefficients and hence positively skewed distributions (most of the values in each variable fall below the mean value) (Table S6). Thus, as variables did not present a normal distribution, the potential relationships among the presence of organic CECs and other water constituents and properties were explored through pairwise correlations using Spearman's Rank correlation test.

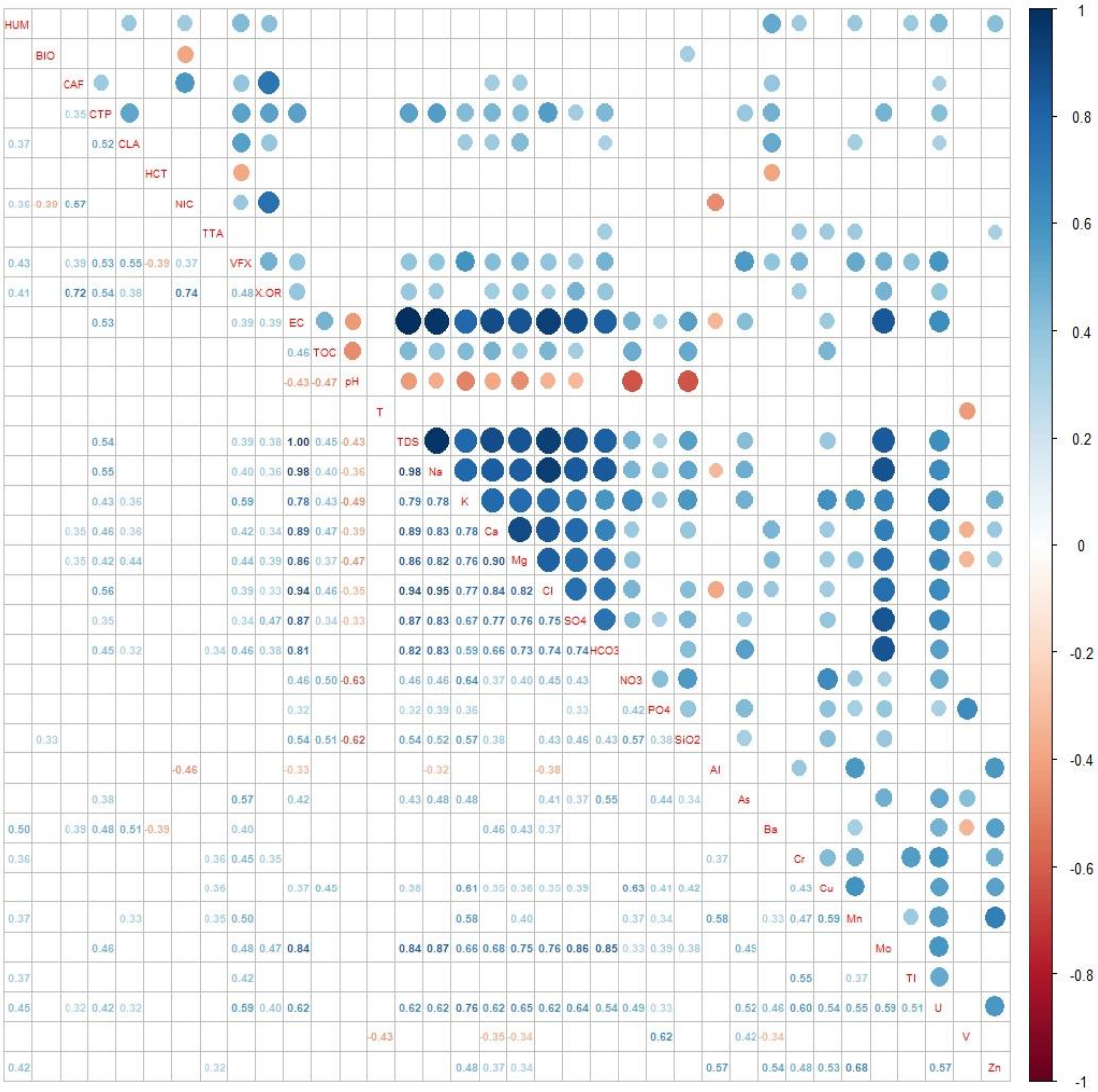
Pairwise correlations among variables

Figure S1 summarizes the results obtained after pairwise correlation tests. Only statistically significant correlations (α=0.05) are shown. The strength of the correlation is indicated by the size of the dot and the intensity of the font color. All correlations above $|0.5|$ were found to be statistically significant, and therefore, they were considered strong correlations. The pH was negatively correlated with nitrate and SiO_2 concentrations. Positive and strong relationships (rho>0.81) were found between electrical conductivity (EC) and total dissolved solids (TDS), Na^+, Ca^{+2}, Mg^{+2}, Cl^-, SO_4^{-2}, and HCO_3^-; between TDS and Na^+, Ca^{+2}, Mg^{+2}, Cl^-, SO_4^{-2} and HCO_3^-; between Na^+ and Ca^{+2}, Mg^{+2}, Cl^-, SO_4^{-2} and HCO_3^-; between Ca^{+2} and Mg^{+2} and Cl^-; and between Mg^{+2} and Cl^-. Overall, the investigated organic CECs did not present strong correlations with the water constituents and characteristics. Among them, weak positive relationships (rho= 0.52-0.57) were observed between caffeine and nicotine, and among clarithromycin, citalopram, and venlafaxine. These relationships are also well illustrated in the network plot shown in Figure S2.

Table S6. Descriptive statistics of the variables included in the statistical analysis

		Mean	St Dev	Median	Min	Max	Skewness	Kurtosis
CAF	ng/L	11	22	0.05	0.05	94	2.26	4.67
CTPM	ng/L	16	49	2.2	0.65	292	4.87	24.47
CLAR	ng/L	7.0	29	0.05	0.05	173	5.14	26.48
HCTZ	ng/L	1.9	2.6	0.28	0.15	10	1.53	1.49
NIC	ng/L	15	27	8.7	0.35	146	3.41	12.82
TTA	ng/L	3.1	3.6	2.2	0.25	20	2.83	9.66
VFX	ng/L	2.0	5.8	0.10	0.10	35	4.63	22.75
EC	µS/cm	7240	18455	93	15	57100	2.10	2.49
TOC	mg/L	1.8	0.6	1.6	0.25	4.0	1.09	2.93
pH		7.3	0.5	7.4	5.4	8.2	-0.91	1.78
T	°C	4.7	9.7	2.8	0.4	55	4.19	17.27
TDS	mg/L	5201	13258	70	14	40795	2.10	2.49
Na	mg/L	1574	4038	14	3.0	13294	2.12	2.64
K	mg/L	65	167	0.00	0.00	528	2.10	2.51
Ca	mg/L	58	141	1.0	0.00	480	2.11	2.66
Mg	mg/L	131	337	1.5	0.00	1100	2.12	2.62
Cl	mg/L	2559	6608	18	2.0	22000	2.13	2.68
SO_4^{-2}	mg/L	415	1043	5.0	1.0	3340	2.12	2.63
HCO_3^-	mg/L	26	30	13	4.0	162	2.70	8.83
NO_3^-	mg/L	3.0	9.3	0.30	0.30	56	4.89	24.60
PO_4^{-2}	mg/L	0.17	0.29	0.00	0.00	1.2	1.80	2.63
SiO_2	mg/L	7.6	16	4.2	0.50	98	5.11	26.63
Al	µg/L	74	115	25	1.6	570	2.57	7.19
As	µg/L	0.95	1.6	0.46	0.07	8.7	3.56	13.55
Ba	µg/L	3.8	8.0	0.55	0.10	45	3.77	16.21
Cr	µg/L	0.41	1.1	0.07	0.03	5.1	3.41	10.94
Cu	µg/L	1.5	2.1	0.41	0.10	7.8	1.42	0.79
Mn	µg/L	41	159	0.78	0.25	880	4.35	18.64
Mo	µg/L	1.1	1.9	0.10	0.10	6.9	1.81	1.67
Tl	µg/L	0.24	0.40	0.10	0.03	1.3	2.07	2.39
U	µg/L	0.38	0.94	0.03	0.03	3.3	2.34	3.78
V	µg/L	11	48	2.7	0.00	301	5.65	30.91
Zn	µg/L	5.4	9.8	1.2	0.05	38	1.90	2.19

CAF: caffeine, CTPM: citalopram, CLAR: clarithromycin; HCTZ: hydrochlorothiazide, NIC: nicotine, TTA: tolytriazole, VFX: venlafaxine, EC: electrical conductivity, TOC: total organic carbon, T: temperature, TDS: total dissolved solids.



HUM: degree of human impact (from 0 to 5 according to the info provided in Table 1), BIO: degree of biological impact (from 0 to 3 according to the info provided in Table 1). CAF: caffeine, CTP: citalopram, CLA: clarithromycin, HCT: hydrochlorothiazide, NIC: nicotine, TTA: tolytriazole, VFX: venlafaxine, X.OR: sum of all organic contaminants, EC: electrical conductivity, TOC: total organic carbon, T: temperature, TDS: total dissolved solids.

Figure S1. Pairwise correlations among the investigated variables. Only statistically significant coefficients are shown. The strength of the correlation is shown by the dote size and the intensity of the font color.

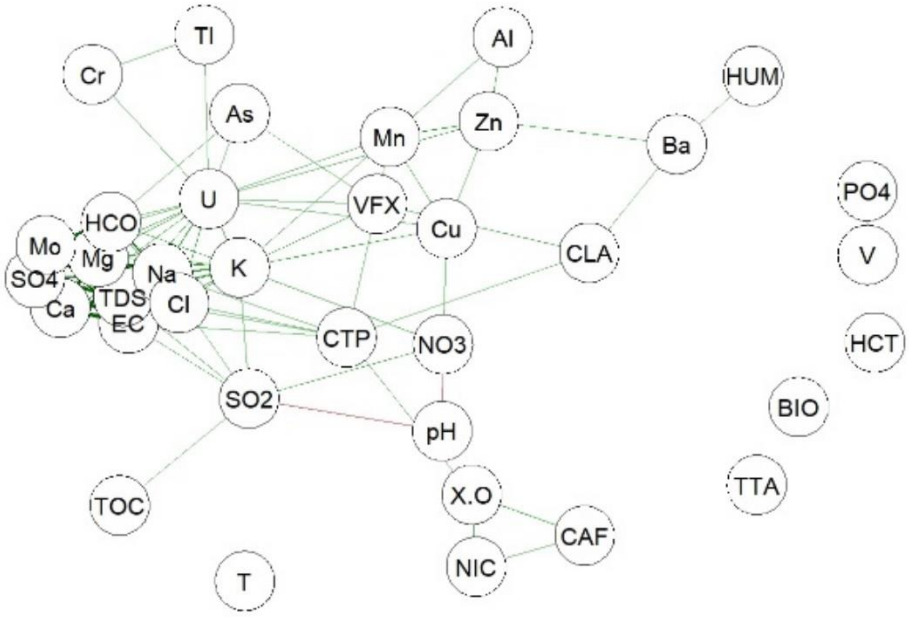


Figure S2. Network plot of the data frame correlation (threshold value of 0.5)

Table S7. Physical-chemical characteristics of the investigated waters (seawater samples are highlighted in blue color).

Sample code	Electrical conductivity (µS/cm)	Total organic carbon (mg/L)	Total dissolved solids (mg/L)	Temperature (° C)	pH	SiO_2 (mg/L)
1_D	40	<0.5	31	1.9	7.90	3.6
2_D	881	1.57	606	1.7	7.05	17.2
3_D	37	1.62	30.5	3.2	7.65	4.2
4_D	52000	1.41	37040	1.9	7.44	6.4
5_D	36	1.63	29.2	1.0	8.12	2.3
6_D	52250	1.86	37310	32.5	6.75	97.5
7_D	99	2.46	79	1.7	6.81	17.7
8_D	62	1.58	45.6	2.9	7.00	5.1
9_D	15	1.38	13.5	1.8	7.16	1.8
10_D	57100	1.65	40795	1.2	7.28	4.6
11_L	91	1.64	67.6	54.5	7.92	2.9
12_L	87	1.41	63.8	2.4	7.41	1.5
13_L	86	1.39	67	3.3	7.38	2.6
14_L	87	1.79	65.4	4.4	6.96	3.3
15_L	54600	2.63	38930	0.9	7.40	3.6
16_L	87	2.68	60.8	3.0	8.05	3.0
17_L	94	2.41	73.6	2.4	7.55	6.8
18_L	64	1.60	48.4	1.7	7.65	1.5
19_L	27	1.25	21.6	0.4	7.52	0.5
20_L	59	1.29	45.2	2.7	7.38	5.1
21_L	31	1.28	24.6	3.6	7.48	0.8
22_L	25	1.40	19.8	3.4	7.46	0.5
23_L	43	1.82	32.8	0.9	7.13	8.5
24_L	40	1.75	30.1	1.2	6.64	7.0
25_B	249	1.65	188	3.5	6.68	4.5
26_B	202	2.80	147	2.5	6.88	8.4
27_B	275	4.01	208	3.4	6.82	9.6
28_B	54000	1.74	39830	3.4	6.98	3.8
29_B	64	1.73	46.8	3.6	8.15	1.5
30_B	983	2.59	694.8	3.8	6.51	9.4
31_B	453	1.51	338.2	3.2	7.31	4.3
32_B	168	1.43	125.6	4.7	7.54	3.4
33_B	135	0.97	93.4	1.7	7.58	3.5
34_B	98	1.32	72	4.1	7.62	4.1
35_B	168	2.02	124.2	2.5	6.96	5.5
36_B	74	1.59	50	1.1	7.42	4.5
37_B	187	2.19	126.8	3.7	5.39	14.3
38_B	116	1.95	77	3.4	6.38	3.4
Min	*15*	*<0.5*	*13.5*	*0.4*	*5.39*	*0.5*
Max	*57100*	*4.01*	*40795*	*54.5*	*8.15*	*97.5*
Average	*7434*	*1.8*	*5201*	*4.8*	*7.23*	*7.7*

Table S8. Concentration (mg/L) of ions in the investigated water samples (seawater samples are highlighted in blue color).

Sample code	Na^{+}	K^{+}	Ca^{+2}	Mg^{+2}	Cl^{-}	SO_4^{-2}	HCO_3^{-}	CO_3^{-2}	NO_3^{-}	NO_2^{-}	NH_4^{+}	PO_4^{-3}	F^{-}	Cn^{-}
1_D	10	n.d.	n.d.	n.d.	9	2	7	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
2_D	227	10	11	3	292	74	35	n.d.	n.d.	n.d.	n.d.	0.27	<0.5	<0.01
3_D	7	n.d.	n.d.	1	5	2	12	n.d.	n.d.	n.d.	n.d.	0.18	<0.5	<0.01
4_D	10551	478	370	900	17100	2880	46	n.d.	2	n.d.	n.d.	0.58	0.78	<0.01
5_D	7	n.d.	n.d.	1	7	2	9	n.d.	n.d.	n.d.	n.d.	0.15	<0.5	<0.01
6_D	11309	476	410	920	18300	2790	162	n.d.	4	n.d.	n.d.	0.71	0.61	<0.01
7_D	15	2	1	1	18	2	5	n.d.	11	n.d.	n.d.	1.19	<0.5	<0.01
8_D	11	n.d.	n.d.	1	11	2	11	n.d.	1	n.d.	n.d.	0.47	<0.5	<0.01
9_D	3	n.d.	n.d.	1	3	2	4	n.d.	1	n.d.	n.d.	0.14	<0.5	<0.01
10_D	13294	528	410	1000	22000	2910	55	n.d.	1	n.d.	n.d.	0.58	0.84	<0.01
11_L	14	n.d.	1	2	21	2	12	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
12_L	14	n.d.	1	2	21	2	11	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
13_L	14	n.d.	1	2	21	2	11	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
14_L	14	n.d.	1	2	20	2	13	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
15_L	11913	471	390	1000	19200	3340	41	n.d.	2	n.d.	n.d.	0.71	0.72	<0.01
16_L	14	n.d.	2	1	21	2	8	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
17_L	12	n.d.	3	1	16	5	12	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
18_L	11	n.d.	n.d.	1	12	2	10	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
19_L	4	n.d.	n.d.	1	6	1	4	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
20_L	8	n.d.	5	n.d.	8	2	19	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
21_L	5	n.d.	n.d.	1	4	1	10	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
22_L	4	n.d.	n.d.	1	2	2	9	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
23_L	7	n.d.	n.d.	1	6	5	7	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
24_L	6	n.d.	n.d.	1	5	2	7	n.d.	2	n.d.	n.d.	n.d.	<0.5	<0.01
25_B	36	1	16	3	27	63	25	n.d.	2	n.d.	n.d.	n.d.	<0.5	<0.01
26_B	40	2	2	3	25	10	55	n.d.	15	n.d.	n.d.	n.d.	<0.5	<0.01

Table S8. (Cont.)

Sample code	Na^{+}	K^{+}	Ca^{+2}	Mg^{+2}	Cl^{-}	SO_4^{-2}	HCO_3^{-}	CO_3^{-2}	NO_3^{-}	NO_2^{-}	NH_4^{+}	PO_4^{--3}	F^{-}	Cn^{-}
27_B	52	4	4	5	29	58	47	n.d.	3	n.d.	n.d.	n.d.	<0.5	<0.01
28_B	11807	486	480	1100	19600	3320	47	n.d.	2	n.d.	n.d.	n.d.	0.83	<0.01
29_B	11	n.d.	1	1	12	9	5	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
30_B	178	9	25	15	300	5	92	n.d.	n.d.	n.d.	8.4	n.d.	<0.5	<0.01
31_B	39	n.d.	63	8	18	194	52	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
32_B	31	n.d.	1	2	22	21	29	n.d.	n.d.	n.d.	n.d.	0.18	<0.5	<0.01
33_B	26	n.d.	1	2	17	11	37	n.d.	n.d.	n.d.	n.d.	0.10	<0.5	<0.01
34_B	19	n.d.	n.d.	1	15	9	16	n.d.	n.d.	n.d.	n.d.	0.16	<0.5	<0.01
35_B	34	n.d.	n.d.	1	27	14	23	n.d.	5	n.d.	n.d.	0.72	<0.5	<0.01
36_B	15	n.d.	n.d.	1	12	2	20	n.d.	n.d.	n.d.	n.d.	0.24	<0.5	<0.01
37_B	20	2	10	5	21	6	8	n.d.	56	n.d.	n.d.	0.15	<0.5	<0.01
38_B	12	n.d.	4	3	13	14	17	n.d.	n.d.	n.d.	n.d.	n.d.	<0.5	<0.01
Freq. detection	*100*	*32*	*63*	*95*	*100*	*100*	*100*	*0*	*37*	*0*	*3*	*42*	*13*	*0*
Min	*3*	*1*	*1*	*1*	*2*	*1*	*4*	*-*	*1*	*-*	*8.4*	*0.1.0*	*0.61*	*-*
Max	*13294*	*528*	*480*	*1100*	*22000*	*3340*	*162*		*56*		*-*	*1.19*	*0.84*	
Average*	*1574*	*206*	*92*	*139*	*2559*	*415*	*26*		*8*			*0.41*	*0.75*	

n.d. not detected. The method detection limit in each case is 10 % of the parametric value established in the Spanish legislation for drinking water (Real Decreto 140/2003, de 7 de febrero, por el que se establecen los criterios sanitarios de la calidad del agua de consumo humano, Ministerio de la Presidencia «BOE» núm. 45, de 21 de febrero de 2003. Referencia: BOE-A-2003-3596).

* n.d. values were not considered to calculate average values.

Table S9. Concentration (µg/L) of metals in the investigated water samples (seawater samples are highlighted in blue color).

Sample code	Al	As	B	Ba	Be	Co	Cr	Cu	Fe	Mn	Mo	Ni	Pb	Sb	Se	Tl	U	V	Zn
1_D	11.2	0.14	< 100	< 0.2	< 0.05	< 0.05	< 0.05	< 0.2	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.12	< 0.05	7.60	1.42
2_D	15.0	8.71	175	0.37	< 0.05	< 0.05	0.06	0.33	< 15	< 0.5	6.86	< 0.5	< 0.2	0.07	0.53	< 0.05	< 0.05	301	1.69
3_D	570	0.52	< 100	0.41	< 0.05	0.31	0.30	1.37	916	11.80	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.12	< 0.05	13.80	1.97
4_D	< 50	< 2.5	< 5000	12.20	< 2.5	< 2.5	4.24	< 10	< 750	< 25	< 10	< 2.5	< 10	< 2.5	< 25	< 2.5	2.73	4.80	< 50
5_D	168	0.36	< 100	< 0.2	< 0.05	0.12	0.10	0.29	285	4.82	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.12	< 0.05	8.54	1.24
6_D	< 50	5.12	< 5000	45.20	< 2.5	< 2.5	< 2.5	< 10	< 750	880	< 10	< 2.5	< 10	< 2.5	< 25	< 2.5	< 2.5	6.21	< 50
7_D	173	0.46	< 100	< 0.2	< 0.05	1.20	< 0.05	5.20	< 15	27.80	< 0.2	0.57	< 0.2	< 0.05	0.78	0.07	< 0.05	4.47	3.92
8_D	28.0	0.19	< 100	< 0.2	< 0.05	< 0.05	0.16	0.43	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.09	< 0.05	4.27	0.96
9_D	248	0.12	< 100	0.20	< 0.05	0.21	0.15	7.81	420	6.25	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.13	< 0.05	5.10	1.87
10_D	< 50	2.45	< 5000	12.2	< 2.5	< 2.5	< 2.5	< 10	< 750	< 25	< 10	< 2.5	< 10	< 2.5	< 25	< 2.5	3.29	4.50	< 50
11_L	34.7	0.07	< 100	12.7	< 0.05	1.58	0.08	0.43	< 15	1.49	0.32	0.81	< 0.2	0.31	< 0.5	0.05	< 0.05	0.31	37.80
12_L	16.4	0.22	< 100	5.96	< 0.05	< 0.05	< 0.05	< 0.2	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	< 0.05	< 0.05	0.75	1.02
13_L	15.0	0.21	< 100	4.63	< 0.05	< 0.05	< 0.05	< 0.2	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	< 0.05	< 0.05	0.92	1.17
14_L	17.1	0.27	< 100	4.16	< 0.05	< 0.05	< 0.05	< 0.2	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	< 0.05	< 0.05	1.10	1.19
15_L	< 50	< 2.5	< 5000	11.6	< 2.5	< 2.5	< 2.5	< 10	< 750	< 25	< 10	< 2.5	< 10	< 2.5	< 25	< 2.5	3.01	2.61	< 50
16_L	14.1	0.27	< 100	4.06	< 0.05	< 0.05	0.05	< 0.2	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.09	< 0.05	1.02	1.35
17_L	47.2	0.79	< 100	2.84	< 0.05	< 0.05	< 0.05	2.84	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.06	< 0.05	2.73	1.72
18_L	225	1.45	< 100	3.74	< 0.05	0.07	0.12	0.88	84.3	3.26	< 0.2	< 0.5	0.28	0.25	< 0.5	0.08	< 0.05	1.92	2.50
19_L	325	0.45	< 100	2.17	< 0.05	0.16	0.26	0.26	156	3.94	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.10	< 0.05	1.04	1.69
20_L	15.1	1.28	< 100	0.84	< 0.05	< 0.05	< 0.05	< 0.2	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.12	< 0.05	2.85	< 1
21_L	115	0.27	< 100	0.57	< 0.05	< 0.05	0.10	0.27	66.7	1.53	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.14	< 0.05	1.08	1.21
22_L	104	0.31	< 100	0.45	< 0.05	< 0.05	0.07	0.23	55.3	1.21	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.14	< 0.05	1.10	1.14
23_L	64.1	0.10	< 100	0.31	< 0.05	< 0.05	0.08	0.68	41.9	0.99	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.13	< 0.05	3.53	1.26
24_L	12.2	0.49	< 100	1.18	< 0.05	< 0.05	< 0.05	0.63	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.13	< 0.05	5.01	< 1
25_B	14.1	0.20	< 100	0.55	< 0.05	< 0.05	< 0.05	0.38	< 15	< 0.5	0.95	< 0.5	< 0.2	< 0.05	< 0.5	0.09	< 0.05	0.72	1.04
26_B	13.6	0.30	< 100	< 0.2	< 0.05	< 0.05	< 0.05	2.69	< 15	< 0.5	0.69	< 0.5	< 0.2	< 0.05	< 0.5	0.10	< 0.05	0.88	< 1

Table S9. (Cont.)

Sample code	Al	As	B	Ba	Be	Co	Cr	Cu	Fe	Mn	Mo	Ni	Pb	Sb	Se	Tl	U	V	Zn
27_B	44.9	1.35	< 100	< 0.2	< 0.05	< 0.05	0.09	2.02	76.1	7.21	0.36	< 0.5	< 0.2	< 0.05	< 0.5	0.08	0.05	3.14	1.96
28_B	< 50	< 2.5	< 5000	11.70	< 2.5	< 2.5	5.12	< 10	< 750	< 25	< 10	< 2.5	< 10	< 2.5	< 25	< 2.5	3.03	n/a	< 50
29_B	10.1	0.07	< 100	< 0.2	< 0.05	< 0.05	0.07	0.24	< 15	< 0.5	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.10	< 0.05	0.38	< 1
30_B	8.80	0.66	< 100	1.08	< 0.05	0.40	< 0.05	0.91	20.50	472	0.44	0.59	< 0.2	< 0.05	< 0.5	< 0.05	< 0.05	0.34	< 1
31_B	40.6	0.10	< 100	1.68	< 0.05	< 0.05	< 0.05	< 0.2	< 15	0.57	1.57	< 0.5	< 0.2	< 0.05	1.17	0.11	< 0.05	0.24	1.22
32_B	18.5	1.04	< 100	< 0.2	< 0.05	< 0.05	0.06	2.06	< 15	< 0.5	0.66	< 0.5	< 0.2	< 0.05	< 0.5	0.09	< 0.05	4.40	1.09
33_B	19.3	1.49	< 100	< 0.2	< 0.05	< 0.05	0.06	< 0.2	< 15	< 0.5	0.56	< 0.5	< 0.2	< 0.05	< 0.5	0.10	< 0.05	2.73	< 1
34_B	22.0	0.65	< 100	< 0.2	< 0.05	< 0.05	0.11	< 0.2	< 15	< 0.5	0.56	< 0.5	< 0.2	< 0.05	< 0.5	0.09	< 0.05	4.28	< 1
35_B	1.62	0.81	< 100	< 0.2	< 0.05	< 0.05	< 0.05	0.44	< 15	< 0.5	0.51	< 0.5	< 0.2	< 0.05	< 0.5	0.06	< 0.05	7.24	< 1
36_B	48.5	1.17	< 100	< 0.2	< 0.05	< 0.05	< 0.05	< 0.2	49.60	1.41	0.39	< 0.5	< 0.2	< 0.05	< 0.5	0.11	< 0.05	6.39	1.01
37_B	220	0.13	< 100	0.55	0.18	0.52	< 0.05	0.38	< 15	64	< 0.2	< 0.5	< 0.2	< 0.05	< 0.5	0.08	< 0.05	0.18	8.99
38_B	5.95	0.09	< 100	< 0.2	< 0.05	< 0.05	0.18	0.26	< 15	< 0.5	0.238	0< 0.5	< 0.2	< 0.05	< 0.5	0.09	< 0.05	1.45	< 1
Freq. detect	*87*	*92*	*3*	*66*	*3*	*24*	*53*	*61*	*29*	*42*	*34*	*8*	*3*	*8*	*8*	*74*	*13*	*97*	*63*
Min	*1.62*	*0.07*	*175*	*0.2*	*0.18*	*0.07*	*0.05*	*0.23*	*20.5*	*0.57*	*0.23*	*0.57*	*0.28*	*0.07*	*0.53*	*0.05*	*0.05*	*0.18*	*0.96*
Max	*570*	*8.71*	*-*	*45.2*	*-*	*1.58*	*5.12*	*7.81*	*916*	*880*	*6.86*	*0.81*	*-*	*0.31*	*1.17*	*0.14*	*3.29*	*301*	*37.8*
Average	*81.4*	*0.92*	*-*	*5.65*	*0.18*	*0.51*	*0.57*	*1.35*	*197*	*93.0*	*1.08*	*0.66*		*0.21*	*0.83*	*0.1*	*2.42*	*11.3*	*3.35*

Ag was <0.05 in all surface water samples and <2.5 in all seawater samples
Cd was <0.2 in all surface water samples and <10 in all seawater samples
Hg was <0.5 in all surface water samples and <25 in all seawater samples
Th was <0.05 in all surface water samples and <2.5 in all seawater samples
n/a: data not available.

Table S10. Concentration (ng/L) of the target organic contaminants detected in the investigated water samples (seawater samples are highlighted in blue color; acetaminophen, bezafibrate, and ibuprofen were not detected in any sample).

Sample code	Target organic contaminants [a]									Total [b]
	BP1	CAF	CTPM	CLAR	DCF	HCTZ	NIC	TTA	VFX	
1_D	n.d.	94	2.4	n.d.	n.d.	8.1	13	<1.4	n.d.	**118**
2_D	n.d.	1.7	13	11	n.d.	n.d.	12	2.5	1. 7	**42**
3_D	n.d.	n.d.	n.d.	3.6	n.d.	5.9	n.d.	5.8	n.d.	**15**
4_D	69	4.6	27	2.0	n.d.	n.d.	12	2.7	5.7	**122**
5_D	17	n.d.	n.d.	n.d.	n.d.	n.d.	72	2.4	3.8	**95**
6_D	n.d.	32	51	4.4	n.d.	n.d.	38	4.5	8.3	**138**
7_D	n.d.	n.d.	7.8	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	**7.8**
8_D	36	n.d.	9.1	0.7	n.d.	2.5	n.d.	<1.4	n.d.	**49**
9_D	n.d.	n.d.	n.d.	n.d.	n.d.	<0.8	n.d.	7.1	n.d.	**7.1**
10_D	95	14	12	2.0	n.d.	n.d.	9.3	2.1	4.1	**138**
11_L	n.d.	28	5.0	n.d.	n.d.	2.4	n.d.	6.4	n.d.	**42**
12_L	n.d.	n.d.	<4.4	2.9	n.d.	n.d.	4.4	<1.4	n.d.	**7.3**
13_L	n.d.	n.d.	<4.4	3.4	n.d.	n.d.	13	<1.4	n.d.	**16**
14_L	n.d.	7.3	<4.4	n.d.	n.d.	2.4	7.8	2.2	n.d.	**20**
15_L	43	26	17	2.5	n.d.	1.8	12	2.3	6.0	**110**
16_L	n.d.	n.d.	5.2	n.d.	n.d.	n.d.	8.5	2.1	n.d.	**16**
17_L	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	6.0	n.d.	**6.0**
18_L	n.d.	n.d.	14	n.d.	n.d.	<0.8	4.2	1.9	n.d.	**20**
19_L	n.d.	n.d.	<4.4	4.9	n.d.	n.d.	8.8	<1.4	<0.5	**14**
20_L	n.d.	2.6	<4.4	n.d.	n.d.	n.d.	6.0	<1.4	0.5	**9.1**
21_L	n.d.	6.1	n.d.	2.3	n.d.	n.d.	6.9	2.2	1.0	**19**
22_L	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	2.0	n.d.	**2.0**
23_L	n.d.	66	n.d.	n.d.	7.1	10	146	5.6	n.d.	**235**
24_L	n.d.	24	n.d.	0.7	n.d.	3.1	31	n.d.	n.d.	**58**
25_B	n.d.	1.8	n.d.	n.d.	n.d.	6.0	8.9	<1.4	n.d.	**17**
26_B	n.d.	n.d.	n.d.	n.d.	n.d.	4.0	n.d.	2.0	n.d.	**6.0**
27_B	n.d.	n.d.	n.d.	n.d.	n.d.	2.8	n.d.	11	n.d.	**14**
28_B	78	7.6	30	3.0	n.d.	n.d.	10	4.6	6.4	**140**
29_B	21	n.d.	n.d.	n.d.	n.d.	n.d.	7.1	2.3	n.d.	**30**
30_B	69	61	292	173	n.d.	1.2	32	20	35	**682**
31_B	n.d.	8.7	80	47	n.d.	n.d.	13	2.8	n.d.	**151**
32_B	57	n.d.	n.d.	n.d.	n.d.	n.d.	9.3	3.3	n.d.	**69**
33_B	21	n.d.	9.9	n.d.	n.d.	1.3	5.7	2.0	<0.5	**40**
34_B	n.d.	n.d.	n.d.	n.d.	n.d.	1.3	13	1.8	n.d.	**16**
35_B	n.d.	n.d.	14	n.d.	n.d.	4.3	13.	n.d.	n.d.	**32**
36_B	n.d.	n.d.	n.d.	n.d.	n.d.	3.0	4.0	3.0	n.d.	**11**
37_B	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	**0**
38_B	n.d.	40	n.d.	n.d.	n.d.	7.4	58	2.2	n.d.	**108**

[a] BP1: benzophenone-1, CAF: caffeine, CTPM: citalopram, CLAR: clarithromycin; DCF: diclofenac, HCTZ: hydrochlorothiazide, NIC: nicotine, TTA: tolytriazole, VFX: venlafaxine

n.d. not detected

[b] Total sum of contaminants in each sample was calculated considering n.d and <LOQ as 0, as suggested by Commission Directive 2009/90/EC of 31 July 2009 Laying Down, Pursuant to Directive 2000/60/EC of the European Parliament and of the Council, Technical Specifications for Chemical Analysis and Monitoring of Water Status. Retrieved from https://bit.ly/2YmkYhb. Accessed in July 2022.

Text S3. Statistical analysis – principal component analysis.

Principal-component analysis (PCA) was used to extract useful information from the data, e.g., to identify potential CEC contamination patterns. Therefore, the variables used in the PCA included only individual CEC concentrations and total CEC concentrations (X.ORG). After PCA, these variables (loadings) were reduced to several uncorrelated orthogonal variables or principal components (PCs), which identify the main sources of variance in the chemical composition of water. The samples (scores) are represented along the PCs, to identify the main samples contributing to the main sources of variance, and thereby, uncover potential spatial contamination patterns of organic CECs. Since the variances of the variables under consideration presented large differences among them, data within each variable were autoscaled or standardized by mean centering and division by the standard deviation: $y= (x - \mu) / \sigma$, where y is the autoscaled data, x is the data itself, μ is the variable mean, and σ is the variable standard deviation. This process contributes to reducing potential collinearity problems.

A large proportion of the variance of the organic pollution data (70 %) was explained by four PCs (Table S11). The loadings plots along the four first PCs are shown in the main manuscript in Figure 4. The score plots along the four first PCs are provided in Figure S3. Biplots including loadings and scores were also created, to identify the distribution of the contamination patterns described by the different PCs (Figure S4).

Table S11. Proportion of the data variance explained by each principal component (only the concentrations of organic chemicals were considered as variables).

	PC1	**PC2**	**PC3**	**PC4**	**PC5**	**PC6**	**PC7**	**PC8**
Std dev	2.17	1.41	0.73	0.64	0.48	0.30	0.15	0.11
Proportion of variance	59.0	24.7	6.6	5.1	2.9	1.1	0.3	0.1
Cumulative proportion	**59.0**	**83.7**	**90.3**	**95.5**	98.4	99.6	99.9	1.00

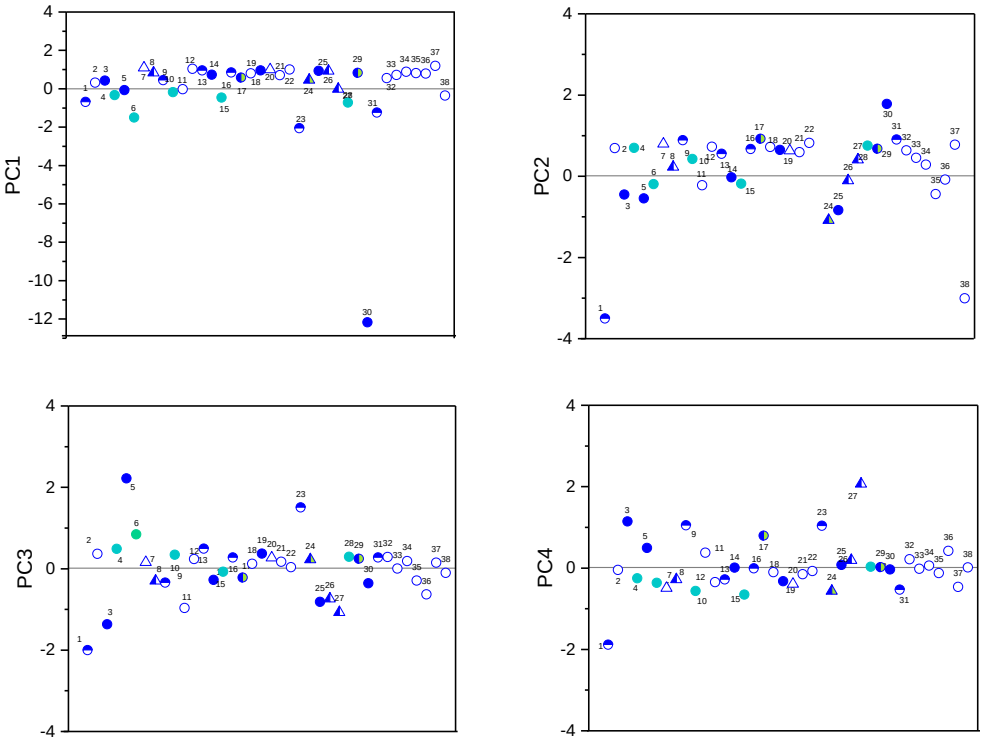


Figure S3. Score plots along the four first principal components (only the concentrations of organic chemicals were considered as variables).

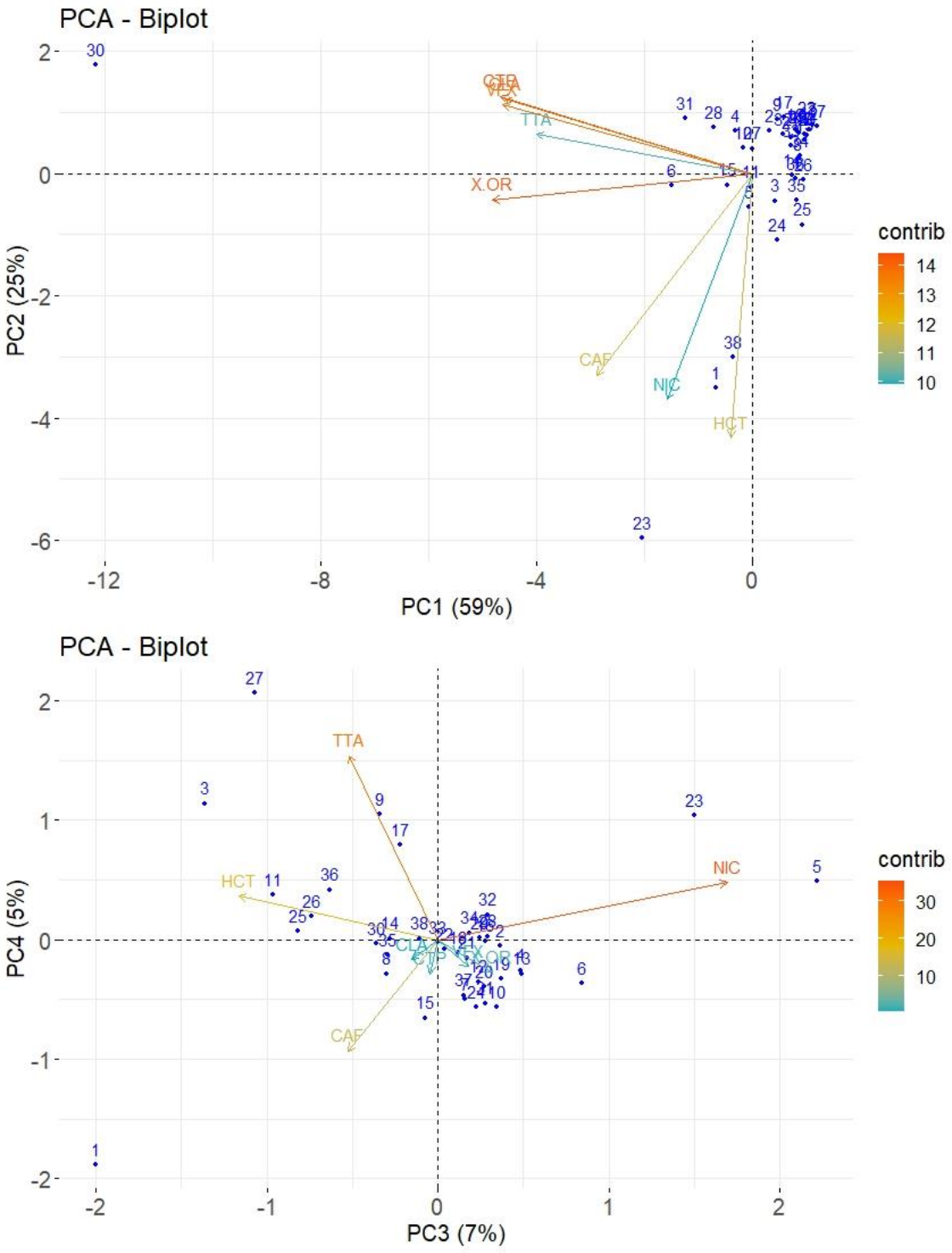
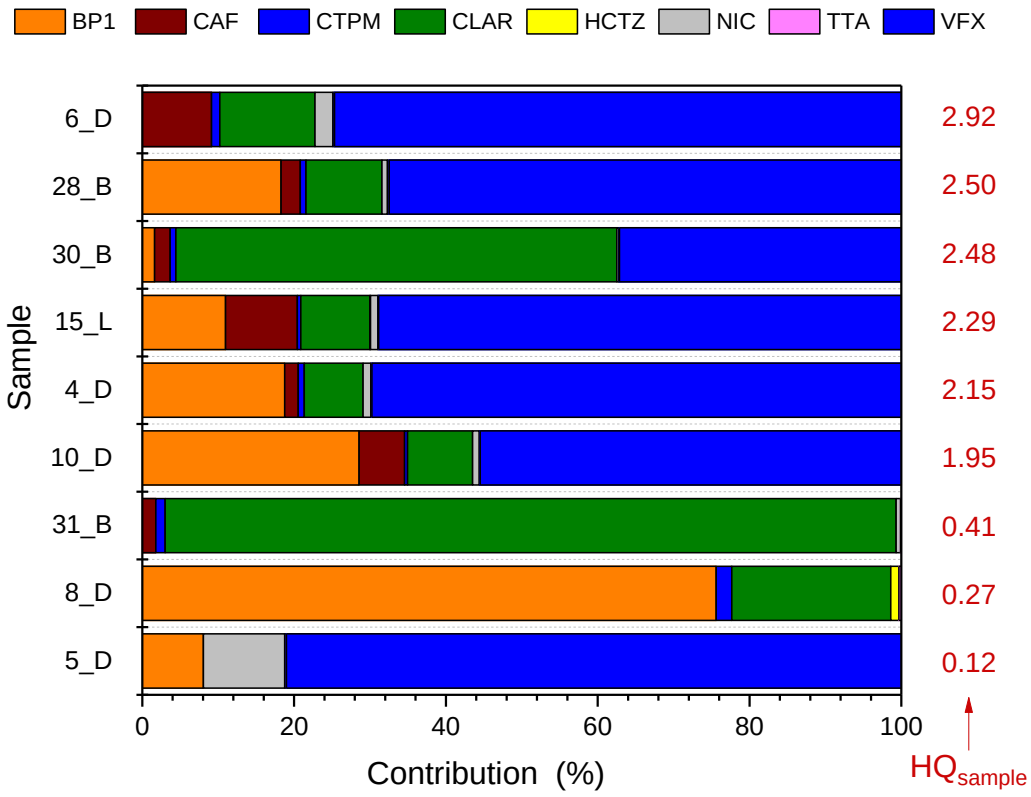


Figure S4. PCA biplots of the investigated samples along (a) PC1 and PC2, (b) PC3 and PC4 (only the concentrations of organic chemicals were considered as variables).



Abbreviations: BP1: benzophenone-1, CAF: caffeine, CTPM: citalopram, CLAR: clarithromycin, HCTZ: hydrochlorothiazide, NIC: nicotine, TTA: tolytriazole, VFX: venlafaxine.

Figure S5. Contribution of the target CECs to the HQ_{sample} values that indicate a low and moderate ecotoxicity risk to exposed aquatic organisms.