Supplementary Materials

A Snapshot on the Occurrence and Risk Assessment of Organic Pollutants in an Urban River

Moisés Canle [1,*] and Ana M. Antão-Geraldes [2,3,*]

[1] React! Department of Chemistry, Faculty of Sciences & CICA, University of A Coruña, E-15071 A Coruña, Spain
[2] Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal
[3] Laboratório Associado para a Sustentabilidade e Tecnologia em Regiões de Montanha (SusTEC), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal
* Correspondence: moises.canle@udc.es (M.C.); geraldes@ipb.pt (A.M.A.-G.)

Table S1. CECs concentrations reported in surface waters and sediments in different European countries.

	River (Country)	Water Concentration ($ng\ L^{-1}$)	Sediment Concentration ($ng\ g^{-1}$)	References
Paracetamol/Acetaminophen	**Fervença River (Portugal)**	**0.05**	**0.05 ($ng\ L^{-1}$)**	**Present study**
	Hogsmill ,Chertsey, Blackwater Rivers (UK)	< 0.93 – 415	< 0.93 – 1.11	[117]
	Thames River (UK)	8.2-12,000		[118]
	Kalamas River, Lake Pamvotis (Greece)	n.d. – 156		[119]
	Lis River (Portugal)	n.d. – 527		[38]
	Dee River (Scotland)	n.d.-658		[120]
	Leitzaran, Mustarre and Oria Rivers (Spain)	n.d.-6.1		[121]
	Guadalhorce River (Spain)	79-200		[122]
	Llobregat Basin (Spain)	0.60-2,420		[123]
	Valencia Mediterranean rivers (Spain)	1,968 (max detected)		[124]
	Llobregat River Basin (Spain)	4.4 – 1060		[125]
	Mijares River (Spain)	n.d.-197		[126]
	Lakes Vänern Vättern Mälaren/associated rivers (Sweden)	34 (max)		[127]
Ibuprofen	**Fervença River (Portugal)**	**0.05-21.91**	**0.05-18.80 ($ng\ L^{-1}$)**	**Present study**
	Elbe basin (Czech Republic)	7.33-3,210.25		[128]
	Thames River (UK)	30-450		[118]
	Lake Päijänne, River Vantaa (Finland)	2.8-187		[129]
	Kalamas River, Lake Pamvotis (Greece)	n.d. – 1,351		[119]
	Lakes Vänern Vättern Mälaren / associated rivers (Sweden)	< 3.1		[127]
	Douro River (Portugal)	n.d.- 232 ± 7		[37]
	Minho River (Portugal)	204 ± 10		[37]
	Ave River (Portugal)	n.d.- 343 ± 19		[37]
	Lima River (Portugal)	40 ± 2-723 ± 6		[37]
	Leça River(Portugal)	n.d. 256 ± 9		[37]

	Rabaçal River (Portugal, Douro tributary)	n.d.		[37]
	Tinhela River (Portugal)	n.d.		[37]
	Tâmega River (Portugal)	81 ± 6- 359 ± 12		[37]
	Uíma River (Portugal)	nd-173 ± 3		[37]
	Cabrum River (Portugal)	nd		[37]
	Lis River (Portugal)	n.d. – 1317		[38]
	Dee River (Scotland)	0.1-17.2		[120]
	Danube Basin (Serbia)	n.d. -163		[18]
	Danube River (Serbia)	n.d-60.1		[130]
	Danube River (Serbia)	<LOQ—346		[95]
	Llobregat Basin (Spain)	160-9,890		[123]
	Valencia Mediterranean rivers (Spain)	2,850 (max detected)		[124]
	Llobregat River Basin (Spain)	29.4-490.4		[131]
	Llobregat River Basin (Spain)	2.7 – 868		[125]
Diclofenac	**Fervença River (Portugal)**	**0.05-398.35**	**0.05-92.93 (ng L^{-1})**	**Present study**
	Elbe basin (Czech Republic)	1.46-1,070.28		[128]
	Hogsmill, Chertsey, Blackwater Rivers (UK)	< 0.96 – 253	< 0.96 – 6.4	[117]
	Thames River (UK)	5.9-380		[118]
	Lake Päijänne, River Vantaa (Filand)	n.d.-227		[129]
	Several streams (Germany)	<5-370		[132]
	Kalamas River, Lake Pamvotis (Greece)	n.d. – 457		[119]
	Several urban streams (Hungry)	0.66-2,070.76	1.43-47.31	[78]
	Lis River (Portugal)	n.d. – 38		[38]
	Sousa River (Portugal)	3,200		[98]
	Ave River (Portugal)	388		[98]
	Danube river (Romenia)	n.d.-166		[133]
	Prut River (Romenia)	2-9		[134]
	Dee River (Scotland)	0.2-29.1		[120]
	Sava River (Slovenia and Croatia)	62		[135]
	Llobregat River Basin (Spain)	0.4 – 786		[125]
	Miño River basin (Spain)	2.8 – 46.0		[136]

	Mijares River (Spain)	n.d.-578		[126]
	Guadalhorce river, Spain	1-83		[122]
	Llobregat Basin (Spain)	0.08-18.78 (ug)		[123]
	Valencia Mediterranean rivers (Spain)	358 (max detected)		[124]
	Llobregat River Basin (Spain)	17.6-358.1		[131]
	Danube river (Serbia)	<LOQ—324		[95]
	Turia River Basin		100	[137]
	Lakes Vänern Vättern Mälaren and associated rivers (Sweden)	200 (max detected)		[127]
Clorofibric acid	**Fervença River (Portugal)**	**0.05**	**0.05-21.47 (ng L^{-1})**	**Present study**
	Danube river (Romenia)	n.d.-4.3		[133]
	Llobregat Basin (spain)	10-7,910		[123]
	Llobregat River Basin (Spain)	21-133		[131]
	Lake Mälaren (Sweden)	<2-3.6	n.d	[139]
Carbamazepine	**Fervença River (Portugal)**	**0.05-52.10**	**0.05-47.10 (ng L^{-1})**	**Present study**
	Lake Päijänne, River Vantaa (Filand)	0.4-65		[129]
	Henares-Jarama-Tajo basin (Madrid, Spain)	n.d-104		[139]
	Danube River (Serbia)	n.d.-130		[140]
	Sava River (Serbia)	29-50		[140]
	Tamis River (Serbia)	30		[140]
	River Foss (UK)	n.d.-195		[141]
	River Ouse (UK)	1-54.4		[141]
	Tâmega River (Portugal)	n.d.		[41]
	Tua River (Portugal)	n.d.		[41]
	Mondego River (Portugal)	n.d.		[41]
	Trancão River (Portugal)	n.d.-<10.90		[41]
	Tagus River (Portugal)	n.d.		[41]
	Xarrama River Portugal)	n.d.		[41]
	Guadiana River (Portugal)	n.d.		[41]
	Ave River (Portugal)	n.d.-24.50		[36]

	Leça River (Portugal)	n.d.-98.59		[36]
	Antuã River (Portugal)	3.43-81.13		[36]
	Cértima River (Portugal)	3.96-177.01		[36]
	Arade River (Portugal)	13-31		[142]
	Lis River (Portugal)	24.9-214		[38]
	Lake Mälaren (Sweden)	2.1-2.9	0.14-0.21	[138]
	Prut River (Romenia)	29-72		[134]
	Several streams (Germany)	<5-68		[132]
	Danube river (Romenia)	n.d.-40		[133]
	Several urban streams (Hungry)	0.34-58,889.6	0.11-395.92	[78]
	Llobregat River Basin (Spain)	1.2 – 266.7		[125]
	Rur River Basin (Germany)	n.d. -400		[143]
	Thames River (England)	5.9-350		[118]
	Dee River (Scotland)	0.1-7		[120]
	Guadalhorce river (Spain)	0.2-185		[122]
	Donets River Basin (Ukreine)	n.d-65.7		[144]
	Danube River (Serbia)	2.56-22.9		[130]
	Lakes Vänern Vättern Mälaren /associated rivers (Sweden)	21 (max detected)		[127]
	Danube basin (Serbia)	94 -473		[18]
	Llobregat Basin (Spain)	80-3,090		[123]
	Douro River (Portugal)	<MDL-n.d.	n.d	[46]
	Leça River (Portugal)	206-354	<MDL	[44]
Ofloxacin	**Fervença River (Portugal)**	**0.05-376.16**	**0.05 (ng L^{-1})**	**Present study**
	Olona (Italy)	n.d. -1.90		[145]
	Lambro (Italy)	19.31-306.10		[145]
	Po (Italy)	n.d.-36.91		[145]
	Lambro river, Italy	306		[146]
	Ave River (Portugal)	n.d.		[36]
	Leça River (Portugal)	n.d.		[36]
	Antuã River (Portugal)	n.d.		[36]

	Cértima River (l Portugal)	n.d.		[36]
	Llobregat River Basin (Spain)	n.d. – 488.4		[125]
	Guadalhorce river, Spain	84		[122]
	Llobregat Basin (spain)	190-887		[123]
	Valencia Mediterranean rivers (spain)	2,850 (max detected)		[124]
	Llobregat River Basin (Spain)	8.0-1,903.6		[131]
	Guadalhorce river, Spain	6-89		[122]
	River Leça (Portugal)	n.d.-120	n.d.	[46]
	River Douro (Portugal)	n.d.	n.d.	[44]
Caffeine	**Fervença River (Portugal)**	**3.17-167.38**	**14.43-92.60 (ng L^{-1})**	**Present study**
	Lake Mälaren (Sweden)	8.7-12	1.1-1.8	[138]
	Kalamas River, Lake Pamvotis (Greece)	125 – 3506		[119]
	Guadalquivir River (Spain)	91.9 (mean)		[147]
	Rur River basin (Germany)	n.d. -170		[146]
	Prut River (Romenia)	26-46		[134]
	Several urban streams (Hungry)	11.36-221,385	15.76-153.61	[78]
	Rivers Leitzaran, Mustarre and Oria (Spain)	n.d.-12		[121]
	Guadalhorce river, Spain	3-568		[122]
	Danube River (Serbia)	1.11-621		[130]
	Lakes Vänern Vättern Mälaren and associated rivers (Sweden)	880 (max)		[127]
	Danube basin (Serbia)	131- 5,540		[30]
	River Liz (Portugal)	25.3-321		[43]
	Danube Basin (Romania)	4,820 (mean value)		[149]
Galaxolide	**Fervença River (Portugal)**	**0.05-224.36**	**0.05 (ng L^{-1})**	**Present study**
	Rur River basin (Germany)	n.d.-170		[143]
	Prut River (Romenia)	59-280		[134]
	Guadalhorce River (Spain)	890-26990		[122]
	Ave River(Portugal)	n.d- 61.6		[45]
	Leça River(Portugal)	8.4-379.2-		[45]
	Antuã River(Portugal)	7.0-121		[45]

	Molgora River (Italy)	up to 1,141	3.5E^{-04} –7,993*	[149]
Tonalide	**Fervença River (Portugal)**	**0.05-231.5**	**0.05 (ng L^{-1})**	**Present study**
	Rur River basin (Germany)	n.d. -30		[143]
	Prut River (Romenia)	10-38		[134]
	Guadalhorce river, Spain	266-1,408		[122]
	Ave River(Portugal)	n.d- 7.3		[45]
	Leça River(Portugal)	2.2-60.6		[45]
	Antuã River(Portugal)	2.7-22.2		[45]
	Molgora River (Italy)	up to 365	< 3.5E^{-04}–4,321*	[149]
Bisphenol A	**Fervença River (Portugal)**	**90.95-212.18**	**134.94-772.85 (ng L^{-1})**	**Present study**
	Ebre river (Spain)	61-101	0.24-117	[150]
	Hogsmill, Chertsey, Blackwater Rivers (UK)	< 3.87 – 1,420	< 3.87 – 67.1	[117]
	Ave river (Portugal)	7.9 – 521.8		[44]
	Svitava / Svratka Rivers (Czech Republic)	0.7-38.7	45.6-62.3	[151]
	Besos basin (Spain)	n.d. -587		[152]
	Seine River basin (France)	7.2-127		[153]
	Study of 124 water courses/18 lakes (France)		8.5-226	[154]
	Aisonas River (Greece)	55-162		[155]
	Turia River Basin (Spain)	4-325		[137]
	Danube basin (Serbia)	28- 407		[18]
	Danube (Serbia)	<LOD-105.7		[77]

* Suspended sediments.

Table S2. PAHs' and PCBs' concentrations reported in sediments in different European countries.

	River (Country)	Σ	Concentration (ng g^{-1} dw)	Reference
PAHs	**Fervença River (Portugal)**	**16**	**10.39-52.91**	**Present study**
	Bardello River (Italy)	18	478.5 ± 319.1	[156]
	Boesio River (Italy)	18	1296.1 ± 2791.4	[156]
	Margorabia River (Italy)	18	422.7 ± 348.6	[156]
	Toce River (Italy)	18	145.7 ± 77.1	[156]
	Tresa River (Italy)	18	4651.2 ± 22,198.3	[156]
	Huveaune River (France)	16	572 - 4235	[64]
	Someşu Mic River (Romania)	16	24.8 - 575.6	[157]
	Durance River(France)	16	57–1528	[65]
	Scheldt Basin (Belgium/ France)	16	9.01 ± 6.69 (mg/kg)	[158]
	Upper Danube basin (Hungry)		8.3 to 1,202.5	[159]
	Donets River Basin (Ukraine)		55.8-367.2	[144]
	Eure River (France)	16	2.27-38.20 (mg/kg)	[160]
	Rhine River (Germany)	16	393-24,434	[162]
	Danube River (Hungry)	17	8.3–1,202.5	[163]
	Danube River (Serbia)	16	29.7–1,047	[30]
PCBs	**Fervença River (Portugal)**	**18**	**5.06-6.76 (total)** **2.21-4.22 (IPCBs)**	**Present study**
	Bardello River (Italy)	14	16.9 ± 18.3	[156]
	Boesio River (Italy)	14	15.2 ± 14.7	[156]
	Margorabia River (Italy)	14	7.1 ± 6.4	[156]
	Toce River (Italy)	14	5.5 ± 7.1	[156]
	Tresa River (Italy)	14	7.7 ± 5.3	[156]
	Huveaune River (France)	7	2.8 - 435	[64]
	Someşu Mic (Romania)	20	2.7 - 252.7	[157]
	Durance River(France)	7	0.03 - 13.13	[65]

Scheldt Basin (Belgium/ France)	28*	0.23–7.34	[158]
Donets River Basin (Ukraine)	7	2 - 15	[144]
Neva River (Russia)	DL PCB	159-24,660 (pg g-1)	[161]
Rhine River (Germany)	(28,53,101,128,153 e 180)	11,8-580	[162]
Danube River (Hungry)	(28,53,101,128,153 e 180	90 and 953	[163]
Danube River (Serbia)	47	0.928 -32.1	[30]
Eure River (France)	-	0.02 - 1.57 (mg kg−1)	[161]
Tiber River (Italy)	32	62.04-79.30	[164]
Loreto River (Mondego Basin-Portugal)	10	0.47–5.3	[51]

* only PCB 153 was detected.

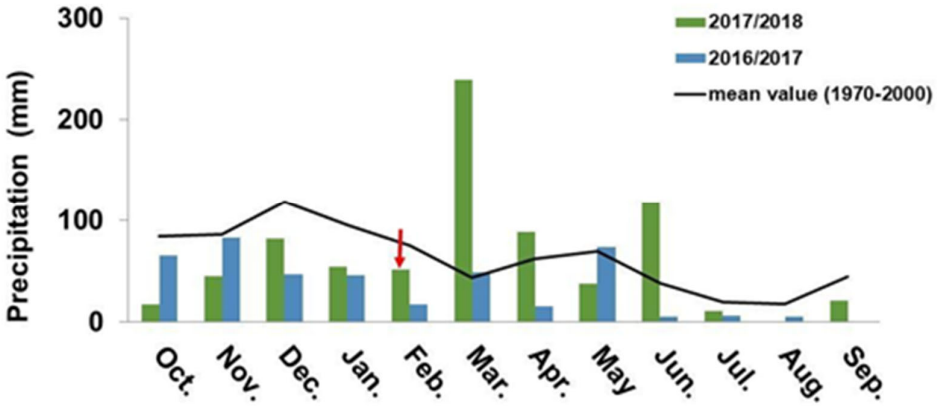

Figure S1. Precipitation during the hydrological years 2016/2017 and 2017/2018 in Bragança. The arrow indicates the month of sampling (February 2018). Source: [165].

Table S3. Toxicological data ng L^{-1} in literature and values of Predicted non Observed Effect Concentrations (PNEC) for the selected CECs dissolved in freshwater.

	Selected organism	Endpoint	Effect Measured	Concentration ng·l^{-1}	Af	Lowest PNEC ng·l^{-1}	References
Paracetamol	Crustacea (*D. magna*)	Immobility	EC50 (a 48 h)	30,100	1000	30	[5,166]
Ibuprofen	Fish (*O. latipes*)	Survival	NOEC (c120 d)	100	10	10	[13,167]
Diclofenac	Fish (*S. trutta*)	monocyte infiltration/accumulation in liver	NOEC (c21 d)	500	10	50	[5,12,83]
Clofibric Acid	Fish (*G. holbrooki*)	Enzymatic activity	NOEC (c28 d)	75,000	10	7,500	[168,169]
Carbamazepine	Crustacea (*C. dubia*)	Reproduction	NOEC (c7 d)	25,000	10	2,500	[170]
Ofloxacin	Algae -	-	NOEC (c-)	1,300	10	130	[5,13]
Caffeine	Annelida *(D. neapolitana)*	Body regeneration	NOEC (c28 d)	500	10	50	[9,15,171]
Galaxolide	Crustacea (*A. tonsa)*	Growth	NOEC (c 5 d)	44,000	10	4,400	[172]
Tonalide	Fish *(P. promelas*)	Survival	NOEC (c36 d)	35,000	10	3,500	[173]
Bisphenol A	Insecta larvae) (*C. riparious*)	Deformities in mouth parts	NOEC (c-)	100	10	10	[8]

a: acute exposure; c: chronic exposure; AF: assessment factor (more information in Methodology); EC50 Half maximal effective concentration; NOEC: No Observed Effect Concentration. PNEC sediment was derived from Lowest PNEC freshwater x2.6 (0.651+ 0.019Koc) according to [33]; Koc values are presented in Table S6. .

Table S4. PAHs' PNEC freshwater, K_{oc} values and PNEC sediment.

	CAS Number	PNEC Water $\mu g \cdot L^{-1}$	K_{oc}	PNEC Sediment $\mu g \cdot kg^{-1}$	PNEC Sediment $\mu g \cdot g^{-1}$	PNEC Sediment $ng \cdot g^{-1}$
Naphtalene	91-20-3	2.00	$2.00 \cdot 10^3$	88.37	0.088	88
Acenaphthylene	208-96-8	0.13	$4.12 \cdot 10^3$	11.72	0.011	11
Acenaphthene	83-32-9	0.38	$7.08 \cdot 10^3$	58.68	0.059	59
Fluorene	86-73-7	0.25	$1.38 \cdot 10^4$	75.06	0.075	75
Phenanthrene	85-01-8	1.30	$1.47 \cdot 10^4$	415.70	0.416	416
Anthracene	120-12-7	0.10	$2.95 \cdot 10^4$	64.09	0.064	64
Fluoranthene	206-44-0	$6.30 \cdot 10^{-3}$	$1.07 \cdot 10^5$	14.63	0.015	15
Pyrene	129-00-0	0.02	$1.05 \cdot 10^5$	52.42	0.052	52
Benz(a)anthracene	56-55-3	$1.20 \cdot 10^{-3}$	$3.98 \cdot 10^5$	10.36	0.010	10
Chrysene	218-01-9	0.01	$3.98 \cdot 10^5$	60.40	0.060	60
Benzo(b+j)fluoranthene	-	-	-	-	-	-
Benzo(k)fluoranthene	207-08-9	$1.70 \cdot 10^{-4}$	$1.23 \cdot 10^6$	4.54	0.005	5
Benzo(a)pyrene	50-32-8	$1.70 \cdot 10^{-4}$	$1.02 \cdot 10^6$	3.76	0.004	4
Dibenz(a.h)anthracene	53-70-3	$1.40 \cdot 10^{-4}$	$3.80 \cdot 10^6$	11.54	0.012	12
Benzo(ghi)perylene	191-24-2	$1.70 \cdot 10^{-4}$	$9.01 \cdot 10^5$	3.32	0.003	3
Indeno(1.2.3-cd) pyrene	193-39-5	$1.70 \cdot 10^{-4}$	$3.47 \cdot 10^6$	12.80	0.013	13

Sources: PNEC freshwater water values: [174]; K_{oc} values: [175]; PNEC sediment was derived according to the methodology proposed by [61]. .

Table S5. PNEC freshwater, K_{oc} values used to derived PNEC sediment of PCBs and TEF values.

	PNEC Water $\mu g \cdot L^{-1}$	**K_{oc}**	**PNEC Sediments** $ng \cdot g^{-1}$	**TEF**
Indicator PCBs				
PCB28	$3.19 \cdot 10^{-5}$	$2.71 \cdot 10^{4}$	0.086	-
PCB52	$3.49 \cdot 10^{-5}$	$4.48 \cdot 10^{4}$	0.015	-
PCB101	$2.76 \cdot 10^{-5}$	$2.71 \cdot 10^{4}$	0.086	-
PCB138	$2.47 \cdot 10^{-5}$	$1.25 \cdot 10^{5}$	0.031	-
PCB153	$2.21 \cdot 10^{-5}$	$1.23 \cdot 10^{5}$	0.027	-
PCB180	$1.63 \cdot 10^{-5}$	$2.07 \cdot 10^{5}$	0.034	-
Dioxin like PCBs				
PCB81	-	-	-	$5 \cdot 10^{-4}$
PCB77	$1.89 \cdot 10^{-6}$	$4.48 \cdot 10^{4}$	0.008	$1 \cdot 10^{-4}$
PCB123	-	-	-	$3 \cdot 10^{-5}$
PCB118	-	-	-	$3 \cdot 10^{-5}$
PCB114	-	-	-	$3 \cdot 10^{-5}$
PCB105	$3.19 \cdot 10^{-5}$	$2.71 \cdot 10^{4}$	0.086	$3 \cdot 10^{-5}$
PCB126	$3.49 \cdot 10^{-5}$	$4.48 \cdot 10^{4}$	0.016	$5 \cdot 10^{-3}$
PCB167	$2.76 \cdot 10^{-5}$	$2.71 \cdot 10^{4}$	0.086	$3 \cdot 10^{-5}$
PCB156	$2.47 \cdot 10^{-5}$	$1.25 \cdot 10^{5}$	0.031	$3 \cdot 10^{-5}$
PCB157	$2.21 \cdot 10^{-5}$	$1.23 \cdot 10^{5}$	0.027	$3 \cdot 10^{-5}$
PCB169	$1.63 \cdot 10^{-5}$	$2.07 \cdot 10^{5}$	0.034	$3 \cdot 10^{-2}$
PCB189	-	-	-	$3 \cdot 10^{-5}$

Sources: PNEC water and PNEC sediment [68]; TEF [71].

Table S6. CAS number and main physical-chemical properties of CECs analyzed, in the present study water and in lixiviates from sediment.

	CAS Number	Molecular Weight $g \cdot mol^{-1}$	log K_{ow}	Henry's Law Const. $atm\text{-}m^3 \cdot mol^{-1}$, 25 ºC	Vapor Pressure mm Hg, 25ºC	Water Solubility $mg \cdot L^{-1}$, 25ºC	pK_a	K_{oc}
ANALGESICS / ANTI-INFLAMMATORIES								
Paracetamol	103-90-2	151.17	0.46	$6.42 \cdot 10^{-13}$	$7.00 \cdot 10^{-6}$	1.40×10^4	9.38	21
Ibuprofen	15687-27-1	206.29	3.97	$1.50 \cdot 10^{-7}$	$1.86 \cdot 10^{-4}$	21	4.91	$3.40 \cdot 10^3$
Diclofenac	15307-86-5	296.15	4.51	$4.73 \cdot 10^{-12}$	$6.14 \cdot 10^{-8}$	2.37	4.15	245
LIPID REGULADOR								
Clofibric Acid	882-09-7	214.64	2.57	$2.19 \cdot 10^{-8}$	$1.13 \cdot 10^{-4}$	583	3.18	-
PSYCHIATRIC DRUGS								
Carbamazepine	298-46-4	236.27	2.45	$1.08 \cdot 10^{-10}$	$1.84 \cdot 10^{-7}$	17.7	13.9	510
ANTIBIOTICS								
Ofloxacin	82419-36-1	361.37	-0.39	$4.98 \cdot 10^{-20}$	$1.55 \cdot 10^{-13}$	$2.83 \cdot 10^4$	5.97	$4.41 \cdot 10^4$
STIMULANT ALKALOID								
Caffeine	58-08-2	194.19	-0.07	$1.90 \cdot 10^{-19}$	15 (89ºC)	$2.16 \cdot 10^4$	10.4	71
MUSK FRAGRANCES								
Galaxolide (HHCB)	1222-05-5	258.40	5.9	$1.06 \cdot 10^{-4}$	$5.45 \cdot 10^{-4}$	1.75	-	$1.90 \cdot 10^4$
Tonalide (AHTN)	1506-02-1	248.40	5.7	$1.40 \cdot 10^{-4}$	$5.10 \cdot 10^{-4}$	1.25	-	$2.00 \cdot 10^4$
PLASTICIZER								
Bisphenol A	80-05-7	228.29	3.32	$1.0 \cdot 10^{-11}$	$3.91 \cdot 10^{-7}$	120	9. 6	251-3886

Sources: [176].

Table S7. CAS number and main physical-chemical properties of the PAHs analyzed in the sediments of the sampling sites.

	CAS Number	Molecular Weight g·mol^{-1}	Log Kow	Henry's Law Constant atm-m^3·mol^{-1}, 25 ºC	Vapour Pressure mm Hg, 25ºC	Water Solubility mg·L^{-1}, 25ºC
Naphtalene	91-20-3	128.17	3.30	$4.40 \cdot 10^{-4}$	$8.5 \cdot 10^{-2}$	31
Acenaphthylene	208-96-8	152.20	3.94	$1.14 \cdot 10^{-4}$	$6.68 \cdot 10^{-3}$	16.1
Acenaphthene	83-32-9	154.21	3.92	$1.84 \cdot 10^{-4}$	$2.15 \cdot 10^{-3}$	3.9
Fluorene	86-73-7	166.22	4.18	$9.62 \cdot 10^{-5}$	$6.00 \cdot 10^{-4}$	1.69
Phenanthrene	85-01-8	178.23	4.46	$4.23 \cdot 10^{-5}$	$1.21 \cdot 10^{-4}$	1.15
Anthracene	120-12-7	178.23	4.45	$5.56 \cdot 10^{-5}$	-	$4{,}34 \cdot 10^{-2}$ (23ºC)
Fluoranthene	206-44-0	202.26	5.16	$8.86 \cdot 10^{-6}$	$9.22 \cdot 10^{-6}$	0.26
Pyrene	129-00-0	202.26	4.88	$1.19 \cdot 10^{-5}$	$1.19 \cdot 10^{-5}$	0.14
Benz(a)anthracene	56-55-3	228.29	5.76	$1.20 \cdot 10^{-5}$	$2.10 \cdot 10^{-7}$	$9.40 \cdot 10^{-3}$
Chrysene	218-01-9	228.29	5.81	$5.23 \cdot 10^{-6}$	$6.23 \cdot 10^{-9}$	$2.00 \cdot 10^{-3}$
Benzo(b+j)fluoranthene	-	-	-	-	-	-
Benzo(k)fluoranthene	207-08-9	252.32	6.11	$5.84 \cdot 10^{-7}$	_	$8.00 \cdot 10^{-4}$
Benzo(a)pyrene	50-32-8	252.31	6.13	$4.57 \cdot 10^{-7}$	-	$1.62 \cdot 10^{-3}$
Dibenz(a.h)anthracene	53-70-3	278.35	6.75	$1.23 \cdot 10^{-7}$	$1.00 \cdot 10^{-10}$	$2.49 \cdot 10^{-3}$
Benzo(ghi)perylene	191-24-2	276.34	6.63	$3.31 \cdot 10^{-7}$	$1.00 \cdot 10^{-10}$	$2.60 \cdot 10^{-4}$
Indeno(1.2.3-cd) pyrene	193-39-5	276.34	6.70	$3.48 \cdot 10^{-7}$	$1.25 \cdot 10^{-10}$	$1.90 \cdot 10^{-4}$

Sources: [176].

Table S8. CAS number and main physical-chemical properties of the PCBs analyzed in the sediments of the sampling sites.

	CAS Number	Molecular Weight g·mol^{-1}	Log K_{ow}	Henry's Law Constant atm-m^3·mol^{-1}, 25 ºC	Vapour Pressure mm Hg, 25ºC	Water Solubility mg L^{-1}, 25ºC
			Indicator PCBs			
PCB28	7012-37-5	257.55	5.62	$2.00 \cdot 10^{-4}$	$1.95 \cdot 10^{-4}$	0.27
PCB52	35693-99-3	291.99	6.09	$2.00 \cdot 10^{-4}$	$8.45 \cdot 10^{-6}$	$1.53 \cdot 10^{-2}$
PCB101	37680-73-2	326.44	6.8	$9.00 \cdot 10^{-5}$	$2.52 \cdot 10^{-5}$	$1{,}54 \cdot 10^{-2}$
PCB138	35065-28-2	360.88	7.44	$2.10 \cdot 10^{-5}$	$3.80 \cdot 10^{-6}$	$1.50 \cdot 10^{-3}$
PCB153	35065-27-1	360.88	7.75	$2.30 \cdot 10^{-5}$	$3.43 \cdot 10^{-6}$	$9.50 \cdot 10^{-4}$
PCB180	35065-29-3	395.33	8.27	$1.00 \cdot 10^{-5}$	$9.77 \cdot 10^{-7}$	$3.85 \cdot 10^{-3}$
			Dioxin like PCBs			
PCB81	70362-50-4	291.99	-	-	-	-
PCB77	32598-13-3	291.99	6.63	$9.40 \cdot 10^{-6}$	$1.64 \cdot 10^{-5}$	$5.69 \cdot 10^{-4}$
PCB123	65510-44-3	326.44	-	-	-	-
PCB118	31508-00-6	326.44	7.12	$2.88 \cdot 10^{-4}$	$8.97 \cdot 10^{-6}$	$1.34 \cdot 10^{-2}$
PCB114	74472-37-0	326.44	6.98	-	-	$1.60 \cdot 10^{-2}$
PCB105	32598-14-4	326.44	6.79	$8.25 \cdot 10^{-4}$	$6.53 \cdot 10^{-6}$	$3.4 \cdot 10^{-3}$
PCB126	57465-28-8	326.44	-	-	-	-
PCB167	52663-72-6	360.88	7.5	$6.85 \cdot 10^{-5}$	$5.81 \cdot 10^{-7}$	$2.23 \cdot 10^{-3}$
PCB156	38380-08-4	360.88	7.6	$1.43 \cdot 10^{-4}$	$1.61 \cdot 10^{-6}$	$5.33 \cdot 10^{-3}$
PCB157	69782-90-7	360.88	7.41	$6.85 \cdot 10^{-5}$	$5.81 \cdot 10^{-7}$	$5.10 \cdot 10^{-4}$
PCB169	32774-16-6	360.88	7.41	$6.85 \cdot 10^{-5}$	$5.81 \cdot 10^{-7}$	$5.10 \cdot 10^{-4}$
PCB189	39635-31-9	395.33	8.27	-	-	$7.53 \cdot 10^{-4}$

Sources: [176].