Supplementary information

For

Novel brominated flame retardants relevant for European aquatic environments: ranking of analytes to monitor and focus on the French Eastern Mediterranean coastline.

Camille Rigal¹, Laurence Asia¹, Stéphanie Lebarillier¹, Pierre Doumenq¹, Pascal Mirleau², Laure Malleret^{1*}

¹ Laboratoire Chimie Environnement, Aix Marseille Univ, CNRS, Europole de l'Arbois, Aix-en-Provence, France

² IMBE – Aix Marseille Univ, Avignon Université, CNRS, IRD, Marseille, France

* Corresponding author : <u>laure.malleret@univ-amu.fr</u>

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Table of contents

Table of contents
Figure S1 : Picture of a suspended matter trap
Table S1 : Information about the ten collected samples of suspended matter : geographical coordinates, depth, exposure periods, fraction sieved and total organic carbon (TOC)
Table S2 : GC/EI-MS/MS (MRM mode) methods for the analysis of CPs and PCBs with a 7890A GC coupled toTriple quadrupole 3000 A MS (Agilent Technologies, Santa Clara, USA) ; EI, 70 eV
Table S3 : Transitions used for quantification and qualification of PCBs and CPs 3
Table S4 : Limits of detection (LODs) and quantification (LOQs) of compounds analysed in this study
Table S5 : OSPAR Background Assessment Concentrations (BAC) and Environmental Assessment Concentrations (EAC) for PCBs in sediments
Table S6 : Federal Environmental Quality Guidelines (FEQGs) established for PBDEs in sediments by the Canadian Environmental Protection Act, 1999
Table S7 : Ranking of the 148 reported nBFRs based on European production or import, occurrence and ecotoxicology
Table S8 : Chemical and physical properties of the 22 nBFRs targeted : molecular weight (MW), log Kow (computed by XLogP3 3.0, PubChem), water solubility (predicted with ECOSAR), ebullition temperature (predicted with ACD/Labs Percepta Platform - PhysChem Module, version: 14.00) and score at the relevance ranking
Table S9 : Concentrations of 38 halogenated flame retardants targeted in the suspended matter samples
Table S10 : Non-parametric Spearman rank correlation across the detected compounds 22
Table S11 : Risk quotients obtained for the detected nBFRs 23

Figure S1 : Picture of a suspended matter trap



Table S1 : Information about the ten collected samples of suspended matter : geographical coordinates, depth, exposure periods, fraction sieved and total organic carbon (TOC)

Sampling	Latitude	Longitude	Depth	Sampling	Collecting	Fraction	СОТ	Mass		
Site	(minutes)	(minutes)	(m)	date	period ¹	sieved ²		analysed		
					(days)	(µm)		(g d.w.)		
FOS	43°	4° 56.478'E	7	24/04/2018	154	< 500	1.0%	10.620		
	25.268'N									
NIO	43°	5° 15.360'E	16	20/02/2018	85	< 500	1.8%	4.896		
	20.260'N									
VEY	43°	5° 15.178'E	27	08/03/2018	100	< 500	3.7%	2.905		
	12.392'N									
EST	43°	5° 17.352'E	13	17/04/2018	56	< 250	5.0%	1.177		
	21.285'N									
MAI	43°	5° 19.842'E	17	26/02/2018	90	< 250	3.2%	8.300		
	12.768'N									
SAM	43°	5° 20.648'E	16	13/02/2018	132	< 500	4.2%	10.018		
	13.409'N									
CHE	43°	5° 21.970'E	10	08/03/2018	108	< 500	5.2%	1.449		
	12.250'N									
SMN	43° 5.117'N	5° 56.413'E	11	20/04/2018	135	< 500	4.7%	2.185		
SMH	43° 4.488'N	5° 57.198'E	12	20/11/2018	125	< 500	5.6%	4.903		
PRA	43° 5.867'N	6° 0.772'E	11	20/04/2018	123	< 500	8.5%	1.900		

¹ The overall monitoring of posidonia meadows and sample collection involves three diving periods each year, leading to 90-130 days sampling intervals for a given site (depending on meteorological conditions, divers and boats availabilities). However, suspended matter traps may be found detached or overturned on the bottom sediment (probably due to net-fishing activities); in that case, suspended matter samples are not recovered, traps are cleaned, placed back to their initial position and further sampled (e.g. the Estaque trap was repaired 20/02/2018 and the SM sample collected 17/04/2018, making the shortest collecting period of 56 days).

 2 Suspended matter samples were initially used to assess trace metals (TM) concentrations and a sieving protocol was developed to compare concentrations obtained in various sieving fractions (similar TM concentrations were obtained in the various sieving fractions). Only fractions < 250 mm of the sampling dates remained in sufficient amount for Estaque and Maïre samples. As required to detect and quantify trace organic contaminants, the sieving protocol was further adjusted to the single fraction < 500 mm, yielding higher suspended matter sample mass.

Table S2 : GC/EI-MS/MS (MRM mode) methods for the analysis of CPs and PCBs with a 7890A GC coupled to Triple quadrupole 3000 A MS (Agilent Technologies, Santa Clara, USA) ; EI, 70 eV

C	CPs								
Injector temperature (°C)	280°C								
Transfer line temperature (°C)	250°C								
Source temperature (°C)	250°C								
Oven progamm	120°C (hold 1 minute)								
	Heat 15°C/min until 300°C (hold 7 minutes)								
PCBs									
Injector temperature (°C)	300°C								
Transfer line temperature (°C)	300°C								
Source temperature (°C)	280°C								
Oven progamm	60°C (hold 1 minute)								
	Heat 20°C/min until 120°C								
	Heat 6°C/min until 250°C								
	Heat 17.5°C/min until 300°C (hold 2 minutes)								

 $\label{eq:solution} Table \, S3: \mbox{Table S3}: \mbox{$

	Quantifier	Collision energy (V)	Qualifier	Collision energy (V)
PCB 30 d5	261 -> 191	15	263 -> 191	15
PCB 28	256 -> 186	15	258 -> 188	15
PCB 52	290 -> 220	20	292 -> 222	15
PCB 101	326 -> 256	20	328 -> 256	20
PCB 116 d5	331 -> 261	20	331 -> 259	20
PCB 118	326 -> 256	20	324 -> 254	20
PCB 153	360 -> 290	20	360 -> 288	20
PCB 138	360 -> 290	20	360 -> 288	20
PCB 156 d3	363 -> 293	20	363 -> 291	20
PCB 180	394 -> 324	20	396 -> 361	20
CPs	101 -> 65	8	115 -> 78	8
			102 -> 78	10
¹³ C ₆ -HCB	290 -> 220	20	292 -> 222	20

	FOS	NIO	VEY	EST	MAI	SAM	CHE	SMN	SMH	PRA	Mean
Sample mass (g d.w.)	10.620	4.896	2.905	1.177	8.300	10.018	1.449	2.185	4.903	1.900	4.032
				nBFRs	(LOD / LOQ	in ng.g ⁻¹ d.w.))				
2,4-DBP	0.04 / 0.13	0.08 / 0.27	0.14 / 0.46	0.34 / 1.14	0.05 / 0.16	0.04 / 0.13	0.28 / 0.92	0.18 / 0.61	0.08 / 0.27	0.21 / 0.70	0.14 / 0.48
2,4,6-TBP	0.02 / 0.07	0.05 / 0.15	0.08 / 0.25	0.19 / 0.63	0.03 / 0.09	0.02 / 0.07	0.15 / 0.51	0.10/0.34	0.05 / 0.15	0.12 / 0.39	0.08 / 0.27
BEH-TEBP	0.68 / 2.26	1.47 / 4.90	2.48 / 8.26	6.12 / 20.39	0.87 / 2.89	0.72 / 2.40	4.97 / 16.56	3.30 / 10.98	1.47 / 4.89	3.79 / 12.63	2.59 / 8.62
BTBPE	0.09 / 0.29	0.19 / 0.63	0.32 / 1.06	0.79 / 2.62	0.11/0.37	0.09 / 0.31	0.64 / 2.13	0.42 / 1.41	0.19/0.63	0.49 / 1.62	0.33 / 1.11
DDDDE	1 72 / 5 72	3.72 /	6.28 /	15.49 /	2 20 / 7 22	1.92/07	12.58 /	8.35 /	3.72 /	9.60 /	6.55 /
DBDFE	1.72/ 5.72	12.41	20.92	51.64	2.2077.32	1.82/0.07	41.95	27.82	12.40	31.99	21.82
DBE-DBCH	0.05 / 0.17	0.11 / 0.38	0.19 / 0.63	0.47 / 1.57	0.07 / 0.22	0.06 / 0.18	0.38 / 1.27	0.25 / 0.84	0.11 / 0.38	0.29 / 0.97	0.20 / 0.66
DBHCTD	0.03 / 0.09	0.06 / 0.19	0.10 / 0.32	0.23 / 0.78	0.03 / 0.11	0.03 / 0.09	0.19 / 0.64	0.13 / 0.42	0.06 / 0.19	0.15 / 0.48	0.10/0.33
EH-TBB	0.12 / 0.39	0.25 / 0.84	0.42 / 1.41	1.05 / 3.48	0.15 / 0.49	0.12 / 0.41	0.85 / 2.83	0.56 / 1.88	0.25 / 0.84	0.65 / 2.16	0.44 / 1.47
HBB	0.02 / 0.06	0.04 / 0.14	0.07 / 0.23	0.17 0.58	0.02 / 0.08	0.02 / 0.07	0.14 / 0.47	0.09 / 0.31	0.04 / 0.14	0.11/0.36	0.07 / 0.24
PBB-Acr	0.03 / 0.10	0.06 / 0.21	0.10 / 0.35	0.26 / 0.86	0.04 / 0.12	0.03 / 0.10	0.21 / 0.70	0.14 / 0.46	0.06 / 0.21	0.16 / 0.53	0.11/0.36
PBBB	0.02 / 0.08	0.05 / 0.18	0.09 / 0.30	0.22 / 0.73	0.03 / 0.10	0.03 / 0.09	0.18 / 0.60	0.12 / 0.40	0.05 / 0.18	0.14 / 0.45	0.09 / 0.31
PBBz	0.02 / 0.05	0.03 / 0.11	0.06 / 0.19	0.14 / 0.47	0.02 / 0.07	0.02 / 0.05	0.11 / 0.38	0.08 / 0.25	0.03 / 0.11	0.09 / 0.29	0.06 / 0.20
PBEB	0.01 / 0.05	0.03 / 0.10	0.05 / 0.17	0.13 / 0.43	0.02 / 0.06	0.02 / 0.05	0.10/0.35	0.07 / 0.23	0.03 / 0.10	0.08 / 0.27	0.05 / 0.18
מממ	1 49 / 4 04	3.22 /	5.42 /	13.38 /	1.00 / 6.22	157/524	10.87 /	7.21 /	3.21 /	8.29 /	5.66 /
PDP	1.46 / 4.94	10.72	18.07	44.60	1.90 / 0.33	1.377 3.24	36.23	24.03	10.71	27.63	18.85
PBT	0.01 / 0.04	0.03 / 0.10	0.05 / 0.16	0.12 / 0.40	0.02 / 0.06	0.01 / 0.05	0.10 / 0.33	0.06 / 0.22	0.03 / 0.10	0.07 / 0.25	0.05 / 0.17
TBBPA	0.59 / 1.98	1.29 / 4.30	2.17 / 7.25	5.37 / 17.89	0.76 / 2.54	0.63 / 2.10	4.36 / 15.53	2.89 / 9.64	1.29 / 4.29	3.32 / 11.08	2.27 / 7.56
TBBPA-BDBPE	1.00 / 3.34	2.17 / 7.24	3.66 / 12.20	9.03 / 30.11	1.28 / 4.27	1.06 / 3.54	7.34 / 24.46	4.87 / 16.22	2.17 / 7.23	5.60 / 18.65	3.82 / 12.73
TBBPS-BME	0.10/0.34	0.22 / 0.75	0.38 / 1.26	0.93 / 3.10	0.13 / 0.44	0.11/0.36	0.76 / 2.52	0.50 / 1.67	0.22 / 0.74	0.58 / 1.92	0.39 / 1.31
TBP-AE	0.01 / 0.05	0.03 / 0.10	0.05 / 0.17	0.13 / 0.43	0.02 / 0.06	0.02 / 0.05	0.11/0.35	0.07 / 0.23	0.03 / 0.10	0.08 / 0.27	0.05 / 0.18
TBX	0.01 / 0.03	0.02 / 0.06	0.03 / 0.10	0.08 / 0.25	0.01 / 0.04	0.01 / 0.03	0.06 / 0.21	0.04 / 0.14	0.02 / 0.06	0.05 / 0.16	0.03 / 0.11
TDBP-TAZTO	0.35 / 1.15	0.75 / 2.50	1.26 / 4.22	3.12 / 10.40	0.44 / 1.48	0.37 / 1.22	2.54 / 8.45	1.68 / 5.60	0.75 / 2.50	1.93 / 6.44	1.32 / 4.40
TTBP-TAZ	0.99 / 3.31	2.15 / 7.18	3.63 / 12.10	8.96 / 29.86	1.27 / 4.23	1.05 / 3.51	7.28 / 24.26	4.83 / 16.09	2.15 / 7.17	5.55 / 18.50	3.79 / 12.62

Table S4 : Limits of detection (LODs) and quantification (LOQs) of compounds analysed in this study

	FOS	NIO	VEY	EST	MAI	SAM	CHE	SMN	SMH	PRA	Mean		
Sample mass (g d.w.)	10.620	4.896	2.905	1.177	0.264	10.018	1.449	2.185	4.903	1.900	4.032		
				PBDEs	(LOD / LOQ	in ng.g ⁻¹ d.w.))						
BDE 28	0.02 / 0.07	0.04 / 0.15	0.08 / 0.25	0.19 / 0.62	0.03 / 0.09	0.02 / 0.07	0.15 / 0.50	0.10 / 0.33	0.04 / 0.15	0.12 / 0.38	0.05 / 0.15		
BDE 47	0.01 / 0.04	0.03 / 0.09	0.05 / 0.15	0.11 / 0.38	0.02 / 0.05	0.01 / 0.04	0.09 / 0.31	0.06 / / 0.20	0.03 / 0.09	0.07 / 0.23	0.03 / 0.09		
BDE 99	0.01 / 0.05	0.03 / 0.10	0.05 / 0.17	0.13 / 0.43	0.02 / 0.06	0.02 / 0.05	0.10 / 0.35	0.07 / 0.23	0.03 / 0.10	0.08 / 0.27	0.03 / 0.10		
BDE 100	0.02 / 0.06	0.04 / 0.13	0.07 / 0.22	0.17 / 0.55	0.02 / 0.08	0.02 / 0.06	0.13 / 0.45	0.09 / 0.30	0.04 / 0.13	0.10 / 0.34	0.04 / 0.13		
BDE 153	0.02 / 0.06	0.04 / 0.14	0.07 / 0.23	0.17 / 0.58	0.02 / 0.08	0.02 / 0.07	0.14 / 0.47	0.09 / 0.31	0.04 / 0.14	0.11 / 0.36	0.04 / 0.14		
BDE 154	0.03 / 0.11	0.07 / 0.25	0.12 / 0.41	0.31 / 1.02	0.04 / 0.14	0.04 / 0.12	0.25 / 0.83	0.16 / 0.55	0.07 / 0.24	0.19 / 0.63	0.07 / 0.25		
BDE 183	0.07 / 0.24	0.16 / 0.53	0.27 / 0.89	0.66 / 2.20	0.09 / 0.31	0.08 / 0.26	0.54 / 1.79	0.36 / 1.19	0.16/0.53	0.41 / 1.36	0.16/0.54		
DDE 200	4.56 /	9.90 /	16.68 /	41.17 /	5.84 /	4.84 /	33.44 /	22.18 /	9.88 /	25.51 /	10.02 /		
BDE 209	15.21	32.99	55.61	137.25	19.46	16.12	111.48	73.93	32.95	85.02	33.41		
	PCBs (LOD / LOQ in ng.g ⁻¹ d.w.)												
PCB 28	0.002 /	0.005 /	0.008 /	0.020 /	0.003 /	0.002 /	0.017 /	0.011 /	0.005 /	0.013 /	0.005 /		
100 20	0.008	0.017	0.028	0.020	0.010	0.008	0.057	0.038	0.017	0.043	0.017		
PCB 52	0.003 /	0.006 /	0.010 /	0.025 /	0.004 /	0.003 /	0.021 /	0.014 /	0.006 /	0.016 /	0.006 /		
	0.009	0.020	0.034	0.085	0.012	0.010	0.069	0.046	0.020	0.053	0.021		
PCB 101	0.003 /	0.007 /	0.011 /	0.027 /	0.004 /	0.003 /	0.022 /	0.015 /	0.007 /	0.017 /	0.007 /		
100 101	0.010	0.022	0.037	0.092	0.013	0.011	0.075	0.049	0.022	0.057	0.022		
PCB 118	0.005 /	0.011 /	0.019 /	0.048 /	0.007 /	0.006 /	0.039 /	0.026 /	0.011 /	0.029 /	0.012 /		
100 110	0.018	0.038	0.065	0.160	0.023	0.019	0.130	0.086	0.038	0.099	0.039		
PCB 138	0.005 /	0.011 /	0.019 /	0.048 /	0.007 /	0.006 /	0.039 /	0.026 /	0.011 /	0.029 /	0.012 /		
I CD 150	0.018	0.038	0.065	0.160	0.023	0.019	0.130	0.086	0.038	0.099	0.039		
DCB 153	0.006 /	0.013 /	0.021 /	0.053 /	0.007 /	0.006 /	0.043 /	0.028 /	0.013 /	0.033 /	0.013 /		
FCD 155	0.019	0.042	0.070	0.173	0.025	0.020	0.141	0.093	0.042	0.107	0.042		
DCB 180	0.004 /	0.008 /	0.013 /	0.032 /	0.005 /	0.004 /	0.026 /	0.017 /	0.008 /	0.020 /	0.008 /		
I CD 100	0.012	0.026	0.043	0.107	0.015	0.013	0.087	0.058	0.026	0.066	0.026		
				CPs (LOD / LOQ in	n ng.g ⁻¹ d.w.)							
CPs	106/352	22.0 / 76.5	38.7 /	95.5 /	135/451	11 2 / 37 4	77.5 /	51.4 /	22.0 / 76.4	59.1 /	23 2 / 77 5		
Crs	10.07 33.3	22.9/10.3	128.9	318.2	13.3 / 43.1	11.2/37.4	258.5	171.4	22.9/ 10.4	197.1	23.2/11.3		

Table S4 (continued) : Limits of detection (LODs) and quantification (LOQs) of compounds analysed in this study

Fable S5 : OSPAR Background Assessment Concer	ntrations (BAC) and Environmental Asse	essment Concentrations (EAC) for PCBs in sediments
-----------------------------------------------	----------------------------------------	----------------------------------------------------

Congener	BAC (µg.kg ⁻¹ d.w.) ¹	EAC (μg.kg ⁻¹ d.w.) ¹
PCB 28	0.22	1.7
PCB 52	0.12	2.7
PCB 101	0.14	3.0
PCB 118	0.17	0.6
PCB 138	0.15	7.9
PCB 153	0.19	40
PCB 180	0.10	12

¹ Values normalized to 1% TOC.

Table S6 : Federal Environmental Quality Guidelines (FEQGs) established for PBDEs in sediments by the Canadian Environmental Protection Act, 1999

Homologue ¹	Congeners	Sediment ² (ng.g ⁻¹ d.w.)
triBDE	total	44
tetraBDE	total	39
pentaBDE	total	0.4
pentaBDE	BDE-99	0.4
pentaBDE	BDE-100	0.4
hexaBDE	total	440
heptaBDE	total	-
octaBDE	total	5600 ³
nonaBDE	total	-
decaBDE	total	19 ^{3,4}

¹ FEQG for triBDE (tribromodiphenyl ether), tetraBDE (tetrabromodiphenyl ether), hexaBDE (hexabromodiphenyl ether), heptaBDE (heptabromodiphenyl ether), nonaBDE (nonabromodiphenyl ether) and decaBDE (decabromodiphenyl ether) are based on data for the congeners: BDE-28, BDE-47, BDE-153, BDE-183, BDE-206, and BDE-209, respectively unless otherwise noted.

² Values normalized to 1% organic carbon.

³ Values adopted from Ecological Screening Assessment Report (Environment Canada 2006). Sediment guidelines for octaBDE and decaBDE were adapted from the SAR by being corrected for the sediment organic carbon in the actual tests, then normalised to 1% organic carbon instead of the 4% in the SAR.

⁴ Values based on commercial decaBDE mixture which is composed mainly of nonaBDE and decaBDE.

Identity	A - Re Pro	gistration / duction	B - Occurrence			C - Ecotoxicology			Score for relevance ranking				
CAS Number (Acronym) 1	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total		
79-94-7 (TBBPA)	Yes	≥ 10 000 - < 100 000	16 [1] [2] [3] [4] [5] [6] [7] [8] [9] [10] [11] [12] [13] [14] [15] [16]	15 [1] [2] [3] [4] [5] [7] [8] [9] [10] [11] [12] [13] [14] [15] [16]	94%	9.5	-	4	3	2	9		
21850-44-2 (TBBPA- BDBPE)	Yes	≥ 1 000 - < 10 000	6 [7] [9] [16] [17] [18] [19]	4 [7] [16] [17] [18]	67%	2.20E-03	-	3	3	3	9		
84852-53-9 (DBDPE)	Yes	≥ 10 000 - < 100 000	88 [1] [8] [12] [13] [14] [18] [19] [20] [21] [22] [23] [24] [25] [26] [27] [28] [29] [30] [31] [32] [33] [34] [35] [36] [37] [38] [39] [40] [41] [42] [43] [44] [45] [46] [47] [48] [49] [50] [51] [52] [53] [54] [55] [56] [57] [58] [59] [60] [61] [62] [63] [64] [65] [66] [67] [68] [69] [70] [71] [72] [73] [74] [75] [76] [77] [78] [79] [80] [81] [82] [83] [84] [85] [86] [87] [88] [89] [90] [91] [92] [93] [94] [95] [96] [97] [98] [99] [100]	71 [1] [8] [12] [13] [14] [18] [20] [21] [22] [23] [24] [28] [29] [30] [31] [32] [33] [34] [35] [36] [38] [39] [40] [41] [42] [44] [46] [47] [48] [49] [50] [51] [52] [53] [54] [55] [56] [58] [59] [60] [61] [62] [63] [64] [65] [66] [68] [69] [70] [71] [72] [73] [74] [76] [77] [79] [80] [81] [83] [84] [85] [88] [89] [93] [94] [96] [97] [98] [99] [100]	81%	2.80E-05	0.47 (95% CI : 0.32–0.66)	4	3	2	9		

Identity	A - Reg Pro	gistration / duction	В - С	B - Occurrence			Ecotoxicology	Score for relevance ranking			
CAS Number (Acronym) 1	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC50 on fish. 96h (µg/L)	Trophic Magnification Factor ³	А	В	С	Total
26040-51-7 (BEH- TEBP)	Yes	≥ 100 – < 1 000	44 [1] [4] [6] [12] [13] [18] [21] [22] [23] [25] [26] [31] [32] [34] [39] [41] [43] [45] [49] [54] [60] [62] [68] [75] [78] [82] [85] [87] [89] [90] [91] [92] [95] [96] [99] [101] [102] [103] [104] [105] [106] [107] [108] [109]	26 [1] [12] [13] [18] [21] [22] [23] [26] [31] [34] [45] [62] [68] [82] [85] [89] [90] [91] [92] [96] [99] [102] [104] [105] [106] [107]	59%	6.70E-04	-	2	3	3	8
37853-59-1 (BTBPE)	Yes	≥ 1 - < 10	80 [1] [4] [6] [7] [8] [12] [13] [15] [18] [19] [20] [21] [22] [23] [25] [26] [31] [33] [34] [35] [39] [40] [41] [42] [43] [44] [45] [46] [47] [48] [49] [50] [51] [52] [53] [54] [57] [58] [60] [62] [63] [64] [65] [67] [68] [69] [70] [71] [75] [77] [78] [79] [80] [82] [85] [87] [88] [89] [90] [91] [92] [94] [96] [99] [100] [101] [102] [103] [104] [106] [107] [108] [109] [110] [111] [112] [113] [114]	61 [1] [4] [7] [8] [12] [13] [15] [18] [19] [21] [22] [23] [26] [31] [33] [34] [35] [40] [41] [42] [43] [44] [45] [46] [47] [48] [49] [50] [51] [52] [53] [57] [62] [63] [65] [67] [68] [69] [70] [71] [77] [78] [79] [80] [82] [88] [89] [90] [94] [96] [97] [98] [99] [100] [104] [107] [109] [110] [112] [113] [114]	76%	0.22	2.3 (95% CI : 1.5–3.5)	0	3	4	7
59447-55-1 (PBB-Acr)	Yes	≥ 100 - < 1 000	15 [4] [25] [26] [54] [67] [79] [82] [90] [91] [96] [98] [99] [108] [109] [110]	6 [4] [67] [91] [96] [98] [110]	40%	19.0	2.0 (95% CI : 1.5–2.8)	2	2	3	7

Identity	A - Reg Pro	gistration / duction	B - Oce	B - Occurrence			C - Ecotoxicology			Score for relevance ranking				
CAS Number (Acronym) 1	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC50 on fish. 96h (µg/L)	Trophic Magnification Factor ³	А	В	С	Total			
52434-90-9 (TDBP- TAZTO)	Yes	$\geq 100 - < 1\ 000$	6 [7] [24] [25] [26] [99] [115]	3 [7] [24] [115]	50%	8.90	-	2	3	2	7			
87-82-1 (HBB)	Yes	≥ 1 - < 10	81 [1] [4] [6] [7] [14] [15] [18] [20] [21] [22] [23] [24] [25] [26] [27] [31] [32] [33] [34] [35] [36] [37] [38] [39] [40] [44] [46] [47] [49] [51] [53] [54] [55] [56] [57] [58] [59] [60] [62] [63] [65] [67] [70] [75] [76] [77] [78] [79] [81] [82] [84] [85] [86] [87] [88] [89] [90] [91] [92] [93] [94] [95] [97] [98] [99] [100] [101] [103] [104] [105] [106] [107] [108] [109] [110] [112] [113] [116] [117] [118]	59 [4] [7] [15] [18] [20] [21] [22] [24] [25] [26] [31] [32] [33] [34] [35] [39] [40] [44] [46] [47] [49] [51] [53] [55] [57] [62] [63] [65] [67] [70] [72] [75] [77] [79] [81] [82] [84] [85] [87] [88] [89] [90] [91] [92] [93] [94] [95] [97] [98] [99] [103] [104] [107] [110] [112] [113] [116] [117] [118]	73%	7.4	2.9 (95% CI: 1.9–4.5)	0	3	3	6			
87-83-2 (PBT)	Yes	≥ 1 - < 10	57 [4] [7] [11] [15] [18] [21] [22] [23] [24] [25] [26] [32] [33] [34] [39] [40] [44] [46] [47] [51] [53] [54] [60] [63] [65] [67] [70] [75] [76] [77] [79] [82] [85] [87] [89] [90] [91] [94] [95] [97] [98] [99] [100] [103] [105] [106] [107] [108] [109] [111] [113] [114] [116] [117] [118] [119] [120]	39 [4] [7] [18] [21] [22] [26] [32] [33] [34] [39] [40] [46] [47] [51] [53] [54] [63] [65] [70] [77] [79] [85] [90] [91] [94] [95] [97] [98] [100] [105] [107] [108] [111] [113] [116] [117] [118]	68%	13	4.5 (95% CI: 3.1–6.3)	0	3	3	6			

Identity	A - Re Pro	egistration / oduction	B - Oc	currence		С	- Ecotoxicology	Scor	e for r ranki	eleva ng	nce
CAS Number (Acronym) ¹	US EPA 2	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	А	В	С	Total
85-22-3 (PBEB)	Yes	≥ 1 - < 10	80 [1] [4] [7] [11] [14] [15] [18] [21] [22] [23] [24] [25] [26] [27] [31] [32] [33] [34] [36] [37] [38] [39] [40] [44] [46] [47] [49] [51] [53] [54] [55] [56] [57] [59] [60] [61] [62] [63] [64] [65] [67] [70] [72] [75] [76] [77] [78] [79] [81] [82] [84] [85] [86] [87] [88] [89] [90] [91] [92] [93] [94] [95] [97] [98] [99] [100] [101] [103] [104] [105] [106] [107] [108] [109] [111] [113] [114] [116] [117] [118]	50 [1] [7] [14] [18] [21] [22] [25] [26] [31] [32] [33] [34] [40] [46] [47] [49] [53] [54] [55] [57] [62] [63] [70] [72] [75] [77] [78] [79] [81] [85] [87] [88] [89] [90] [91] [93] [94] [95] [97] [98] [100] [104] [105] [106] [107] [108] [109] [111] [113] [118]	63%	4.9	4.0 (95% CI: 2.1–7.6)	0	3	3	6
183658-27-7 (EH-TBB)	Yes	< 1	53 [1] [4] [6] [7] [12] [13] [18] [21] [22] [23] [24] [25] [26] [32] [33] [34] [39] [41] [43] [44] [45] [49] [51] [53] [54] [58] [60] [62] [67] [68] [75] [78] [82] [85] [87] [89] [90] [91] [92] [99] [100] [101] [102] [103] [104] [106] [107] [108] [109] [111] [112] [114] [117]	33 [7] [12] [13] [18] [21] [22] [23] [25] [26] [33] [34] [39] [41] [43] [44] [45] [49] [51] [53] [62] [67] [68] [82] [91] [92] [99] [100] [104] [107] [108] [111] [112] [117]	62%	0.39	_	0	3	3	6
608-90-2 (PBBz)	Yes	< 1	25 [7] [20] [21] [25] [26] [39] [53] [62] [67] [76] [82] [90] [91] [92] [94] [98] [99] [103] [104] [106] [107] [109] [110] [111] [118]	15 [7] [20] [21] [26] [53] [62] [91] [94] [98] [99] [104] [107] [110] [111] [118]	60%	40	1.7 (95% CI : 1.4–2.1)	0	3	3	6

Table S7	(continued)	: Ranking of t	he 148 repo	orted nBFRs base	d on European	production or imp	port. occurrence and	ecotoxicology
	(P	· · · · , · · · · · · · · · · · · · · ·	

Identity	A - Re Pro	egistration / oduction	B - Oo	ccurrence		С	- Ecotoxicology	Scor	e for r rank	eleva ing	nce
CAS Number (Acronym) ¹	US EPA 2	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	А	В	С	Total
51936-55-1 (DBHCTD)	Yes	≥ 1 - < 10	25 [4] [11] [13] [22] [23] [25] [26] [31] [47] [54] [60] [67] [75] [76] [79] [82] [89] [90] [98] [99] [101] [102] [106] [108] [117]	8 [13] [22] [31] [47] [79] [90] [98] [108]	33%	0.48	3.9 (95% CI: 3.1–5.0)	0	2	4	6
35109-60-5 (TBP-DPTE)	Yes	≥ 1 - < 10	32 [21] [25] [26] [32] [33] [39] [41] [44] [47] [49] [51] [54] [58] [60] [75] [76] [87] [89] [91] [94] [98] [99] [100] [103] [105] [106] [107] [108] [109] [110] [111] [116]	20 [21] [25] [26] [32] [33] [41] [44] [47] [49] [51] [91] [94] [98] [100] [103] [105] [106] [107] [108] [110]	63%	55	2.8 (95% CI : 1.9–4.0)	0	3	3	6
25713-60-4 ⁴ (TTBP-TAZ)	Yes	≥1 - < 10	1 [24]	1 [24]	100%	0.0028	-	2	1	3	6
32588-76-4 (EHTEBPI)	Yes	$\geq 100 - < 1\ 000$	-	-	-	0.078	-	2	1	3	6
34571-16-9 (HCTBPH)	Yes	≥ 1 - < 10	29 [11] [20] [21] [25] [27] [31] [36] [37] [38] [49] [53] [55] [56] [58] [59] [62] [67] [72] [82] [85] [86] [90] [92] [93] [95] [105] [106] [107] [111]	11 [31] [37] [38] [53] [58] [62] [82] [85] [92] [93] [111]	38%	0.0052	-	0	2	3	5
39569-21-6 (TBCT)	Yes	≥1 - < 10	17 [4] [7] [25] [26] [54] [67] [79] [82] [90] [91] [92] [96] [99] [108] [109] [110] [118]	10 [7] [54] [79] [82] [90] [92] [96] [108] [110] [118]	59%	20	-	0	3	2	5
118-79-6 (2.4.6-TBP)	Yes	$\geq 100 - < 1\ 000$	10 [1] [2] [3] [4] [5] [6] [18] [24] [25] [121]	8 [1] [2] [3] [4] [5] [18] [24] [121]	80%	1420	-	2	3	0	5

Identity	A - Re Pro	egistration / oduction	B - Oo	ccurrence		(C - Ecotoxicology	Sco	ore for ran	rele [.] king	vance
CAS Number (Acronym) ¹	US EPA 2	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total
3322-93-8 (DBE-DBCH)	Yes	≥ 1 - < 10	26 [1] [4] [18] [19] [20] [21] [22] [23] [25] [26] [39] [54] [76] [79] [82] [90] [96] [98] [99] [101] [108] [110] [113] [114] [122] [123]	13 [18] [21] [22] [23] [26] [54] [79] [90] [96] [98] [110] [122] [123]	50%	434	β-TBECH : 2.6 (95% CI : 1.9–3.5) α-TBECH : 1.9 (95% : 1.5–2.5)	0	3	2	5
3072-84-2 (TBBPA- BGE)	No	≥ 100 - < 1 000	1 [9]	0	0%	7.50	-	2	1	2	5
23488-38-2 (TBX)	Yes	≥ 1 - < 10	26 [4] [7] [11] [20] [25] [26] [40] [46] [54] [62] [67] [76] [77] [79] [82] [83] [90] [91] [98] [99] [107] [108] [109] [117] [118] [119]	20 [4] [7] [26] [40] [54] [62] [77] [79] [82] [83] [90] [91] [98] [99] [107] [108] [109] [117] [118] [119]	77%	23	0.97 (95% CI : 0.82–1.2)	0	3	1	4
3278-89-5 (TBP-AE)	Yes	≥ 1 - < 10	19 [4] [21] [25] [26] [39] [49] [54] [67] [79] [82] [90] [91] [96] [98] [99] [105] [107] [108] [109]	9 [21] [26] [49] [54] [67] [90] [96] [98] [107]	47%	182	1.8 (95% : 1.3–2.6)	0	2	2	4
608-71-9 (PBP)	Yes	≥ 1 - < 10	6 [2] [3] [4] [5] [18] [108]	3 [2] [3] [18]	50%	111	-	0	3	1	4

Identity	A - Re Pre	egistration / oduction	В - О	ocurrence		C - 1	Ecotoxicology	Sco	ore for ran	rele [.] king	vance
CAS Number (Acronym) ¹	US EPA 2	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total
58965-66-5 (4'-PeBPOBDE208)	Yes	≥1 - < 10	2 [58] [120]	0	0%	4.8E-08	-	0	1	3	4
1084889-51-9 1025956-65-3 893843-07 (OBTMPI)	Yes	< 1	16 [4] [7] [11] [44] [47] [54] [76] [85] [89] [91] [95] [98] [106] [108] [109] [118]	5 [7] [47] [89] [98] [118]	31%	0.000089	0.44 (95% CI : 0.32–0.60)	0	2	2	4
3194-57-8 (TBCO)	Yes	< 1	11 [4] [25] [26] [49] [76] [82] [90] [98] [99] [108] [110]	4 [25] [26] [98] [110]	36%	434	α-TBCO : 2.5 (95% CI : 1.9–3.2) β-TBCO : 2.5 (95% CI : 1.9–3.2)	0	2	2	4
19186-97-1 ⁴ (TTBNPP)	Yes	< 1	2 [4] [45]	2 [4] [45]	100%	3.10	-	1	1	2	4
25327-89-3 (TBBPA-BAE)	No	≥1 - < 10	4 [9] [16] [17] [19]	3 [16] [17] [19]	75%	0.032	-	0	1	3	4
37853-61-5 (TBBPA-BME)	Yes	< 1	3 [7] [9] [10]	2 [7] [10]	67%	0.98	-	0	1	3	4
42757-55-1 (TBBPS-BDBPE)	Yes	≥ 1 - < 10	3 [9] [16] [124]	2 [16] [124]	67%	0.48	-	0	1	3	4
66710-97-2 (TBBPA-BHEEBA)	No	≥1 - < 10	-	-	-	0.26	-	0	1	3	4
106-93-4	Yes	$\geq 1\ 000\ - < 10\ 000$	-	-	-	1.51E+05	-	3	1	0	4
125904-11-2	Yes	$\geq 1\ 000 - < 10\ 000$	-	-	-	3500	-	3	1	0	4
49690-63-3	Yes	≥ 1 - < 10	-	-	-	0.039	-	0	1	3	4
497107-13-8	Yes	< 1	-	-	-	0.00038	-	0	1	3	4
61262-53-1	Yes	$\geq 1 - < 10$	-	-	-	0.0002	-	0	1	3	4
82001-21-6	Yes	≥ 1 - < 10	-	-	-	1.3E-08	-	0	1	3	4
90075-91-5	Yes	< 1	-	-	-	0.000016	-	0	1	3	4

Table S7 (continued) : Ranking of the 148 reported nBFRs based on European production or import, occurrence and ecotoxicology

Identity	A - R Pr	egistration / oduction]	B - Occurrence		С	- Ecotoxicology	Sco	re for) rar	• rele 1king	vance
CAS Number (Acronym) ¹	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total
39635-79-5 (TBBPS)	Yes	≥ 1 - < 10	3 [9] [12] [19]	1 [19]	33%	373	-	0	2	1	3
3555-11-1 (PBP-AE)	Yes	< 1	2 [4] [54]	0	0%	6.5	-	0	1	2	3
3296-90-0 ⁴ (DBNPG)	Yes	≥ 1 - < 10	1 [4]	0	0%	2.32E+06	-	2	1	0	3
4162-45-2 (TBBPA-BHEE)	Yes	≥ 1 - < 10	1 [9]	0	0%	26	-	0	1	2	3
57829-89-7 (DBP-TAZTO)	No	< 1	-	-	-	109	-	0	1	2	3
70156-79-5 (TBBPS-BME)	No	< 1	-	-	-	63	-	0	1	2	3
37419-42-4 (TBBPA-BP)	No	< 1	-	-	-	1.1	-	0	1	2	3
143-15-7	Yes	< 1	-	-	-	16	-	0	1	2	3
1715-40-8	Yes	≥ 1 - < 10	-	-	-	8.6	-	0	1	2	3
18300-04-4	Yes	≥ 1 - < 10	-	-	-	6.3	-	0	1	2	3
21609-90-5	Yes	≥ 1 - < 10	-	=	-	3.9	-	0	1	2	3
25495-98-1	Yes	< 1	-	-	-	21	-	0	1	2	3
33798-02-6	Yes	≥ 1 - < 10	-	-	-	8	-	0	1	2	3
39568-99-5	Yes	≥ 1 - < 10	-	-	-	7.7	-	0	1	2	3
4824-78-6	Yes	≥ 1 - < 10	-	-	-	6.2	-	0	1	2	3
52-51-7	Yes	$\geq 100 - < 1000$	-	-	-	1.00E+04	-	2	1	0	3
55205-38-4	Yes	< 1	-	-	-	1.9	-	0	1	2	3
57117-31-4	Yes	$\geq 1 - < 10$	-	-	-	10	-	0	1	2	3
59447-57-3	Yes	< 1	-	-	-	19	-	0	1	2	3
6386-73-8	Yes	≥ 1 - < 10	-	-	-	51	-	0	1	2	3
75-25-2	Yes	$\geq 100 - < 1000$	-	=	-	3.21E+05	-	2	1	0	3

Identity	A - R Pr	egistration / oduction	B - Oce	currence		С	- Ecotoxicology	Sco	ore foi rar	rele: rele:	vance
CAS Number (Acronym) ¹	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC ₅₀ on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total
38521-51-6 (PBBB)	Yes	≥ 1 - < 10	9 [4] [25] [67] [79] [82] [90] [92] [107] [108]	1 [79]	11%	7.5	-	0	0	2	2
87-84-3 (PBCCH)	Yes	≥1 - < 10	3 [4] [13] [108]	1 [13]	33%	1560	-	0	1	1	2
607-99-8 (2.4.6-TBA)	Yes	< 1	2 [6] [25]	0	0%	973	-	0	1	1	2
636-28-2 (TeBB)	Yes	≥ 1 - < 10	2 [15] [113]	1 [113]	50%	208	-	0	1	1	2
31780-26-4 (DBS)	No	≥ 1 - < 10	1 [4]	0	0%	600	-	0	1	1	2
632-79-1 (TEBP-Anh)	Yes	≥ 10 - < 100	1 [4]	1 [4]	100%	210	-	0	1	1	2
105-36-2	Yes	≥ 1 - < 10	-	-	-	790	-	0	1	1	2
31454-48-5	Yes	≥ 1 - < 10	-	-	-	434	-	0	1	1	2
36678-45-2	Yes	≥ 1 - < 10	-	-	-	445	-	0	1	1	2
5445-17-0	Yes	≥ 1 - < 10	-	-	-	806	-	0	1	1	2
5445-19-2	Yes	≥ 1 - < 10	-	-	-	672	-	0	1	1	2
55481-60-2	Yes	< 1	-	-	-	533	-	0	1	1	2
66108-37-0	Yes	≥ 1 - < 10	-	-	-	620	-	0	1	1	2
7347-19-5	Yes	$\geq 1 - < 10$	-	-	-	544	-	0	1	1	2
7436-90-0	Yes	< 1	-	-	-	600	-	0	1	1	2
93-52-7	Yes	≥ 1 - < 10	-	-	-	920	-	0	1	1	2
96-32-2	Yes	< 1	-	-	-	829	-	0	1	1	2
106-41-2 (4-BP)	Yes	≥ 1 - < 10	3 [6] [121] [125]	2 [121] [125]	67%	12500	-	0	1	0	1
608-33-3 (2.6-DBP)	Yes	≥ 1 - < 10	3 [3] [4] [6]	1 [3]	33%	4430	-	0	1	0	1
615-58-7 (2.4-DBP)	Yes	≥1 - < 10	5 [3] [4] [5] [6] [121]	2 [3] [121]	40%	4430	-	0	1	0	1

Table S7 (continued) : Ranking of the 148 reported nBFRs based on European production or import, occurrence and ecotoxicology

Identity	A - R Pr	egistration / oduction	B - Oc	currence		C - F	Ccotoxicology	Sco	ore foi rar	r rele 1king	vance
CAS Number (Acronym) ¹	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC50 on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total
126-72-7 (TDBPP)	Yes	≥ 1 - < 10	1 [13]	1 [13]	100%	4040	-	0	1	0	1
1522-92-5 36483-57-5 (TBNPA)	Yes	< 1	1 [4]	0	0%	159000	-	0	1	0	1
168434-45-5 (TBPD-TBP)	No	< 1	-	-	-	Not found	-	0	1	0	1
20566-35-2 (HEEHP-TEBP)	Yes	< 1	-	-	-	5990	-	0	1	0	1
75795-16-3 (BDBP-TAZTO)	No	< 1	-	-	-	Not found	-	0	1	0	1
103-63-9	Yes	≥ 1 - < 10	-	-	-	8850	-	0	1	0	1
109678-33-3	Yes	Confidential	-	-	-	114000	-	0	1	0	1
124-73-2	Yes	≥ 1 - < 10	-	-	-	29300	-	0	1	0	1
13810-83-8	Yes	< 1 t	-	-	-	17200	-	0	1	0	1
147-82-0	Yes	≥ 1 - < 10	-	-	-	2580	-	0	1	0	1
14925-39-4	Yes	≥ 1 - < 10	-	-	-	64300	-	0	1	0	1
1837-91-8	Yes	< 1 t	-	-	-	1410	-	0	1	0	1
19660-16-3	Yes	≥ 1 - < 10	-	-	-	3180	-	0	1	0	1
20217-01-0	Yes	≥ 1 - < 10	-	-	-	5.35E+03	-	0	1	0	1
2623-87-2	Yes	≥ 1 - < 10	-	-	-	4620000	-	0	1	0	1
3234-02-4	Yes	≥ 1 - < 10	-	-	-	14100	-	0	1	0	1
353-59-3	Yes	≥ 1 - < 10	-	-	-	165000	-	0	1	0	1
40703-79-5	Yes	≥ 1 - < 10	-	-	-	14300	-	0	1	0	1
42597-49-9	Yes	≥ 1 - < 10	-	-	-	2360	-	0	1	0	1
52907-07-0	Yes	≥ 1 - < 10	-	-	-	23800	-	0	1	0	1
5324-12-9	Yes	< 1	-	-	-	2470000	-	0	1	0	1
5412-25-9	Yes	$\geq 1 - < 10$	-	-	-	136000	-	0	1	0	1
58495-09-3	Yes	< 1	-	-	-	Not found	-	0	1	0	1
591-20-8	Yes	$\geq 1 - < 10$	-	-	-	12500	-	0	1	0	1

Identity	A - R	egistration /	B - Oc	currence		С - Е	cotoxicology	Sco	ore for	rele	vance
	Pr	oduction							rar	ıking	
CAS Number (Acronym) ¹	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC50 on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	С	Total
593-60-2	Yes	< 1	-	-	-	9340	-	0	1	0	1
59789-51-4	Yes	< 1	-	-	-	Not found	-	0	1	0	1
598-72-1	Yes	< 1	-	-	-	1460000	-	0	1	0	1
7415-86-3	Yes	≥ 1 - < 10	-	-	-	1270	-	0	1	0	1
75-63-8	Yes	< 1	-	-	-	285000	-	0	1	0	1
75-95-6	Yes	≥ 1 - < 10	-	-	-	13800	-	0	1	0	1
79-08-3	Yes	< 1	-	-	-	3130000	-	0	1	0	1
79-27-6	Yes	≥ 1 - < 10	-	-	-	90900	-	0	1	0	1
79-28-7	Yes	≥ 1 - < 10	-	-	-	4580	-	0	1	0	1
95-56-7	Yes	≥ 1 - < 10	-	-	-	12500	-	0	1	0	1
102739-99-1	Yes	Not registered	-	-	-	-	-	-	-	-	-
103582-29-2	Yes	Not registered	-	-	-	-	-	-	-	-	-
107555-93-1	Yes	Not registered	-	-	-	-	-	-	-	-	-
107555-94-2	Yes	Not registered	-	-	-	-	-	-	-	-	-
107555-95-3	Yes	Not registered	-	-	-	-	-	-	-	-	-
109333-34-8	Yes	Not registered	-	-	-	-	-	-	-	-	-
110999-44-5	Yes	Not registered	-	-	-	-	-	-	-	-	-
110999-45-6	Yes	Not registered	-	-	-	-	-	-	-	-	-
110999-46-7	Yes	Not registered	-	-	-	-	-	-	-	-	-
110999-47-8	Yes	Not registered	-	-	-	-	-	-	-	-	-
129880-08-6	Yes	Not registered	-	-	-	-	-	-	-	-	-
131166-92-2	Yes	Not registered	-	-	-	-	-	-	-	-	-
1403456-28-9	Yes	Not registered	-	-	-	-	-	-	-	-	-
161880-49-5	Yes	Not registered	-	-	-	-	-	-	-	-	-
161880-50-8	Yes	Not registered	-	-	-	-	-	-	-	-	-
161880-51-9	Yes	Not registered	-	-	-	-	-	-	-	-	-
1991993-66-8	Yes	Not registered	-	-	-	-	-	-	-	-	-
1991993-68-0	Yes	Not registered	-	-	-	-	-	-	-	-	-
1991993-69-1	Yes	Not registered	=	-	_	-	=	-	-	-	-

Identity	A - R Pi	legistration / roduction	B - Oc	currence		C - F	Ccotoxicology	Sco	ore fo rai	r rele 1king	vance
CAS Number (Acronym) ¹	US EPA ²	ECHA (ton/year)	nBFR analyzed (number of studies)	nBFR detected (number of studies)	%	LC50 on fish. 96h (µg/L)	Trophic Magnification Factor ³	A	В	C	Total
1991993-70-4	Yes	Not registered	-	-	-	-	-	-	-	-	-
2167063-57-0	Yes	Not registered	-	-	-	-	-	-	-	-	-
2170-45-8	Yes	Not registered	-	-	-	-	-	-	-	-	-
24173-07-7	Yes	Not registered	-	-	-	-	-	-	-	-	-
26657-83-0	Yes	Not registered	-	-	-	-	-	-	-	-	-
3066-70-4	Yes	Not registered	-	-	-	-	-	-	-	-	-
31611-84-4	Yes	Not registered	-	-	-	-	-	-	-	-	-
50585-41-6	Yes	Not registered	-	-	-	-	-	-	-	-	-
52434-59-0	Yes	Not registered	-	-	-	-	-	-	-	-	-
57011-47-9	Yes	Not registered	-	-	-	-	-	-	-	-	-
67733-57-7	Yes	Not registered	-	-	-	-	-	-	-	-	-
7046-64-2	Yes	Not registered	-	-	-	-	-	-	-	-	-
79755-43-4	Yes	Not registered	-	-	-	-	-	-	-	-	-
71245-27-7	Yes	Not registered	-	-	-	-	-	-	-	-	-
860302-33-6	Yes	Not registered	-	-	-	-	-	-	-	-	-

¹ Acronyms given by Bergman et al., 2012 [126]. For compounds not reported by Bergman et al., 2012, commonly used accronyms were given.

² nBFRs not registered by the US EPA (« No ») were found in the litterature [126]

³ Trophic Magnification Factor was established in a zooplankton – invertebrate – fish – bird food chain in the litterature [127]

⁴ TTBNPP, TTBP-TAZ and DBNPG were ranked according to their production quantities registered by the ECHA in 2021 rather than 2023

Table S8 :	Chemical and physical prop	perties of the 22 nBI	FRs targeted : mo	olecular weight (MW), log Kow (computed by X	KLogP3 3.0, I	PubChem), wa	ter solubility (predicted
with ECOS	AR), ebullition temperature	e (predicted with A	CD/Labs Percept	ta Platform - Phy	Chem Module,	version: 14.00)) and score at	the relevance	ranking	

(Acronym) ¹	CAS Number	Full name	MW (g.mol ⁻¹)	Log Kow	Water solubility (µg.L ⁻¹)	Boiling Point (°C at 760 mmHg)	Score
2,4-DBP	615-58-7	2,4-Dibromophenol	251.90	3.2	1.131E+06	238.5±0.0 °C	1
2,4,6-TBP	118-79-6	2,4,6-Tribromophenol	330.80	4.4	3.3224E+04	286.8±0.0	5
BEH-TEBP	26040-51-7	Bis(2-ethylhexyl) tetrabromophthalate	706.1	10.6	1.9828E-06	584.8±45.0	8
BTBPE	37853-59-1	1,2-Bis(2,4,6-tribromophenoxy)ethane	687.6	7.7	6.5509E-04	566.4±50.0	7
DBDPE	84852-53-9	Decabromodiphenyl ethane	971.2	11.1	1.1612E-09	676.2±50.0	9
DBE-DBCH	3322-93-8	4-(1,2-Dibromoethyl)-1,2- dibromocyclohexane	427.80	4.6	6.9147E+01	371.2±22.0	5
DBHCTD	51936-55-1	Hexachlorocyclopentadienyl- dibromocyclooctane	540.8	6.4	6.8425E-02	480.7±45.0	6
EH-TBB	183658-27-7	2-Ethylhexyl 2,3,4,5-tetrabromobenzoate	549.9	7.7	1.1437E-02	477.5±40.0	6
HBB	87-82-1	Hexabromobenzene	551.5	6.1	1.2778E-01	417.5±40.0	6
PBB-Acr	59447-55-1	Pentabromobenzyl acrylate	556.7	5.7	4.062E-01	477.7±40.0	7
PBBB	38521-51-6	Pentabromobenzyl bromide	565.5	5.9	1.4737E-01	460.4±40.0	2
PBBz	608-90-2	Pentabromobenzene	472.59	5.4	2.8292	376.1±37.0	6
PBEB	85-22-3	Pentabromoethylbenzene	500.64	6.2	3.9697E-01	413.3±40.0	6
PBP	608-71-9	Pentabromophenol	488.59	5	1.5962E+01	352.3±37.0	4
PBT	87-83-2	Pentabromotoluene	486.62	5.7	5.2712E-02	394.4±37.0	6
TBBPA	79-94-7	Tetrabromobisphenol A	543.9	6.8	2.1461	417.9±40.0	9
TBBPA- BDBPE	21850-44-2	Tetrabromobisphenol A bis(2,3dibromopropyl) ether	943.6	10.6	1.1642E-07	676.5±55.0	9
TBBPS- BME	70156-79-5	Tetrabromobisphenol S bismethyl ether	593.9	5.4	6.9385E-01	590.9±50.0	3
TBP-AE	3278-89-5	2,4,6-Tribromophenyl allyl ether	370.86	4.7	7.7929E+01	339.5±37.0	4
TBX	23488-38-2	2,3,5,6-Tetrabromo-p-xylene	421.75	5.4	4.7168	361.3±37.0	4
TDBP- TAZTO	52434-90-9	1,3,5-Tris(2,3-dibromopropyl) isocyanurate	728.7	4.1	1.1401E-02	618.8±55.0	7
TTBP-TAZ	25713-60-4	Tris(2,4,6-tribromophenoxy)-s-triazine	1067.4	11.8	1.8493E-08	812.2±75.0	6

¹ Acronyms given by Bergman et al., 2012 [126]. For compounds not reported by Bergman et al., 2012, commonly used accronyms were given.

	FOS	NIO	VEY	EST	MAI	SAM	СНЕ	SMH	SMN	PRA
				nBFI	Rs (ng.g ⁻¹ d.w.)					
2.4-DBP	3.80	4.89	3.42	4.14	6.75	0.16	1.86	12.49	9.61	2.16
2.4.6-TBP	0.57	0.89	1.46	2.44	0.94	0.12	1.40	3.19	1.28	1.64
BEH-TEBP	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
BTBPE	< LOD	< LOD	2.37	< LOD	0.86	< LOD				
DBDPE	< LOD	< LOD	< LOQ	< LOD	7.51	< LOQ	< LOD	< LOQ	< LOQ	< LOD
DBE-DBCH	0.09	0.14	0.33	2.56	0.05	0.08	0.15	0.53	0.24	1.48
DBHCTD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
EH-TBB	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
HBB	< LOD	< LOD	< LOD	< LOD	0.10	< LOD	< LOD	< LOD	< LOD	< LOQ
PBB-Acr	0.35	0.73	1.27	2.98	0.51	< LOD	2.39	1.89	0.83	1.85
PBBB	0.18	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOQ	0.19	< LOD
PBBz	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
PBEB	< LOD	< LOQ	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD
PBP	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
PBT	< LOQ	< LOQ	< LOD	< LOD	< LOQ	< LOD				
TBBPA	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
TBBPA-BDBPE	< LOD	< LOD	< LOQ	< LOD	< LOQ	< LOD	< LOD	< LOQ	< LOQ	< LOD
TBBPS-BME	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
TBP-AE	< LOD	< LOD	< LOD	0.37	< LOQ	< LOD				
TBX	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
TDBP-TAZTO	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
TTBP-TAZ	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
				PBD	Es (ng.g ⁻¹ d.w.)					
BDE 28	< LOQ	< LOQ	< LOD	< LOD	0.09	< LOD				
BDE 47	0.16	3.35	< LOD	0.41	2.16	< LOQ	< LOD	0.30	0.25	11.71
BDE 99	< LOQ	0.18	< LOD	< LOQ	0.13	0.06	3.54	0.60	0.70	< LOQ
BDE 100	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
BDE 153	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
BDE 154	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
BDE 183	< LOD	< LOD	< LOD	< LOD	< LOD	< LOD				
BDE 209	17.74	< LOQ	< LOQ	< LOD	19.96	< LOQ				

Table S9 : Concentrations of 38 halogenated flame retardants targeted in the suspended matter samples

	FOS	NIO	VEY	EST	MAI	SAM	CHE	SMH	SMN	PRA				
	PCBs $(ng.g^{-1} d.w.)$													
PCB 28	0.28	0.39	0.59	1.47	1.07	0.13	1.18	0.38	0.76	0.80				
PCB 52	0.10	0.27	0.17	0.61	1.28	0.25	0.41	0.13	0.41	0.31				
PCB 101	0.21	0.75	0.55	1.92	2.40	0.12	1.37	0.36	0.97	0.82				
PCB 118	0.26	1.08	0.74	3.11	3.67	0.13	1.92	0.59	1.64	1.07				
PCB 138	0.38	1.83	1.56	5.16	6.84	0.11	3.43	0.93	2.65	1.12				
PCB 153	0.42	1.94	1.37	5.66	8.14	0.12	3.26	0.96	2.74	1.24				
PCB 180	0.32	0.92	1.26	3.91	3.39	0.16	2.34	0.75	1.88	1.06				
				CP	s (ng.g ⁻¹ d.w.)									
CPs	184	257	< LOD	267	42	< LOD	323	< LOD	233	< LOD				

Table S9 (continued) : Concentrations of 38 halogenated flame retardants targeted in the suspended matter samples

		nBFRs						PBE	DEs					PCBs				CPs						
		2,4-DBP	2,4,6-TBP	BTBPE	DBDPE	DBE- DBCH	HBB	PBB-Acr	PBBB	PBT	TBBPA- BDBPE	TBP-AE	BDE 28	BDE 47	BDE 99	BDE 209	PCB 28	PCB 52	PCB 101	PCB 118	PCB 138	PCB 153	PCB 180	CPs
	2,4-DBP																							
	2,4,6- TBP	0,297																						
	BTBPE	0,0519	0,0259																					
	DBDPE	0,3551	-0,0804	0,5977																				
Rs	DBE- DBCH	0,1152	0,8788***	-0,2076	-0,3618																			
ΒFI	HBB	0,0432	0,0519	0,3642	0,2582	-0,1557																		
-	PBB-Acr	0,103	0,8909***	-0,147	-0,3551	0,8303	-0,1211																	
	PBBB	0,5443	-0,0373	-0,3193	0,1237	0,0075	-0,3193	-0,1566																
	PBT	0,2659	-0,5698	0,1627	-0,042	-0,6458*	0,2711	-0,5698	0,0467															
	TBBPA- BDBPE	0,6396*	0,2843	0,6086	0,825**	0	0,1521	0	0,3497	-0,0891														
	TBP-AE	0,4719	0,5394	-0,3208	0,1615	0,4944	0,1123	0,2922	0,5254	-0,4226	0,3953													
	BDE 28	0,2922	-0,5394	0,2566	0,0745	-0,6742*	0,3849	-0,5618	0	0,986****	0	-0,4167												
DEs	BDE 47	0,4073	0,1824	-0,1865	-0,1579	0,1885	0,59	0,0486	-0,1271	0,3429	-0,1069	0,3156	0,3607											
PBI	BDE 99	0,3252	-0,0429	-0,3941	0,1085	-0,2147	-0,1489	0,1288	0,2793	-0,0385	0,1439	0,2958	-0,0228	-0,0492										
	BDE 209	0,1268	-0,5294	0,3725	0,371	-0,7531*	0,4789	-0,6636*	0,2294	0,7011*	0,2623	-0,1383	0,7466*	0,0075	0,0377									
	PCB 28	0,0424	0,503	0,147	-0,1876	0,3939	0,3546	0,6848*	-0,3654	-0,1899	0	-0,0899	-0,1124	0,2128	0,1043	-0,2908								
	PCB 52	0,0973	0,1337	0,1128	0,0907	0,0243	0,4685	0,2979	-0,3665	-0,0381	0,0356	-0,1465	0,0676	0,3262	0,2708	-0,1421	0,8389**							
s	PCB 101	0,2485	0,3333	0,2076	0	0,1636	0,4671	0,4788	-0,2759	0,038	0,1421	-0,0899	0,1348	0,3343	0,2393	-0,082	0,9394****	0,924***						
g	PCB 118	0,297	0,2727	0,2076	0	0,103	0,3892	0,4424	-0,2759	0,114	0,1421	-0,1573	0,2023	0,3222	0,2884	-0,082	0,903***	0,9119***	0,9879****					
H	PCB 138	0,3091	0,2606	0,3027	0,0603	0,0788	0,3114	0,4303	-0,2759	0,114	0,2132	-0,2247	0,2023	0,2188	0,2638	-0,082	0,8788***	0,8754***	0,9636****	0,9879****				
	PCB 153	0,3091	0,2606	0,3027	0,0603	0,0788	0,3114	0,4303	-0,2759	0,114	0,2132	-0,2247	0,2023	0,2188	0,2638	-0,082	0,8788***	0,8754***	0,9636****	0,9879****	1****			
	PCB 180	0,2	0,4303	0,32	0,0268	0,2848	0,2941	0,5758	-0,2759	-0,114	0,2132	-0,1573	-0,0225	0,1277	0,1043	-0,2162	0,9515****	0,8511**	0,9515****	0,9394****	0,9515****	0,9515****		
CPs	CPs	0,0688	-0,0688	-0,3347	-0,515	-0,0063	-0,2901	0,3314	-0,0077	0,196	-0,3666	-0,3826	0,1623	-0,0282	0,4305	-0,2231	0,544	0,4955	0,5565	0,6253*	0,6253*	0,6253*	0,5378	

Table S10 : Non-parametric Spearman rank correlation across the detected compounds

p-values are indicated with the respective symbols : * for 0.05>p>0.01,** for 0.01>p>0.001, *** for 0.001>p>0.0001 and **** for p<0.0001. Significant correlations are displayed for p-values < 0,05.

Table S11 : Toxicity of the detected nBFRs (a) and risk quotients (RQ) obtained with EMP method (b) and C_{PW} method (c)

a) Toxicity of the detected nBFRs

	K _{OC} (pH 7.4) ¹	Toxicity (µg/L)	PNEC _{water} (µg.L ⁻¹) ⁶	PNEC _{sediment} (µg.kg ⁻¹) ⁷
2,4-DBP	1101.8	790 ²	0.79	19.5
2,4,6-TBP	314.7	260 ³	0.26	2.0
DBDPE	1000000	19 ⁴	0.019	4123.0
HBB	54002.4	10700 5	10.7	12547.2

¹ K_{OC} obtained with Chemspider (<u>https://www.chemspider.com/</u>), predicted with ACD/Labs Percepta Platform - PhysChem Module, version: 14.00

² LC₅₀, 96h, Green algae, Saltwater, obtained from ECOSAR

³ EC₅₀, 48h, Daphnia magna, obtained from SIDS Initial Assessment Report, 2,4,6-Tribromophenol, 2003 (https://hpvchemicals.oecd.org/UI/handler.axd?id=4b0a638b-3346-4217-8549-94637f6c0d32)

⁴ EC₅₀, 48h, Daphnia magna, obtained from Xiong, et al., 2019, DOI: 10.1021/acs.est.9b03159

⁵ LC₅₀, embryo mortality, Zebrafish, obtained from Xiong, et al., 2019, DOI: 10.1021/acs.est.9b03159

 6 PNEC_{water} = LC₅₀ or EC₅₀ / 1000

⁷ PNEC_{sediment} = $(0.783 + 0.0217 * K_{OC}) * PNEC_{water}$

b) Risk quotients obtained with the EPM method (RQ = MEC / PNEC_{sediments})

	FOS	NIO	VEY	EST	MAI	SAM	CHE	SMH	SMN	PRA
2,4-DBP	0.2	0.3	0.2	0.2	0.3	0.008	<mark>0.095</mark>	0.6	0.5	0.1
2,4,6-TBP	0.3	0.4	0.7	1.2	0.5	<mark>0.06</mark>	0.7	1.6	0.6	0.8
DBDPE	-	-	-	-	0.002	-	-	-	-	-
HBB	-	-	-	-	0.00001	-	-	-	-	-

RQ < 0.01: very low risk $0.01 \le RQ < 0.1$: low risk $0.1 \le RQ < 1$: medium risk $RQ \ge 1$: high risk

c) Risk quotients obtained with the C_{PW} * method from Di Toro et al., 1991 (RQ = C_{PW} / PNEC_{water})

	FOS	NIO	VEY	EST	MAI	SAM	CHE	SMH	SMN	PRA
2,4-DBP	0.4	0.3	0.1	<mark>0.095</mark>	0.2	0.004	<mark>0.04</mark>	0.3	0.2	<mark>0.03</mark>
2,4,6-TBP	0.7	0.6	0.5	0.6	0.4	<mark>0.035</mark>	0.3	0.8	0.3	0.2
DBDPE	-	-	-	-	0.00124	-	-	-	-	-
HBB	-	-	-	-	0.00001	-	-	-	-	-

RQ < 0.01 : very low risk

 $\frac{0.01 \le RQ < 0.1}{0.1 \le RQ < 1} : \text{low risk}$

 $0.1 \leq KQ < 1$. Integrating the

<mark>RQ≥1</mark> : high risk

* $C_{PW} = \frac{C_S}{f_{OC} * K_{OC}}$, with C_S the concentration in sediments (Table S9), f_{OC} the TOC (Table S1) and K_{OC} given in Table S11a

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