SUPPLEMENTARY MATERIAL

The (eco)toxicological effects of flame retardants emerging in water and sediment

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Abbreviations:

FR – flame retardant
OPFRs – organophosphorus flame retardants
TCPP – tris(2-chloropropyl) phosphate
TDCPP – tris(1,3-dichloro-2-propyl) phosphate
TCEP – tris(2-chloroethyl) phosphate
TPrP – tripropyl phosphate
TBOEP – tris(2-butoxyethyl) phosphate
TMP – trimethyl phosphate
TnBP – tri-n-butyl phosphate
TIBP – tri-iso-butyl phosphate
TEP – triethyl phosphate
TEHP – tris(2-ethylhexyl) phosphate
TPHP – triphenyl phosphate
TPPO – triphenylphosphine oxide
RDP – tetraphenyl m-phenylene bis(phosphate)
EHDPP – 2-ethylhexyl diphenyl phosphate
NBFRs – novel brominated flame retardants
HBCD – hexabromocyclododecane
DPTE – 2,3-dibromopropyl 2,4,6-tribromophenyl ether
HBB – hexabromobenzene
BTBPE – 1,2-bis(2,4,6-tribromophenoxy)ethane
EHTBB – 2-ethylhexyl-2,3,4,5-tetrabromobenzoate
DBDPE – decabromodiphenylethane
TBP – 2,4,6-tribromophenol
PBP – pentabromophenol
PBBz – pentabromobenzene
PBEB – 2,3,4,5,6-pentabromoethylbenzene
TBX – 2,3,5,6-tetrabromo-p-xylene
PBT – pentabromotoluene
α-TBCO – 1,2,5,6-tetrabromocyclooctane
DBE-DBCH –1,2-dibromo-4-(1,2-dibromoethyl) cyclohexane
BEHP – bis(2-ethylhexyl) phthalate
BEH-TEBP – bis(2-ethylhexyl) tetrabromophthalate
K_{OW} – octanol-water partition coefficient
EC_{50} – half maximal effective concentration
LC_{50} – median lethal concentration

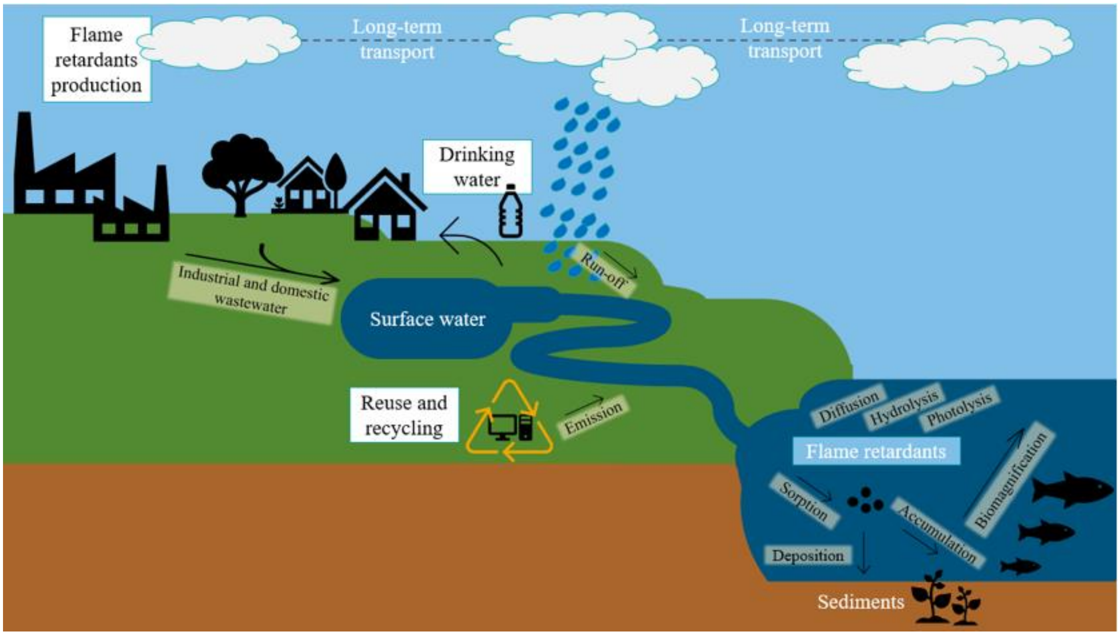

Fig. S1. Occurrence of flame retardants in the environment; source: own elaboration based on: Hou *et al*. (2021), Miranda *et al*. (2022) and Wang *et al*. (2023)

Table S1. Selected physicochemical properties of flame retardants including organophosphorus (OPFRs) and novel brominated flame retardants (NBFRs)

Group	Flame retardant	Molecular weight ($g{\cdot}mol^{-1}$)	Water solubility ($mg{\cdot}dm^{-3}$) at 25°C	Vapour pressure (Pa) at 25°C	log K_{OW}
OPFRs	TCPP	327.57	$1.20{\cdot}10^{-3}$	$7.52{\cdot}10^{-3}$	2.59
	TDCPP	430.89	7.00	$3.81{\cdot}10^{-5}$	3.65
	TCEP	285.49	$7{\cdot}10^{-3}$	$4.25{\cdot}10^{-2}$	1.78
	TBOEP	398.47	$1.10{\cdot}10^{-3}$	$1.64{\cdot}10^{-4}$	3.75
	TnBP	266.31	7.35	$4.65{\cdot}10^{-1}$	4.00
	TEP	182.15	$5.00{\cdot}10^{-5}$	$2.2{\cdot}10^{-1}$	0.87
	TPrP	224.24	$6.45{\cdot}10^{-3}$	3.08	2.35
NBFRs	DBDPE	971.22	$2.10{\cdot}10^{-7}$	$6.00{\cdot}10^{-15}$	11.1
	BTBPE	687.64	$1.90{\cdot}10^{-5}$	$3.88{\cdot}10^{-10}$	8.31
	EHTBB	549.92	$1.10{\cdot}10^{-5}$	$4.57{\cdot}10^{-6}$	7.73
	TBP	330.8	–	$1.50{\cdot}10^{-3}$	4.40
	PBP	448.6	–	$1.91{\cdot}10^{-5}$	5.22
	HBB	551.5	$1.6{\cdot}10^{-7}$	$1.14{\cdot}10^{-4}$	6.07
	PBT	486.6	$7.80{\cdot}10^{-4}$	$1.22{\cdot}10^{-3}$	6.99
	PBEB	500.7	$3.5{\cdot}10^{-4}$	$3.2{\cdot}10^{-4}$	6.40

Source: own elaboration based on: Al-Omran (2018), Xiong *et al.* (2019) and Kung *et al.* (2022).

Table S2. Concentrations of flame retardants including organophosphorus (OPFRs) and novel brominated flame retardants (NBFRs) in water and sediment

Group	Flame retardant	Water concentration ($ng \cdot dm^{-3}$)	Sediment concentration ($ng \cdot g^{-1}$)	Details, location	Reference
OPFRs (Cl-alkyl)	TCPP	651.65	4.77	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		217.5	3.5	surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		594	637	Lake Shikwa, Korea	Lee *et al.* (2018)
		85.44	29.65	Yangtze River, China	Zha *et al.* (2018)
		5120	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		864–3277	NS	influent wastewater, Greece	Wang *et al.* (2023)
		6750	NS	influent wastewater, Spain	Cristale *et al.* (2016)
		NS	6.42	influent wastewater, Evrotas River, Greece	Giulivo *et al.* (2017)
		NS	17.0	Adige River, Italy	Giulivo *et al.* (2017)
	TDCPP	308.14	20.76	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		12.6	–	Surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		48.1	103	Lake Shikwa, Korea	Lee *et al.* (2018)
		0.65	2.23	Yangtze River, China	Zha *et al.* (2018)
		1720	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		29.8–310	NS	influent wastewater, Greece	Wang *et al.* (2023)
		290	NS	influent wastewater, Spain	Cristale *et al.* (2016)
	TCEP	4776.73	103.52	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		144.8	1.0	surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		706	57.9	Lake Shikwa, Korea	Lee *et al.* (2018)
		5.92	4.80	Yangtze River, China	Zha *et al.* (2018)
		1430	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		50.3–186	NS	influent wastewater, Greece	Wang *et al.* (2023)
		320	NS	influent wastewater, Spain	Cristale *et al.* (2016)
		NS	1.64	Adige River, Italy	Giulivo *et al.* (2017)

Group	Flame retardant	Water concentration ($ng\cdot dm^{-3}$)	Sediment concentration ($ng\cdot g^{-1}$)	Details, location	Reference
OPFRS (non–Cl alkyl)	TPrP	7.21	–	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		7.6	0.4	surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		1.42	2.30	Yangtze River, China	Zha *et al.* (2018)
		21.2	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
	TBOEP	27.22	3.25	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		436	213	Lake Shikwa, Korea	Lee *et al.* (2018)
		30100	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		476–4037	NS	influent wastewater, Greece	Wang *et al.* (2023)
		1200	NS	influent wastewater, Spain	Cristale *et al.* (2016)
		NS	1.60	influent wastewater, Evrotas River, Greece	Giulivo *et al.* (2017)
		NS	0.96	Adige River, Italy	Giulivo *et al.* (2017)
	TMP	206.87	–	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
	TnBP	18.96	–	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		18.3	3.2	surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		40.3	6.44	Lake Shikwa, Korea	Lee *et al.* (2018)
		1.29	6.27	Yangtze River, China	Zha *et al.* (2018)
		18.96	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		28.9–129.8	NS	influent wastewater, Greece	Wang *et al.* (2023)
		210	NS	influent wastewater, Spain	Cristale *et al.* (2016)
		NS	4.73	influent wastewater, Evrotas River, Greece	Giulivo *et al.* (2017)
	TIBP	35.26	–	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		1.2	0.2	surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		57.9	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		1340	NS	influent wastewater, Spain	Cristale *et al.* (2016)

Group	Flame retardant	Water concentration ($ng \cdot dm^{-3}$)	Sediment concentration ($ng \cdot g^{-1}$)	Details, location	Reference
OPFRS (non–Cl alkyl)	TEP	86.25	–	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		2.9	0.2	surface seawater, Qinzhou Bay, China	Zhang *et al.* (2021)
		459	23.2	Lake Shikwa, Korea	Lee *et al.* (2018)
		501	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
	TEHP	–	33.02	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		4.96	9.21	Lake Shikwa, Korea	Lee *et al.* (2018)
		392	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		69.5–1299.0	NS	influent wastewater, Greece	Wang *et al.* (2023)
		131	NS	influent wastewater, Spain	Cristale *et al.* (2016)
		NS	4.73	influent wastewater, Evrotas River, Greece	Giulivo *et al.* (2017)
		NS	9.63	Adige River, Italy	Giulivo *et al.* (2017)
OPFRs (aryl)	TPHP	8.83	2.70	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		25.6	59.4	Lake Shikwa, Korea	Lee *et al.* (2018)
		0.24	2.22	Yangtze River, China	Zha *et al.* (2018)
		491	NS	influent wastewater, New York, USA	Kim *et al.* (2017)
		250	NS	influent wastewater, Spain	Cristale *et al.* (2016)
	TPPO	190.81	13.47	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
		17.12	1.63	Yangtze River, China	Zha *et al.* (2018)
	RDP	177.02	–	Maozhou and Guanlan rivers, China	Liu *et al.* (2022)
	EHDPP	9.87	10.3	Lake Shikwa, Korea	Lee *et al.* (2018)
		153	NS	influent wastewater, Spain	Cristale *et al.* (2016)
		NS	6.42	Adige River, Italy	Giulivo *et al.* (2017)

Group	Flame retardant	Water concentration (ng·dm^{-3})	Sediment concentration (ng·g^{-1})	Details, location	Reference
NBFRs	HBCD	1770	16.1	Vaal River, South Africa	Chokwe *et al.* (2015)
	DPTE	67	36	Ulsan and Onsan Bays, Korea	Lee *et al.* (2020)
	HBB	100	86	Ulsan and Onsan Bays, Korea	Lee *et al.* (2020)
		48	53	influent wastewater, Spain	Cristale *et al.* (2015)
	BTBPE	60	88	Ulsan and Onsan Bays, Korea	Lee *et al.* (2020)
	EHTBB	–	45	Ulsan and Onsan Bays, Korea	Lee *et al.* (2020)
		21	11	influent wastewater, Spain	Cristale *et al.* (2015)
	DBDPE	–	48	Ulsan and Onsan Bays, Korea	Lee *et al.* (2020)
		230	353	influent wastewater, Spain	Cristale *et al.* (2015)
	TBP	0.18	0.15	the Beijiang River, China	Xiong *et al.* (2016)
	PBP	0.16	–		
	PBBz	0.0015	–	Archipelago Svalbard, Norway	Carlsson *et al.* (2018)
	PBEB	–	0.0025	Archipelago Svalbard, Norway	Carlsson *et al.* (2018)
		18	3.7	influent wastewater, Spain	Cristale *et al.* (2015)
	TBX	–	0.0008	Archipelago Svalbard, Norway	Carlsson *et al.* (2018)
	PBT	0.0002	–	Archipelago Svalbard, Norway	Carlsson *et al.* (2018)
		12	14	influent wastewater, Spain	Cristale *et al.* (2015)
	α-TBCO	0.030	–	Archipelago Svalbard, Norway	Carlsson *et al.* (2018)
	DBE-DBCH	0.0003	0.0024	Archipelago Svalbard, Norway	Carlsson *et al.* (2018)

*NS – not studied.

Source: own study.