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Spatial distribution and potential ecological risk of traditional and emerging organic toxic substances in sediments along the Yangtze River, China☆

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ABSTRACT

This study investigated 63 persistent toxic substances (PTSs) in surface sediments along the Yangtze River, analyzing contamination levels, spatial distribution, sources, and ecological risks. High PTS levels were observed in Nanjing due to organic pollution, with significant regional variations in styrene oligomers (SOs), alkylphenols (APs), and polyhalogenated carbazoles (PHCZs) in Nantong, Changzhou, and Shanghai, respectively. These patterns were linked to local anthropogenic activities, with higher contamination in more densely populated and industrialized areas. PCBs persisted due to legacy products and combustion sources, while fresh inputs of SOs and APs were common. Hazard quotient (HQ) analysis revealed high risks in Nanjing ($HQ \geq 10$) and moderate risks ($1.0 \leq HQ < 10$) in Taizhou, Suzhou, and Nantong. Polycyclic aromatic hydrocarbons were the primary contributors to HQ, with SOs, APs, and PHCZs also impacting specific regions. This study highlights the need for continued monitoring and management of both traditional and emerging PTSs, emphasizing the growing environmental relevance of emerging contaminants along the Yangtze River.

1. Introduction

Human activities have historically been concentrated along major rivers and coastal areas, utilizing these water resources for various purposes (Geyer et al., 2017; Gleick, 2000). In recent decades, rapid development and industrialization have significantly exacerbated the pollution of adjacent aquatic environments (Cheng et al., 2013; Müller et al., 2008). High population densities in metropolitan and industrial areas generate substantial volumes of domestic and industrial wastewater, which are treated in wastewater treatment facilities before discharge (Acir and Guenther, 2018). However, persistent toxic substances (PTSs) that are difficult to decompose and chemicals used in sewage treatment processes continue to impact aquatic ecosystems negatively, along with hazardous substances introduced through non-point sources (Thiele et al., 1997). Among the pollutants entering aquatic environments, PTSs pose a significant threat due to their physicochemical properties, including hydrophobicity and resistance to degradation (Bhavya et al., 2021). PTSs typically exhibit a high log octanol-water partition coefficient (log K_{OW}) of approximately 4 or greater, which facilitates strong adsorption to suspended particles and ultimately leads to their accumulation in sediments (Wang et al., 2021a). These PTSs, once accumulated in sediments, can have direct ecotoxic effects on benthic organisms and cause secondary pollution through resuspension, biotransformation, and decomposition (Sanganyado et al., 2021).

As concerns about environmental pollution have grown, numerous studies have been conducted to identify and manage the environmental impacts of hazardous substances. Early research primarily focused on monitoring the distribution of compounds with direct and adverse effects on aquatic ecosystems (Kaimoussi et al., 2002). These substances were recognized for their significant ecological risks and regulated as priority control substances in many countries. A notable example is

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polychlorinated biphenyls (PCBs), which were industrially utilized in products such as insulating oils and transformers. Between 1930 and 1993, approximately 1.3 million tons of PCBs were produced and used globally (Breivik et al., 2002). Due to their hepatotoxicity and neurotoxicity to aquatic organisms and humans and their persistence and bioaccumulation characteristics, PCBs were designated as persistent organic pollutants (POPs) under the Stockholm Convention in 2001 (Stockholm Convention, 2001; Yin et al., 2017). Similarly, alkylphenols (APs), widely used in detergents and antioxidants, exhibited strong estrogenic activity, posing significant ecological risks. Consequently, regulations introduced in the 2000s promoted the adoption of alternative compounds and aimed to reduce their usage (Guenther et al., 2002).

In addition to previously regulated compounds such as PCBs and APs, increasing attention has been drawn to the environmental impacts of unregulated compounds with similar origins, molecular structures, and toxicological properties. The environmental impact of these unregulated toxic substances is often comparable to, or even greater than, that of regulated compounds in certain regions (Hong et al., 2023). Moreover, the ongoing development and application of various chemicals in manufacturing processes continue to exacerbate the influence of unregulated PTSs, emphasizing the critical need for monitoring and research to understand better their environmental implications. Recent studies have identified compounds such as styrene oligomers (SOs), which leach from plastics and expandable polystyrene, as emerging contaminants. These compounds have been shown to induce genotoxic and reproductive toxic effects in organisms, with high concentrations detected in aquatic environments due to the widespread use of their source materials (Hong et al., 2016). Similarly, polyhalogenated carbazoles (PHCZs), which are byproducts of electronics and dye manufacturing, exhibit high persistence and bioaccumulation potential (Riddell et al., 2015). Due to their structural similarity to dioxins, PHCZs have been recently recognized as substances that pose significant risks to aquatic ecosystems (Kuehl et al., 1984).

The objectives of this study are: (i) to evaluate the spatial distribution and concentration levels of traditional and emerging PTSs in sediments of the Yangtze River, spanning approximately 350 km through several major cities in China; (ii) to compare the concentrations and compositions of PTSs across different cities to identify potential sources; and (iii) to assess the potential ecological risks associated with traditional and emerging PTSs using hazard quotient (HQ) analysis based on the ECOSAR model.

2. Materials and methods

2.1. Study area and sample collection

The sampling sites of this study correspond to that examined by Hong et al. (2022). Surface sediments were collected from nine cities along the Yangtze River (Latitude: 30°85′–32°28′ N; Longitude: 118°49′–121°90′ E) (Fig. 1). This region has the highest population density among river basin cities worldwide, and numerous substances are discharged into the nearby Yangtze River through anthropogenic activities (Yang et al., 2012). In addition, based on abundant local water resources, it has become one of China's representative heavy industrial areas, with major industries such as coal, steel, cement, and chemical fibers, as well as a well-developed automobile sector (Cheng et al., 2013). The area experiences a subtropical, warm, and humid climate, with an average annual precipitation of approximately 1050 mm, contributing to significant inputs of terrestrial materials, suspended particles, and precipitation into the nearby East China Sea (Liu et al., 2022). Surface sediments (0–2 cm) were collected using pre-cleaned glass containers and stored at −20 °C until further processing. Prior to analysis, the samples were homogenized and freeze-dried. Detailed location data, as well as analyses of total organic carbon (TOC), total nitrogen (TN), and carbon stable isotope ratios ($\delta^{13}C$) were conducted and partially reported in a previous study (Hong et al., 2022).

2.2. Analyses of PCBs, SOs, and APs

The methods for analyzing PTSs in sediments were adapted from previously established protocols (Kim et al., 2024). A total of 32 PCB congeners, 10 SO compounds, and 6 AP compounds were analyzed. PCB

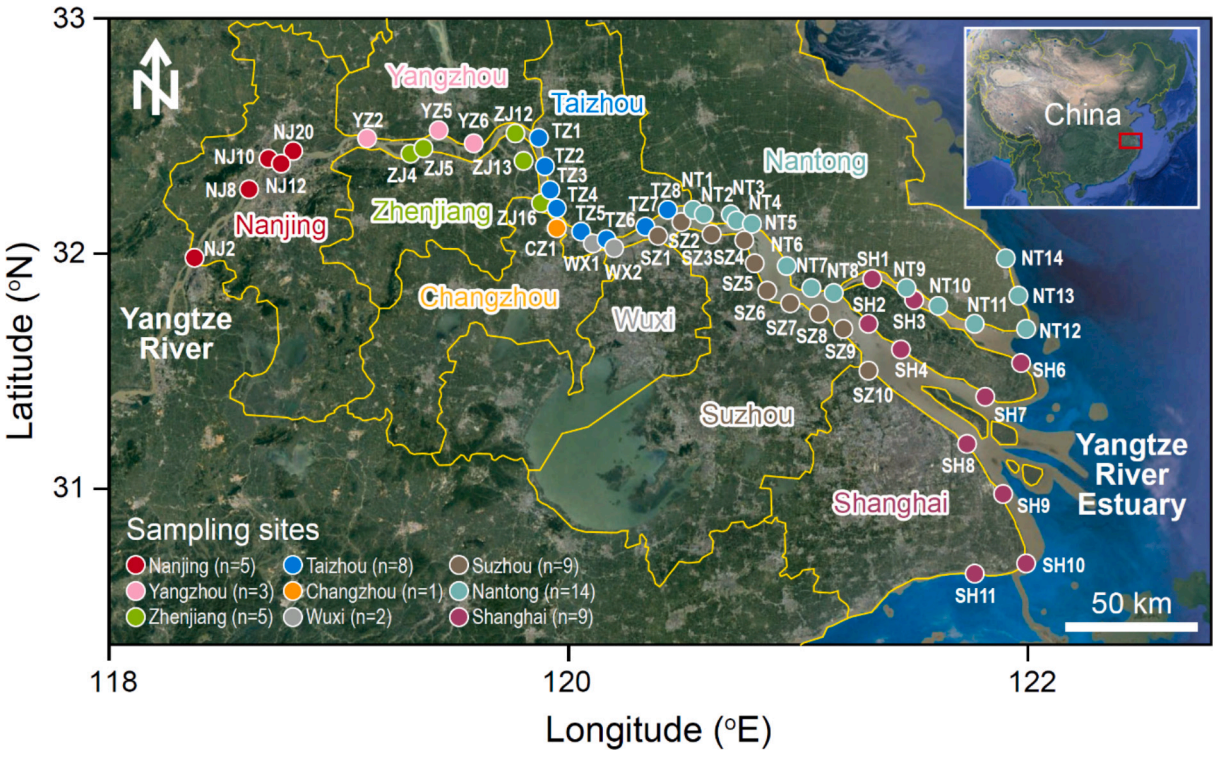

Fig. 1. Map showing the sampling sites of sediments along the Yangtze River in China.

congener standard materials were purchased from Sigma-Aldrich (Saint Louis, MO), and SOs were obtained from Wako Pure Chemical Ind. (Osaka, Japan) and Hayashi Pure Chemical Ind. (Osaka, Japan). AP standards were purchased from Sigma-Aldrich. Approximately 10 g of freeze-dried sediment samples were extracted using an accelerated solvent extractor (Dionex ASE 350, Thermo Scientific, Salt Lake City, UT) with dichloromethane (DCM, Burdick & Jackson, Muskegon, MI). To ensure accurate recovery rates, isotopically labeled surrogate standards with similar chemical properties but distinguishable by mass were spiked into each sample to validate the experimental procedure (Table S1). Procedural blanks were also included in each analytical batch to check for potential contamination, and no contamination was detected throughout the analysis. Organic extracts were concentrated using a TurboVap concentrator (TurboVap LV, Biotage, Uppsala, Sweden), and the solvent was exchanged for hexane (Burdick & Jackson). Sulfur compounds were removed by treating the extracts with activated copper (Merck, Darmstadt, Germany) for 1 h.

The extracts were then purified and fractionated using open-column chromatography with activated silica gel (70–230 mesh, Sigma-Aldrich). The first fraction (F1) was eluted with 30 mL hexane to obtain PCBs. The second fraction (F2) was eluted with 60 mL hexane: DCM (8:2, *v/v*) for SOs. The third fraction (F3) was eluted with 50 mL of 60% DCM in acetone (J.T. Baker, Center Valley, PA) to obtain APs. Each fraction was concentrated to 1 mL under a flow of N_2 gas (TurboVap), and 100 ng of an internal standard (2-fluorobiphenyl, ChemService, West Chester, PA) was added to each sample. The target PTSs were quantified using an Agilent 7890B gas chromatograph (GC) coupled with a 5977B mass selective detector (MSD, Agilent Technologies, Santa Clara, CA). Detailed recovery rates and instrumental conditions are provided in the Supplementary Materials (Table S2).

2.3. Analysis of PHCZs

The analytical method for PHCZs was slightly modified from that described in the previous study (Wu et al., 2017a). A total of 15 PHCZs were analyzed. Freeze-dried sediment samples (5 g) were extracted using an accelerated solvent extractor with DCM. Elemental sulfur was removed by treatment with activated copper, and the extract was concentrated to 0.5 mL. Before clean-up using a solid-phase extraction (SPE) cartridge, the cartridge was conditioned and activated by washing with 10 mL of hexane. The concentrated extract was then loaded onto an ISOLUTE® SI cartridge (2 g, 6 mL, Biotage), and the cartridge was eluted with 10 mL of hexane:DCM (4:6, *v/v*). The eluate was then concentrated to 0.5 mL under a stream of N_2 gas. An internal standard was added to each sample prior to GC–MS/MS (7000C Quadrupole MS/MS, Agilent Technologies) analysis to assess instrumental sensitivity. Detailed recovery rates and instrumental conditions are provided in Tables S3 and S4.

2.4. Data analysis and statistics

To identify the sources of PCBs, principal component analysis (PCA) was performed using the compositional profiles of PCBs in sediments and those released from industrial products and combustion-related sources. The concentration data of PCBs used for PCA were standardized using *Z*-scores, and their normality was verified. The validity of the PCA was confirmed using varimax rotation, along with Bartlett's test of sphericity and the Kaiser-Meyer-Olkin (KMO) measure of sampling adequacy. The correlation matrix was deemed appropriate for PCA as the KMO index exceeded 0.6, indicating sufficient suitability for the analysis.

2.5. Potential ecological risk assessment

The HQ approach was employed to evaluate and compare the potential ecological risks of PTSs in sediments of the Yangtze River. The HQ was calculated using the predicted no-effect concentration (PNEC) and the measured environmental concentration (MEC) of PTSs, as defined in Eq. (1):

$$HQ = \frac{MEC}{PNEC_{sediment}} \tag{1}$$

The toxicity data currently used are largely based on tests with aquatic organisms, which limits their direct applicability to sediment environments. Moreover, key parameters in the risk calculation are derived from estimations rather than direct measurements, introducing additional uncertainty. The ecological effects of PTSs in sediments were assessed using the equilibrium partitioning approach, which accounts for the distinct forms and impacts of PTSs in sediment compared to their dissolved or particulate forms in the aquatic environment (Li et al., 2016). Due to limited experimental toxicity data for the PTSs analyzed in this study, toxicity information for individual compounds was derived from ECOSAR model predictions. The PNEC for sediments ($PNEC_{sediment}$) was calculated using Eqs. (2), (3), and (4):

$$K_{susp-water} = F_{water,susp} + F_{solid,susp} \times \frac{F_{oc,susp} \times K_{oc}}{1000} \times \rho_{solid} \tag{2}$$

$$PNEC_{water} = \frac{L(E)C50}{AF} \tag{3}$$

$$PNEC_{sediement} = \frac{K_{susp-water}}{\rho_{susp}} \times PNEC_{water} \times 1000 \tag{4}$$

Where, $K_{susp\text{-}water}$: Suspended solid-water partition coefficient ($m^3\ m^{-3}$); $F_{water,susp}$: Proportion of water in suspension (0.9 $m^3\ m^{-3}$); $F_{solid,susp}$: Proportion of solid matter in suspension (0.1 $m^3\ m^{-3}$); $F_{oc,susp}$: Organic carbon mass percentage in suspended solids (0.1 kg kg^{-1}); K_{oc}: Organic carbon–water partition coefficient (L kg^{-1}) (Gao et al., 2019); ρ_{solid}: Density of the solid phase (2500 kg m^{-3}); AF: Assessment factor; and ρ_{susp}: Density of wet suspended matter (1150 g L^{-1}). Ecological risks were classified into four levels based on existing literature (Lemly, 1996): acceptable risk (HQ < 0.1), low risk (0.1 ≤ HQ < 1), moderate risk (1 ≤ HQ < 10), and high risk (HQ ≥ 10).

3. Results and discussion

3.1. Spatial distributions of PTSs in sediments along the Yangtze River

3.1.1. Polychlorinated biphenyls (PCBs)

PCBs were detected in sediments at all sampling sites along the Yangtze River, with concentrations ranging from 0.96 to 38 ng g^{-1} dry weight (dw) (mean: 4.7 ng g^{-1} dw). Significant variations in PCB concentrations were observed across different sampling locations (Table S5). Sites NJ12, SZ1, SZ8, and SH1, located in Nanjing, Suzhou, and Shanghai, exhibited relatively high levels of PCB contamination (Fig. 2a). Notably, PCB concentrations at NJ12 and SH1 exceeded the threshold effects level guidelines of NOAA (21.5 ng g^{-1} dw), indicating potential ecological risks (Fig. 3a). Excluding site NJ12, which exhibited elevated levels of organic matter and all PTSs, a comparative analysis of PCB contamination across different cities was conducted. The average PCBs concentration across the study area was 6.3 ng g^{-1} dw, with the highest levels observed in Shanghai, followed by Suzhou (5.8 ng g^{-1} dw) (Fig. 3a). Both cities are highly populated and industrialized, with Shanghai serving as a major maritime transport hub and hosting numerous industrial complexes (Chen et al., 2001; Liu et al., 2022). Consequently, PCBs derived from insulating oil products were detected at elevated concentrations. The pollution levels in Shanghai and Suzhou were relatively lower than those reported in the Pearl River and Qiantang River regions but were comparable to earlier studies conducted along the Yangtze River (Wang et al., 2011b, 2017; Yang et al., 2012) (Table 1). The composition of PCBs revealed tetra-CBs as the most prevalent congeners overall, while Shanghai exhibited a higher

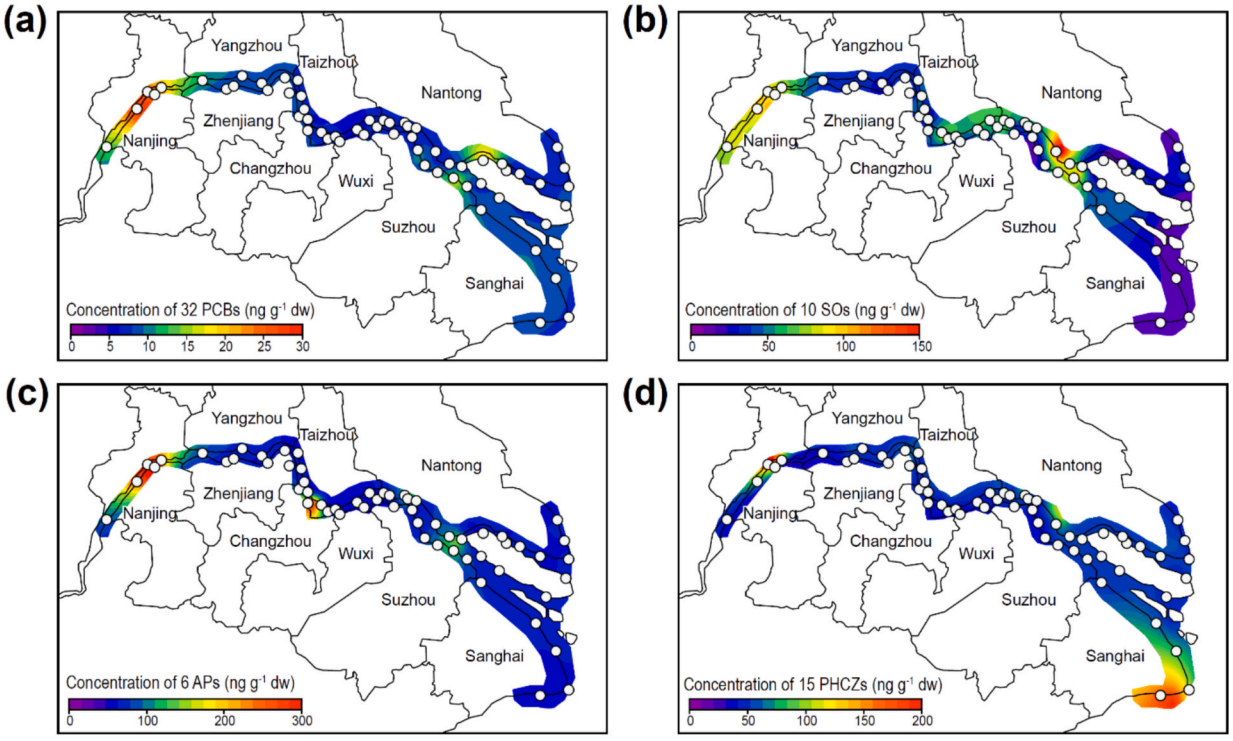

Fig. 2. Distributions of (a) polychlorinated biphenyls (PCBs), (b) styrene oligomers (SOs), (c) alkylphenols (APs), and (d) polyhalogenated carbazoles (PHCZs) in sediments along the Yangtze River, China.

proportion of penta-CBs compared to other regions. This suggests that the sources and inputs of PCBs in Shanghai differ from those in other areas (Wang et al., 2017).

The distribution and fate of organic pollutants, including PCBs, are known to correlate with organic carbon contents (Bergamaschi et al., 1997). In this study, highly chlorinated PCBs showed a positive correlation with TOC and TN contents, while no significant correlation was observed for less chlorinated PCBs (Fig. 4a). These differences are likely due to the lower environmental persistence of low-molecular-weight chlorinated biphenyls (Wang et al., 2023). Additionally, substantial differences in PCB concentrations were observed between hotspot areas and their surroundings. A significant negative correlation was observed between highly chlorinated PCBs among PTSs and $\delta^{13}C$ values, indicating that these compounds may have been introduced alongside terrestrial organic matter (Hong et al., 2022). This spatial distribution pattern suggests that PCBs introduced from pollution sources tend to accumulate near the sources rather than being transported extensively with organic matter or particles (Fig. S1).

3.1.2. Styrene oligomers (SOs)

The contamination levels of SOs in the Yangtze River sediments ranged from 5.7 to 180 ng g^{-1} dw, with a mean concentration of 31 ng g^{-1} dw (Table S6). The highest contamination level was observed at site NT6 in Nantong, followed by elevated levels at sites NJ12 and SZ8 (Fig. 2b). Nantong is known for its high concentration of plastic-derived materials, including polypropylene and polyethylene, compared to other study areas (Xiong et al., 2019). Additionally, site NT12, which also exhibited high SO concentrations, is located near major water sources, such as the Yangtze River, where significant levels of plastic-derived materials have been detected. These findings suggest that SO contamination, known to be influenced by waterborne transport, is closely associated with nearby land use and pollution sources (Kim et al., 2021).

Among the study regions, cities such as Changzhou (41 ng g^{-1} dw), Taizhou (38 ng g^{-1} dw), and Nantong (35 ng g^{-1} dw) displayed relatively higher SO pollution levels (Fig. 3b). These cities are characterized by high population density, proximity to significant water sources, and industrial activities. The contamination levels of SOs in Yangtze River sediments were higher than those reported in Qingdao and Tianjin, but lower than levels found in Saemangeum and Sihwa Lake, South Korea (Tian et al., 2020; Yoon et al., 2017, 2020) (Table 1). SOs are primarily transported through aquatic systems, and their presence is strongly linked to the use of plastic-based materials, including packaging (Kwon et al., 2015). The composition of SOs showed no significant regional variation, with styrene trimers (STs) being predominant, accounting for an average of 75% of the detected SOs. The presence of styrene dimers (SDs), which are byproducts of the weathering process of STs, indicates that the high proportion of STs reflects ongoing SOs contamination in the study area (Tian et al., 2020).

3.1.3. Alkylphenols (APs)

The contamination levels of APs in sediments across the Yangtze River basin ranged from 9.6 to 430 ng g^{-1} dw, with a mean concentration of 44 ng g^{-1} dw (Table S7). The highest concentration, 430 ng g^{-1} dw, was recorded at the NJ12 site, with relatively high levels also observed in Changzhou (Fig. 2c). Significant spatial variations in AP concentrations were noted, with lower levels detected outside of Nanjing and Changzhou. The elevated concentrations at NJ12 are likely influenced by sludge, as AP concentrations are strongly correlated with organic matter content (Soares et al., 2008). In contrast, despite its lower organic matter content, Changzhou exhibited high AP concentrations, attributed to its status as a major industrial hub for pesticide, dye, and fine chemical production (Liu et al., 2016). Similarly, high levels of APs have been detected in nearby water bodies, such as Taihu, located near Changzhou and Wuxi (Gao et al., 2019). Changzhou exhibited the highest AP contamination levels among the study areas, followed by Nantong and Suzhou (Fig. 3c). Suzhou and Nantong, located in the lower reaches of the Yangtze River, are densely populated regions where phenolic compounds from upstream cities are likely to accumulate (Li et al., 2016). Although Shanghai showed relatively high AP levels, it did

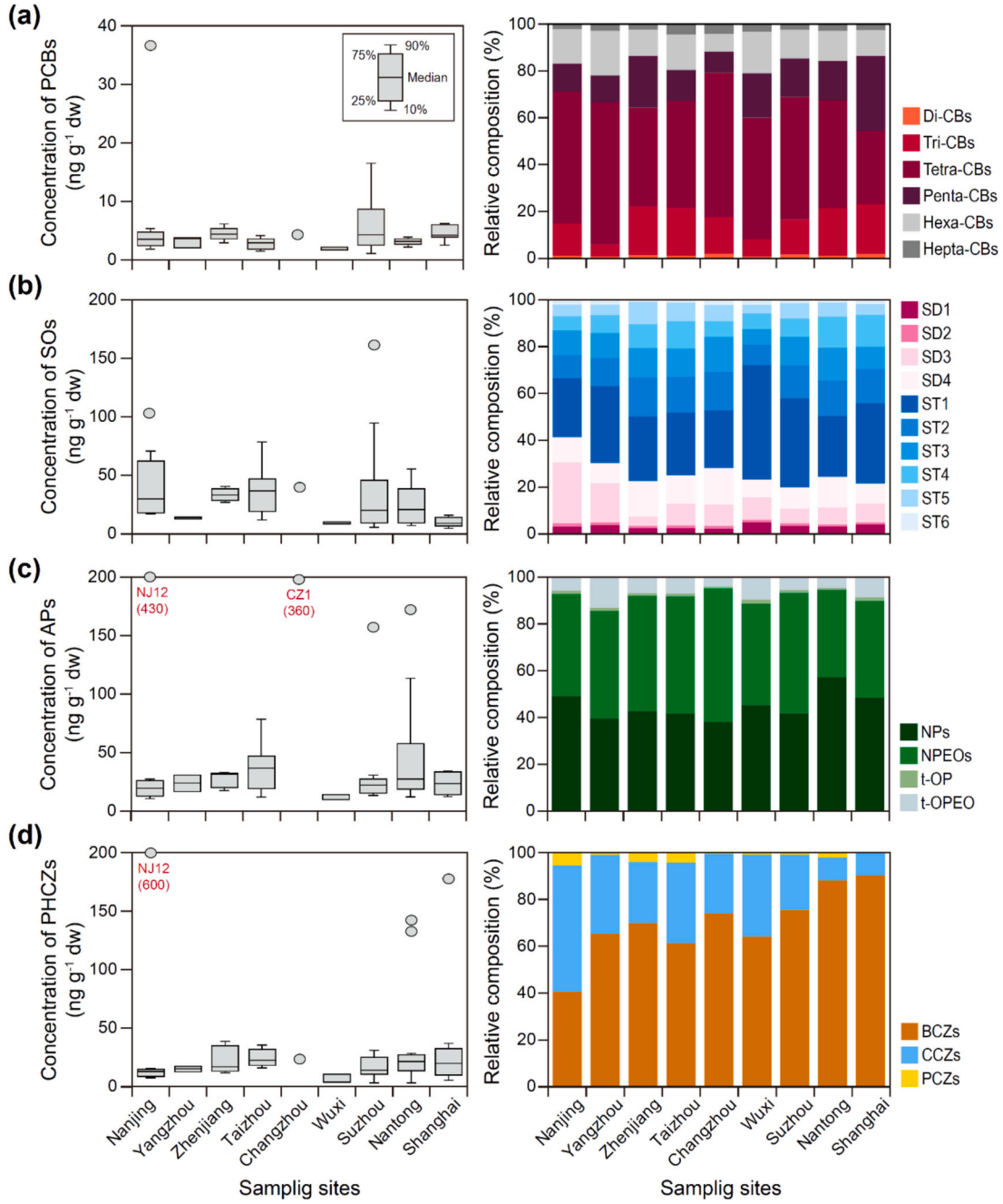

Fig. 3. Average concentrations and relative compositions of persistent toxic substances, including (a) PCBs, (b) SOs, (c) APs, and (d) PHCZs, in sediments along the Yangtze River, China.

not exhibit the highest contamination, likely due to the dilution effect caused by sediment accumulation in coastal areas with slower flow rates (Wang et al., 2020). Similar to SOs, APs are waterborne and influenced by nearby water sources (Kim et al., 2021).

The elevated AP levels in Suzhou are also likely influenced by surrounding water bodies, consistent with the patterns observed for SOs (Li et al., 2016). However, the limited number of sampling points in Changzhou represents a limitation of this study. The AP concentrations observed in this study were higher than those reported in Tianjin and Qingdao, China, but lower than levels in the South China Sea (Yoon et al., 2020) (Table 1). Compared with international regions, the contamination levels were higher than those found in the Adriatic and Baltic Seas (Combi et al., 2016; Koniecko et al., 2014). The composition of APs across all sampling sites was predominantly composed of nonylphenol compounds, with octylphenol compounds contributing a smaller proportion (Sharma et al., 2009). The relatively recent implementation of regulations on APs in China and the broader industrial and commercial use of nonylphenol compared to octylphenol likely explain the observed differences in usage and contamination levels (Kim et al., 2021).

3.1.4. *Polyhalogenated carbazoles (PHCZs)*

The contamination levels of PHCZs ranged from 2.6 to 600 ng g^{-1} dw, with a mean of 36 ng g^{-1} dw (Table S8). Similar to other organic pollutants, the highest PHCZs concentration was observed at the site NT12, with relatively high levels detected at several sites in Nantong and Shanghai (Fig. 2d). Apart from certain sites in Nanjing with high organic matter content, elevated concentrations were primarily found in the

Table 1
Concentration ranges of persistent toxic substances in sediments of rivers, estuaries, and coastal areas obtained from this study and previous studies.

PTSs	Regions	Sampling year	# of Sites	# of target compounds	Concentration (ng g^{-1} dw)			References
					Min	Max	Mean	
PCBs	Daliao River	2007	39	41	0.83	7.3	1.8	Men et al. (2014)
	Minjiang River	1999	9	21	15	58	34	Zhang et al. (2003)
	Pearl River	2008	29	37	5.1	11	8.0	Wang et al. (2011b)
	Qiantang River	2007	50	22	5.1	20	10	Yang et al. (2012)
	Tonghui River	2022	16	12	0.78	8.5	3.3	Zhang et al. (2004)
	Yangtze River	2005	27	39	1.2	45	9.2	Yang et al. (2009)
		2012	14	14	1.5	46	9.1	Wang et al. (2017)
		2016	34	16	0.36	69	6.6	Cui et al. (2020)
		2020	18	7	< LOD	3.4	0.37	Wang et al. (2023)
		2019	56	32	0.96	38	4.7	This study
SOs	Arabian Gulf	2017	3	10	0.9	6.0	2.8	Yoon et al. (2019)
	Gyeonggi Bay	2015	4	10	20	35	25	Hong et al. (2016)
	Lake Sihwa	2015–2016	9	10	< LOD	150	57	Tian et al. (2020)
	Qingdao Coast	2018	7	10	3.2	18	9.1	Yoon et al. (2020)
	Saemangeum Coast	2014	28	10	0.4	260	22	Yoon et al. (2017)
	Tianjin Coast	2018	7	10	7.6	29	14	Yoon et al. (2020)
	Yangtze River	2019	56	10	5.7	180	31	This study
APs	Adriatic Sea	2014	48	1	< LOD	40	10	Combi et al. (2016)
	Baltic Sea	2011–2012	5	2	< LOD	270	8.9	Koniecko et al. (2014)
	Qingdao Coast	2018	7	10	2.4	45	23	Yoon et al. (2020)
	South China Sea	2002	24	2	61	580	270	Chen et al. (2005)
	Yellow Sea	2017	18	6	3.1	20	5.7	Kim et al. (2021)
	Tianjin Coast	2018	7	10	1.8	22	13	Yoon et al. (2020)
	Yangtze River	2019	56	6	9.6	430	44	This study
PHCZs	Jiaozhou Bay	–	25	10	6.9	33	14	Zhu et al. (2019)
	Jiulong Estuary	2017	9	10	1.6	7.0	5.7	Zhou et al. (2019)
	South China Sea	2009–2012	28	8	0.25	3.1	1.5	Zhou et al. (2021)
	Tai Lake	2013–2014	22	11	< LOD	16	1.5	Wu et al. (2017a, 2017b)
	Yangtze River	2020	15	10	1.6	5.5	3.1	Da et al. (2023)
		2019	56	15	2.6	600	36	This study

< LOD: Limit of detection, –: no information.

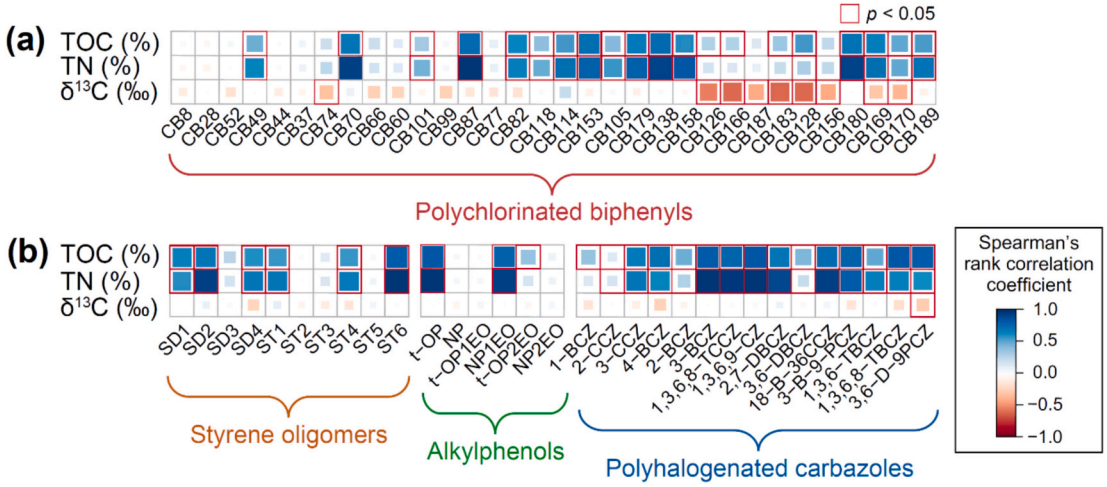

Fig. 4. Spearman rank correlation analysis between sediment properties [total organic carbon (TOC), total nitrogen (TN), and carbon stable isotope ratio ($\delta^{13}C$)] and persistent toxic substances, including (a) PCBs and (b) SOs, APs, and PHCZs, in sediments along the Yangtze River, China.

industrially active areas of Nantong and Shanghai. Unlike PCBs and APs, PHCZs exhibited a strong correlation with organic matter, suggesting that the high concentrations at the NJ12 site in Nanjing were influenced by organic matter contents (TOC and TN) (Fig. 4b) (Da et al., 2023). PHCZs are predominantly generated from industrial activities, such as pharmaceutical production, dye manufacturing, and waste treatment processes (Parette et al., 2015). The relatively high PHCZ levels in Nantong and Shanghai are consistent with the spatial distribution patterns reported by Da et al. (2023), further supporting the industrial origin of these compounds. PHCZs, which are widely used in dyes and coatings, have recently been recognized as compounds posing significant ecological risks (Wang et al., 2021b). The highest contamination levels were observed in Shanghai, followed by Nantong (Fig. 3d). Despite the high sedimentation rates in Shanghai, the elevated PHCZ levels suggest substantial industrial leakage of these compounds. While several sites showed contamination levels similar to previous Yangtze River studies, the overall levels reported here were relatively higher, likely due to the broader range of analyzed compounds (Da et al., 2023) (Table 1).

Among PHCZs, phenylcarbazole (PCZs) exhibited consistently low proportions across all regions, likely due to their greater susceptibility to photodegradation and oxidation compared to other PHCZs (Lin et al., 2012; Musa and Eriksson, 2009). In contrast, bromocarbazoles (BCZs) accounted for the largest proportion, which can be attributed to their

high environmental persistence, frequent detection, and extensive industrial application (Riddell et al., 2015). BCZs are also recognized as compounds that naturally form in marine environments (Zhu and Hites, 2005). The composition analysis of PHCZs revealed that BCZs represented the dominant proportion, ranging from 52.9% to 90.3% across all cities, while chlorocarbazoles (CCZs) contributed 9.5% to 46.3%. Notably, the proportion of BCZs increased progressively from the upper to the lower reaches of the Yangtze River. This trend suggests that the abundant suspended particles and organic matter in the river facilitate the downstream transport and sediment accumulation of PHCZs. Furthermore, the environmental persistence of BCZs and the salinity increase in estuarine areas may have contributed to the elevated concentrations of both anthropogenic and naturally formed BCZs (Deng et al., 2024).

3.2. Identification of potential sources and ongoing contamination of PTSs

PCA was applied to PCBs to identify potential sources, and diagnostic ratios were employed to assess recent inputs of SOs and APs. For PCBs, the PCA utilized compositional profiles of industrial products and combustion sources based on existing literature (Fig. S2). Although the potential sources of PCBs pollution in the Yangtze River did not perfectly align or distinctly separate, they exhibited relative similarities to Kaneclor, Aroclor, and combustion sources (Ikonomou et al., 2002; Pedersen et al., 2015). Kaneclor and Aroclor, which are among the most widely used PCB products, were historically heavily used in China. However, following the ban on PCB products in the 1970s and the gradual restriction of e-waste disposal, combustion processes have become a more prevalent source of PCBs influx, resulting in compositional similarities to various combustion-related sources (Zhu et al., 2022).

For SOs, the diagnostic ratio of STs to their degradation byproducts, SDs was used to evaluate recent styrene inputs (Tian et al., 2020). Results indicated ongoing styrene pollution at 65% of the analyzed sampling points, suggesting active recent inputs (Fig. S2). Styrene, produced during the degradation of plastics and other widely used materials, showed higher levels of ongoing input than other compounds. For APs, the ratio of nonylphenol ethoxylates (NPEOs) to their degradation byproduct, nonylphenols (NPs), was used to assess recent inputs (Isobe et al., 2001) (Fig. S2). Most sampling sites indicated ongoing APs inputs; however, NJ12, NT3, and NT4 showed evidence of older inputs. Although APs exhibit environmental behaviors similar to SOs, their input trends differ. This divergence is likely due to the decreasing use of APs in China due to regulatory measures similar to PCBs. Importantly, none of the sampling points in this study showed AP contamination levels exceeding the Canadian environmental standard of 1000 ng g^{-1} dw. This suggests that recent inputs or ongoing pollution of APs are limited to a few localized sites.

Due to the lack of methods for assessing potential sources of PHCZs, such as diagnostic ratios, regional composition changes were examined (Fig. 3d). The source of PHCZs is known to differ between chlorinated and brominated carbazoles. CCZs are byproducts of industrial processes involving chlorine treatment or aqueous chlorination for water disinfection (Xu et al., 2017). In contrast, BCZs are primarily linked to anthropogenic activities, such as the production of brominated flame retardants and indigo dye (Parette et al., 2015). Additionally, PHCZs can form naturally in aquatic environments (Zhu and Hites, 2005). For example, BCZs, are often naturally formed in marine environments, where they constitute a significant proportion (Flury and Papritz, 1993). In freshwater environments with limited BCZs inputs, CCZs are frequently observed to dominate (Stumm and Morgan, 2013). In this study, the composition of PHCZs revealed that CCZs accounted for a relatively higher proportion in the upper reaches of the Yangtze River, while the proportion of BCZs increased downstream (Fig. 3d). Although this composition cannot be attributed to a single factor, the higher proportion of BCZs in the downstream is thought to result from increased industrial and commercial activities and elevated salinity levels in estuarine areas. Overall, the Yangtze River experiences continuous pollution from SOs and APs, with some areas showing intensified contamination. For PCBs, the primary source has shifted from product-based origins to combustion sources following regulatory measures. Meanwhile, PHCZs are influenced by industrial activities and environmental factors such as salinity.

3.3. Potential ecological risks of PTSs in sediments

The HQ approach was employed to evaluate the potential ecological risks of PTSs and identify priority toxic substances. Since experimentally measured LC50 values were unavailable for all PTSs, the ECOSAR model was utilized to estimate the values required for HQ calculations, ensuring consistent comparison (Table S9). The ECOSAR-derived values were supported by comparison with experimentally determined data for compounds such as PCBs and PAHs, and align with values reported in previous studies (Li et al., 2016). Additionally, concentrations of polycyclic aromatic hydrocarbons (PAHs) were included in HQ calculations [data from Hong et al. (2022)]. Among the analyzed sampling sites, a hotspot in Nanjing (NJ12) exhibited a high risk, with HQ values exceeding 10 (Fig. 5a). This elevated risk was primarily due to PAH levels that exceeded the threshold values established by NOAA and the US EPA (Hong et al., 2022). Several sites also exceeded the moderate risk threshold, including Nanjing (NJ12), Taizhou (TZ6), Suzhou (SZ1 and SZ8), and Nantong (NT6). Regionally, Nanjing had the highest average HQ value (4.97), followed by Taizhou (0.68), Suzhou (0.62), and Nantong (0.47) (Fig. 5a). These findings align with the spatial distribution of PTSs and suggest that regions with higher populations and industrial outputs, such as Nanjing, Taizhou, Suzhou, and Nantong, along the Yangtze River, face elevated ecological risks.

Analysis of the contribution of PTSs to HQ in each region revealed significant variability in dominant pollutants. For instance, in Nanjing, Yangzhou, Taizhou, Changzhou, Suzhou, and Shanghai, traditional PAHs (t-PAHs) accounted for over 50% of the HQ values (Fig. 5b). In contrast, Zhenjiang and Wuxi showed relatively higher contributions from SOs, while in Changzhou, APs contributed more significantly than in other regions. Despite monitoring compounds such as PCBs, t-PAHs, and APs, the contributions of emerging contaminants like emerging PAHs (e-PAHs), SOs, and PHCZs were notable and varied according to regional land use. PAHs were identified as the predominant hazardous compounds at the six sites where HQ values exceeded the moderate risk threshold. Among the PTSs, although emerging PTSs may have relatively lower PNEC values due to their solubility and toxicity compared to traditionally monitored compounds, they appear to have a significant impact on overall distribution and contamination levels (Table S9). Specifically, 4–6 ring PAHs dominated in Nanjing (NJ12), Taizhou (TZ6), and Suzhou (SZ1) (Fig. 5c). At NJ12, contributions to the HQ were relatively balanced across the six analyzed PTSs groups, though 3–5 ring PAHs were the primary contributors among the t-PAHs. In contrast, SZ8 and NT6 exhibited high contributions from SOs, exceeding 80%, with significant proportions also attributed to STs. These results suggest ongoing contamination by SOs in these areas. These results indicate that not only traditionally regulated PTSs but also emerging and previously unregulated PTSs may pose considerable ecological risk, highlighting the need for their inclusion in future environmental monitoring and management frameworks. Furthermore, given the diverse contributions of PTSs and the variability of contamination sources across regions, these findings emphasize the importance of region-specific management strategies that can inform urban planning and policy decisions aimed at reducing ecological risks in densely populated and industrialized river basins.

Fig. 5. (a) Hazardous quotients (HQ) for each site and (b) relative contributions of persistent toxic substances, including PCBs, traditional PAHs (t-PAHs), emerging PAHs (e-PAHs), APs, SOs, and PHCZs, for each city (PAHs data from Hong et al., 2022). (c) Contributions of the top five PTSs at six sampling sites (NJ2, NJ12, TZ6, SZ1, SZ8, and NT6) exceeding the moderate risk level ($1.0 \leq HQ < 10$) and high risk level ($HQ \geq 10$).

4. Conclusions

This study investigated 63 PTSs in surface sediments from the extensive Yangtze River Basin to evaluate contamination levels, spatial distribution, potential sources, and ecological risks. Elevated PTS levels were observed in Nanjing, Nantong, Changzhou, and southern Shanghai, with contamination patterns closely associated with local industrial activities and population densities. PCBs were found to originate primarily from legacy uses and combustion processes post-ban. Continuous SO inputs were observed across most locations, while fresh AP inputs were limited. HQ analysis identified high-risk sites in Nanjing, with moderate risks in Taizhou, Suzhou, and Nantong. t-PAHs were the major contributors to HQ values, while SOs, APs, and PHCZs showed region-specific distributions related to population density and land use. These findings underscore the need for targeted control measures and enhanced monitoring of emerging pollutants in areas under high anthropogenic pressure. The results provide a comprehensive overview of contamination and ecological risks across key urban centers of the Yangtze River Basin, supporting the development of effective and regionally tailored pollution management strategies. This study also highlights the limitations of focusing solely on traditional compounds and recommends future research on monitoring and experimental toxicity testing of emerging, unregulated PTSs to improve ecological risk assessments and inform regulatory frameworks.

CRediT authorship contribution statement

Youngnam Kim: Writing – original draft, Visualization, Investigation, Formal analysis, Data curation, Conceptualization. **Jihyun Cha:** Investigation, Formal analysis. **Gyubin Shin:** Investigation, Formal analysis. **Tieyu Wang:** Writing – review & editing, Investigation, Conceptualization. **Wenyou Hu:** Writing – review & editing, Investigation, Conceptualization. **Jong Seong Khim:** Writing – review & editing, Project administration, Investigation, Funding acquisition, Conceptualization. **Seongjin Hong:** Writing – review & editing, Visualization, Project administration, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence

the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.marpolbul.2025.118283.

Data availability

Data will be made available on request.

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Supplementary materials for

Spatial distribution and potential ecological risk of traditional and emerging organic toxic substances in sediments along the Yangtze River, China

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Supplementary Tables

Table S1. Target compounds (polychlorinated biphenyls, styrene oligomers, and alkylphenols), abbreviations, monitoring ions in the instrumental analysis, method detection limits, and recoveries of surrogate standards.

Target compounds	Abbreviation	Monitoring ions		Method detection limit (ng g^{-1} dw)
		Quantification ion	Confirmation ion	
Polychlorinated biphenyl (PCBs)				
2,4,4'-Trichlorobiphenyl	CB28	256	258	0.03
2,2',5,5'-Tetrachlorobiphenyl	CB52	292	290	0.02
2,2',4,5'-Tetrachlorobiphenyl	CB49	292	290	0.02
2,2',3,5'-Tetrachlorobiphenyl	CB44	292	290	0.03
3,4,4'-Trichlorobiphenyl	CB37	256	258	0.02
2,4,4',5-Tetrachlorobiphenyl	CB74	292	290	0.02
2,3',4',5-Tetrachlorobiphenyl	CB70	292	290	0.01
2,3',4,4'-Tetrachlorobiphenyl	CB66	292	290	0.03
2,3,4,4'-Tetrachlorobiphenyl	CB60	292	290	0.03
2,2',4,5,5'-Pentachlorobiphenyl	CB101	326	324	0.02
2,2',4,4',5-Pentachlorobiphenyl	CB99	326	328	0.02
2,2',3,4,5'-Pentachlorobiphenyl	CB87	292	290	0.02
3,3',4,4'-Tetrachlorobiphenyl	CB77	326	256	0.01
2,2',3,3',4-Pentachlorobiphenyl	CB82	338	340	0.03
2,3',4,4',5-Pentachlorobiphenyl	CB118	326	328	0.03
2,3,4,4',5-Pentachlorobiphenyl	CB114	326	328	0.02
2,2',4,4',5,5'-Hexachlorobiphenyl	CB153	360	362	0.02
2,3,3',4,4'-Pentachlorobiphenyl	CB105	326	324	0.02
2,2',3,3',5,6,6'-Heptachlorobiphenyl	CB179	396	398	0.03
2,2',3,4,4',5'-Hexachlorobiphenyl	CB138	360	362	0.02
2,3,3',4,4',6-Hexachlorobiphenyl	CB158	326	328	0.03
3,3',4,4',5-Pentachlorobiphenyl	CB126	360	362	0.02
2,3,4,4',5,6-Hexachlorobiphenyl	CB166	394	396	0.02
2,2',3,4',5,5',6-Heptachlorobiphenyl	CB187	394	396	0.02
2,2',3,4,4',5',6-Heptachlorobiphenyl	CB183	360	362	0.02
2,2',3,3',4,4'-Hexachlorobiphenyl	CB128	440	442	0.02
2,3,3',4,4',5-Hexachlorobiphenyl	CB156	360	362	0.02
2,2',3,4,4',5,5'-Heptachlorobiphenyl	CB180	394	396	0.03
3,3',4,4',5,5'-Hexachlorobiphenyl	CB169	360	362	0.03
2,2',3,3',4,4',5-Heptachlorobiphenyl	CB170	394	396	0.03
2,3,3',4,4',5,5'-Heptachlorobiphenyl	CB189	476	478	0.03
Styrene oligomers (SOs)				
1,3-Diphenylpropane	SD1	105	196	0.19
cis-1,2-Diphenylcyclobutane	SD2	78	208	0.19
2,4-Diphenyl-1-butene	SD3	104	208	0.89
trans-1,2-Diphenylcyclobutane	SD4	78	208	0.11
2,4,6-Triphenyl-1-hexene	ST1	117	194	0.63
1e-Phenyl-4e-(1-phenylethyl)-tetralin	ST2	129	207	0.66
1a-Phenyl-4e-(1-phenylethyl)-tetralin	ST3	129	207	0.31
1a-Phenyl-4a-(1-phenylethyl)-tetralin	ST4	129	207	0.70
1e-Phenyl-4a-(1-phenylethyl)-tetralin	ST5	207	105	0.41
1,3,5-Triphenylcyclohexane	ST6	117	104	0.88
Alkylphenols (APs)				
4-*tert*-Octylphenol	t-OP	207	221	0.12
4-*tert*-Octylphenol monoethoxylate	t-OP1EO	251	265	0.61

4-*tert*-Octylphenol diethoxylate	t-OP2EO	295	309	0.08
Nonylphenols	NPs	207	221	3.7
Nonylphenol monoethoxylates	NP1EOs	251	265	0.45
Nonylphenol diethoxylates	NP2EOs	295	309	1.5
Internal standard				
2-Fluorobiphenyl	IS	172	171	
Surrogate standards	**Abbreviation**	**Quantification ion**	**Confirmation ion**	**Surrogate recovery (%, mean ± SD)**
Polychlorinated biphenyl (PCBs)				
^{13}C-labeled CB 28		268	270	106 ± 7
^{13}C-labeled CB 52		304	302	99 ± 6
^{13}C-labeled CB 101		326	328	102 ± 6
^{13}C-labeled CB 153		372	374	109 ± 7
^{13}C-labeled CB 138		360	362	110 ± 6
^{13}C-labeled CB 180		406	408	114 ± 7
^{13}C-labeled CB 209		510	512	115 ± 8
Alkylphenols (APs)				
Bisphenol A-d16	BPA-d16	368	386	75 ± 17

Table S2. GC/MSD conditions for analyzing polychlorinated biphenyls, polycyclic aromatic hydrocarbons, styrene oligomers, and alkylphenols in this study.

Instrument	**Agilent 7890B GC / 5977B MSD**	
Column	DB-5ms (30 m × 250 μm × 0.25 μm)	
Gas flow	1 $mLmin^{-1}$ He	
Injection mode	Splitless	
Injection volume	1 μL	
Oven temperature program	PCBs	60 °C (hold 1 min) → 5 °C min^{-1} to 140 °C (hold 1 min) → 30 °C min^{-1} to 200 °C (hold 1 min) → 4 °C min^{-1} to 250 °C (hold 5 min) → 10 °C min^{-1} to 300 °C (hold 1 min)
	SOs	60 °C (hold 2 min) → 6 °C min^{-1} to 300 °C (hold 3 min)
	APs	60 °C (hold 5 min) → 10 °C min^{-1} to 100 °C → 20 °C min^{-1} to 300 °C (hold 6 min)

Table S3. GC/MSMS conditions for analyzing polyhalogenated carbazoles in this study.

Instrument	**Agilent 7890B GC / 7000C MS Triple Quad**	
Column	DB-5ms (30 m × 250 μm × 0.25 μm)	
Gas flow	1 mL min^{-1} He	
Injection mode	Splitless	
Injection volume	1 μL	
Oven temperature program	PHCZs	60 °C (hold 1 min) → 5 °C min^{-1} to 140 °C (hold 1 min) → 20 °C min^{-1} to 300 °C (hold 6 min)

Table S4. Target polyhalogenated carbazoles, abbreviations, monitoring ions and instrumental conditions of GC-MSMS, and recoveries of surrogate standard.

Target compounds	Abbreviation	Molecular weight	Precursor ion	Collision energy	Product ion
Polyhalogenated carbazoles (PHCZs)					
1-Bromocarbazole	1-BCZ	246.1	244.9	20	167.2
2-Chlorocarbazole	2-CCZ	201.7	200.9	20	166.1
3-Chlorocarbazole	3-CCZ	201.7	200.9	20	166.1
4-Bromocarbazole	4-BCZ	246.1	246.9	20	167.2
2-Bromocarbazole	2-BCZ	246.1	244.9	20	166.9
3-Bromocarbazole	3-BCZ	246.1	246.9	30	167.1
1,3,6,8-Tetrachloro-9H-carbazole	1,3,6,8-TCCZ	304.9	304.9	30	270
1-Bromo-3,6-dichloro-9H-carbazole	1,3,6,9-CZ	314.9	314.8	20	233.9
2,7-Dibromocarbazole	2,7-DBCZ	324.9	324.8	40	165
3,6-Dibromocarbazole	3,6-DBCZ	324.9	324.9	40	165
1,8-Dibromo-3,6-dichloro-9H-carbazole	18-B-36CCZ	393.8	392.8	40	198.2
3-Bromo-9-phenylcarbazole	3-B-9-PCZ	322.2	323	40	241.2
1,3,6-Tribromocarbazole	1,3,6-TBCZ	403.8	404.9	30	323.7
1,3,6,8-Tetrabromocarbazole	1,3,6,8-TBCZ	482.8	482.9	30	322.8
3,6-Dibromo-9-phenylcarbazole	3,6-D-9PCZ	401.1	401	30	241.1
Surrogate standard		**Precursor ion**	**Collision energy**	**Product ion**	**Surrogate recovery (%, mean ± SD)**
1,3,6,8-Tetrachloro-9H-[$^{13}C_{12}$]carbazole	SS1	316.9	30	282.0	87 ± 11

Table S5. Concentrations of 32 polychlorinated biphenyls in sediments along the Yangtze River, China.

City	Sites	Concentration of PCBs (ng g^{-1} dw)															
		8	**28**	**52**	**49**	**44**	**37**	**74**	**70**	**66**	**60**	**101**	**99**	**87**	**77**	**82**	**118**
Nanjing	NJ2	0.03	0.95	0.09	1.34	0.31	0.07	0.03	0.10	0.16	0.14	0.10	0.08	0.07	0.19	0.10	0.18
	NJ8	0.04	0.16	0.04	0.41	0.32	0.02	0.05	0.05	0.09	0.07	0.00	0.00	0.00	0.01	0.01	0.01
	NJ10	0.02	0.24	0.38	0.79	0.25	0.02	0.03	0.11	0.10	0.14	0.03	0.01	0.01	0.08	0.02	0.04
	NJ12	0.26	2.65	1.21	7.67	8.32	0.14	1.25	1.30	2.52	2.06	0.07	0.12	0.20	0.44	0.08	0.11
	NJ20	0.03	0.63	0.23	0.60	0.45	0.12	0.01	0.06	0.06	0.11	0.03	0.02	0.01	0.09	0.13	0.08
Yangzhou	YZ2	0.01	0.02	0.14	0.38	0.39	0.03	0.04	0.06	0.05	0.07	0.02	0.00	0.01	0.09	0.02	0.04
	YZ5	0.03	0.22	0.07	1.08	0.29	0.04	0.14	0.09	0.09	0.16	0.02	0.07	0.06	0.03	0.18	0.05
	YZ6	0.03	0.18	0.35	0.96	0.61	0.00	0.02	0.06	0.08	0.09	0.01	0.04	0.01	0.03	0.04	0.02
Zhenjiang	ZJ4	0.03	0.49	0.07	1.07	0.68	0.08	0.02	0.07	0.10	0.10	0.01	0.01	0.03	0.08	0.18	0.18
	ZJ5	0.03	0.28	0.17	0.60	0.47	0.02	0.05	0.09	0.09	0.07	0.01	0.02	0.08	0.04	0.10	0.08
	ZJ12	0.03	1.16	0.34	0.46	0.06	0.22	0.04	0.05	0.06	0.21	0.04	0.03	0.06	0.15	0.18	0.11
	ZJ13	0.13	1.05	0.08	1.23	0.34	0.20	0.07	0.10	0.06	0.12	0.10	0.05	0.04	0.25	0.26	0.15
	ZJ16	0.08	0.99	0.25	0.46	0.40	0.16	0.08	0.11	0.08	0.10	0.04	0.05	0.02	0.03	0.18	0.14
Taizhou	TZ1	0.01	0.97	0.04	0.41	0.42	0.28	0.03	0.03	0.04	0.12	0.02	0.04	0.05	0.10	0.18	0.14
	TZ2	0.01	0.08	0.02	0.26	0.32	0.01	0.03	0.06	0.05	0.06	0.00	0.01	0.01	0.02	0.03	0.04
	TZ3	0.04	0.61	0.18	0.63	0.39	0.02	0.02	0.05	0.07	0.04	0.04	0.02	0.04	0.06	0.07	0.00
	TZ4	0.03	0.92	0.19	0.49	0.39	0.10	0.03	0.04	0.06	0.03	0.02	0.01	0.01	0.11	0.13	0.04
	TZ5	0.07	0.60	0.27	0.91	0.16	0.02	0.05	0.08	0.09	0.14	0.03	0.01	0.06	0.02	0.03	0.02
	TZ6	0.02	0.09	0.04	0.22	0.06	0.07	0.03	0.09	0.03	0.06	0.01	0.00	0.01	0.05	0.01	0.02
	TZ7	0.02	0.49	0.38	0.35	0.27	0.05	0.03	0.06	0.05	0.08	0.07	0.05	0.03	0.02	0.03	0.01
	TZ8	0.01	0.56	0.30	0.51	0.16	0.04	0.04	0.05	0.08	0.05	0.03	0.02	0.01	0.04	0.06	0.02
Changzhou	CZ1	0.08	0.61	0.41	1.35	0.34	0.06	0.02	0.11	0.14	0.17	0.03	0.01	0.05	0.09	0.13	0.01
Wuxi	WX1	0.01	0.08	0.11	0.24	0.29	0.02	0.02	0.02	0.05	0.04	0.02	0.01	0.03	0.05	0.06	0.03
	WX2	0.01	0.15	0.15	0.31	0.22	0.00	0.03	0.09	0.02	0.06	0.02	0.01	0.02	0.06	0.07	0.03
Suzhou	SZ1	0.13	0.51	0.25	5.24	1.37	0.02	0.14	0.13	0.18	0.17	0.02	0.01	0.14	0.04	0.05	0.04
	SZ2	0.03	0.69	0.23	0.69	0.47	0.04	0.03	0.06	0.08	0.07	0.05	0.00	0.08	0.04	0.07	0.02
	SZ3	0.01	0.09	0.06	0.14	0.16	0.01	0.02	0.03	0.02	0.03	0.01	0.00	0.02	0.07	0.03	0.02
	SZ4	0.02	0.04	0.10	0.33	0.05	0.04	0.12	0.07	0.06	0.07	0.04	0.02	0.02	0.02	0.01	0.00
	SZ5	0.23	0.59	0.07	1.06	0.91	0.37	0.15	0.18	0.13	0.06	0.07	0.05	0.06	0.25	0.47	0.28
	SZ6	0.06	0.49	0.38	1.30	0.31	0.01	0.03	0.11	0.11	0.13	0.06	0.02	0.02	0.04	0.09	0.02
	SZ8	0.48	3.86	0.32	4.23	1.20	0.58	0.13	0.36	0.36	0.45	0.15	0.13	0.11	0.11	0.51	0.27
	SZ9	0.03	0.82	0.20	0.48	0.30	0.12	0.05	0.07	0.02	0.09	0.05	0.05	0.05	0.03	0.12	0.10
	SZ10	0.07	0.48	0.47	1.62	0.35	0.19	0.28	0.10	0.09	0.09	0.04	0.07	0.02	0.03	0.14	0.02
Nantong	NT1	0.02	0.67	0.33	1.08	0.27	0.02	0.11	0.06	0.07	0.07	0.04	0.01	0.05	0.02	0.03	0.03
	NT2	0.03	0.38	0.27	0.89	0.44	0.04	0.05	0.05	0.06	0.09	0.05	0.01	0.03	0.01	0.10	0.06
	NT3	0.06	0.33	0.08	1.12	0.25	0.05	0.10	0.10	0.08	0.10	0.01	0.03	0.01	0.03	0.11	0.02

	NT4	0.02	0.70	0.27	0.91	0.18	0.05	0.03	0.09	0.05	0.12	0.04	0.04	0.02	0.03	0.07	0.07
	NT5	0.03	0.23	0.43	0.39	0.28	0.01	0.02	0.08	0.06	0.06	0.05	0.03	0.00	0.07	0.04	0.02
	NT6	0.04	0.30	0.29	0.96	0.19	0.01	0.03	0.05	0.09	0.09	0.03	0.05	0.03	0.10	0.07	0.01
	NT7	0.06	0.30	0.04	0.93	0.16	0.03	0.02	0.09	0.09	0.10	0.04	0.04	0.02	0.02	0.05	0.06
	NT8	0.02	0.65	0.45	0.40	0.30	0.07	0.01	0.06	0.03	0.04	0.02	0.00	0.01	0.02	0.09	0.05
	NT9	0.02	1.00	0.37	0.34	0.12	0.10	0.03	0.05	0.06	0.08	0.06	0.02	0.01	0.07	0.12	0.09
	NT10	0.02	0.44	0.05	0.50	0.35	0.03	0.07	0.05	0.06	0.01	0.05	0.01	0.01	0.03	0.03	0.03
	NT11	0.02	0.29	0.18	0.37	0.25	0.04	0.04	0.06	0.06	0.07	0.06	0.02	0.06	0.02	0.06	0.05
	NT12	0.02	1.10	0.33	0.30	0.27	0.08	0.04	0.06	0.02	0.09	0.05	0.06	0.01	0.07	0.13	0.13
	NT13	0.02	0.61	0.18	0.15	0.19	0.31	0.02	0.01	0.01	0.01	0.04	0.01	0.01	0.02	0.11	0.06
	NT14	0.02	0.64	0.17	0.16	0.23	0.15	0.05	0.03	0.04	0.08	0.06	0.03	0.02	0.03	0.22	0.07
Shanghai	SH1	0.11	0.80	0.27	0.55	0.37	0.16	0.09	0.03	0.03	0.11	0.04	0.03	0.03	0.03	0.17	1.88
	SH2	0.06	0.92	0.20	0.29	0.28	0.22	0.06	0.10	0.03	0.09	0.06	0.02	0.02	0.12	0.13	0.10
	SH3	0.06	0.90	0.25	0.44	0.35	0.15	0.06	0.03	0.04	0.11	0.06	0.03	0.01	0.05	0.18	0.13
	SH4	0.20	0.70	0.05	0.78	0.39	0.17	0.04	0.04	0.08	0.10	0.05	0.06	0.04	0.08	0.23	0.10
	SH6	0.10	0.77	0.27	0.60	0.14	0.15	0.03	0.07	0.03	0.12	0.05	0.02	0.03	0.04	0.20	0.16
	SH7	0.02	0.26	0.22	0.35	0.32	0.03	0.04	0.08	0.05	0.05	0.04	0.02	0.02	0.10	0.07	0.03
	SH8	0.12	1.19	0.59	0.54	0.37	0.19	0.10	0.10	0.07	0.16	0.06	0.02	0.01	0.03	0.18	0.14
	SH10	0.04	1.01	0.02	0.19	0.27	0.15	0.08	0.04	0.05	0.07	0.09	0.03	0.04	0.03	0.13	0.12
	SH11	0.10	1.33	0.19	0.30	0.32	0.21	0.06	0.08	0.04	0.17	0.06	0.03	0.05	1.58	0.25	0.12

< LOD: Limit of detection.

Table S5. Continued.

City	Sites	Concentration of PCBs (ng g^{-1} dw)															
		114	**153**	**105**	**179**	**138**	**158**	**126**	**166**	**187**	**183**	**128**	**156**	**180**	**169**	**170**	**189**
Nanjing	NJ2	0.12	0.09	0.14	0.01	0.03	0.01	0.10	0.12	0.03	0.01	0.10	0.25	0.03	0.04	0.01	0.04
	NJ8	0.04	0.03	0.03	0.01	0.01	0.01	0.11	0.00	0.00	0.00	0.07	0.13	0.00	0.02	0.01	0.02
	NJ10	0.03	0.03	0.07	0.00	0.02	0.02	0.06	0.01	0.02	0.03	0.08	0.27	0.01	0.02	0.01	0.02
	NJ12	0.09	1.60	0.35	0.01	0.51	0.51	0.25	0.19	0.03	0.01	0.44	0.64	0.03	4.35	0.07	0.11
	NJ20	0.10	0.03	0.16	0.00	0.03	0.02	0.08	0.01	0.01	0.01	0.05	0.14	0.00	0.03	0.02	0.02
Yangzhou	YZ2	0.01	0.04	0.05	0.00	0.02	0.02	0.03	0.02	0.01	0.01	0.13	0.19	0.00	0.02	0.00	0.00
	YZ5	0.05	0.11	0.14	0.01	0.03	0.01	0.07	0.02	0.02	0.02	0.03	0.36	0.02	0.02	0.02	0.02
	YZ6	0.05	0.04	0.06	0.01	0.05	0.05	0.03	0.05	0.05	0.02	0.18	0.21	0.01	0.06	0.03	0.01
Zhenjiang	ZJ4	0.12	0.20	0.16	0.00	0.01	0.02	0.15	0.02	0.00	0.02	0.07	0.23	0.01	0.09	0.04	0.03
	ZJ5	0.05	0.06	0.05	0.00	0.01	0.01	0.04	0.04	0.03	0.04	0.03	0.21	0.01	0.01	0.01	0.01
	ZJ12	0.13	0.02	0.36	0.02	0.01	0.01	0.09	0.03	0.01	0.00	0.05	0.22	0.00	0.03	0.01	0.03
	ZJ13	0.47	0.04	0.40	0.01	0.01	0.02	0.22	0.01	0.00	0.02	0.15	0.31	0.01	0.03	0.01	0.02
	ZJ16	0.26	0.05	0.25	0.00	0.03	0.03	0.08	0.04	0.01	0.01	0.04	0.21	0.01	0.04	0.01	0.05
Taizhou	TZ1	0.18	0.05	0.28	0.01	0.01	0.01	0.08	0.04	0.04	0.06	0.04	0.19	0.01	0.07	0.03	0.02
	TZ2	0.02	0.02	0.03	0.00	0.01	0.01	0.08	0.02	0.01	0.03	0.03	0.12	0.00	0.08	0.01	0.02
	TZ3	0.05	0.10	0.01	0.02	0.02	0.01	0.02	0.01	0.03	0.02	0.04	0.06	0.00	0.01	0.02	0.02
	TZ4	0.03	0.05	0.06	0.01	0.02	0.02	0.44	0.01	0.02	0.04	0.05	0.11	0.01	0.05	0.01	0.01
	TZ5	0.02	0.13	0.06	0.04	0.04	0.01	0.03	0.01	0.03	0.03	0.03	0.15	0.03	0.12	0.01	0.01
	TZ6	0.01	0.04	0.01	0.00	0.01	0.01	0.03	0.03	0.04	0.02	0.07	0.14	0.02	0.05	0.01	0.03
	TZ7	0.02	0.15	0.03	0.04	0.02	0.02	0.10	0.01	0.00	0.00	0.04	0.21	0.01	0.07	0.01	0.01
	TZ8	0.01	0.06	0.02	0.01	0.03	0.03	0.04	0.04	0.01	0.01	0.10	0.07	0.00	0.02	0.01	0.02
Changzhou	CZ1	0.05	0.09	0.08	0.01	0.03	0.03	0.02	0.02	0.03	0.02	0.04	0.05	0.07	0.05	0.02	0.03
Wuxi	WX1	0.03	0.07	0.07	0.02	0.02	0.02	0.08	0.03	0.02	0.00	0.06	0.10	0.00	0.06	0.01	0.01
	WX2	0.03	0.05	0.04	0.00	0.01	0.01	0.11	0.01	0.00	0.01	0.03	0.12	0.01	0.01	0.01	0.00
Suzhou	SZ1	0.03	0.05	0.02	0.00	0.01	0.02	0.04	0.02	0.02	0.05	0.14	0.03	0.01	0.04	0.01	0.01
	SZ2	0.04	0.18	0.03	0.00	0.02	0.02	0.04	0.03	0.02	0.02	0.03	0.25	0.04	0.03	0.01	0.01
	SZ3	0.02	0.02	0.02	0.00	0.01	0.01	0.04	0.01	0.00	0.00	0.02	0.06	0.01	0.01	0.01	0.01
	SZ4	0.03	0.04	0.04	0.00	0.01	0.01	0.07	0.02	0.00	0.01	0.06	0.12	0.01	0.02	0.00	0.01
	SZ5	0.83	0.13	0.82	0.03	0.02	0.02	0.20	0.10	0.02	0.03	0.19	0.52	0.01	0.08	0.02	0.05
	SZ6	0.02	0.17	0.03	0.01	0.01	0.03	0.25	0.02	0.01	0.02	0.11	0.23	0.03	0.02	0.02	0.01
	SZ8	0.85	0.43	0.65	0.01	0.13	0.11	0.12	0.07	0.02	0.02	0.16	0.31	0.07	0.06	0.06	0.03
	SZ9	0.04	0.13	0.22	0.01	0.01	0.01	0.11	0.01	0.00	0.00	0.07	0.16	0.01	0.07	0.02	0.06
	SZ10	0.04	0.06	0.10	0.00	0.03	0.03	0.53	0.01	0.02	0.03	0.06	0.25	0.04	0.05	0.03	0.01
Nantong	NT1	0.07	0.13	0.01	0.00	0.01	0.01	0.04	0.05	0.00	0.07	0.04	0.17	0.01	0.02	0.01	0.01
	NT2	0.08	0.17	0.15	0.02	0.01	0.01	0.05	0.04	0.01	0.00	0.03	0.18	0.02	0.03	0.01	0.01
	NT3	0.02	0.06	0.23	0.00	0.02	0.02	0.03	0.06	0.01	0.01	0.04	0.23	0.00	0.08	0.01	0.03

	NT4	0.03	0.13	0.19	0.00	0.05	0.05	0.07	0.01	0.02	0.01	0.05	0.17	0.02	0.05	0.01	0.01
	NT5	0.01	0.05	0.05	0.02	0.01	0.02	0.03	0.02	0.01	0.01	0.04	0.02	0.00	0.01	0.01	0.02
	NT6	0.03	0.02	0.03	0.00	0.01	0.01	0.09	0.04	0.01	0.00	0.05	0.09	0.01	0.02	0.01	0.02
	NT7	0.06	0.09	0.16	0.00	0.03	0.03	0.04	0.06	0.02	0.07	0.11	0.28	0.04	0.03	0.01	0.01
	NT8	0.01	0.16	0.09	0.00	0.01	0.01	0.14	0.01	0.02	0.02	0.02	0.05	0.02	0.03	0.02	0.03
	NT9	0.23	0.13	0.22	0.01	0.01	0.01	0.07	0.04	0.03	0.02	0.09	0.13	0.01	0.02	0.01	0.03
	NT10	0.03	0.07	0.04	0.00	0.02	0.01	0.04	0.06	0.00	0.00	0.02	0.16	0.01	0.04	0.01	0.05
	NT11	0.02	0.04	0.09	0.00	0.01	0.00	0.03	0.05	0.02	0.03	0.03	0.13	0.01	0.08	0.01	0.01
	NT12	0.09	0.11	0.16	0.02	0.02	0.02	0.11	0.01	0.01	0.01	0.04	0.03	0.01	0.07	0.01	0.01
	NT13	0.25	0.04	0.06	0.01	0.01	0.01	0.16	0.00	0.00	0.00	0.14	0.10	0.01	0.01	0.00	0.01
	NT14	0.26	0.07	0.24	0.00	0.01	0.01	0.08	0.01	0.01	0.00	0.02	0.20	0.01	0.02	0.02	0.01
Shanghai	SH1	0.39	0.57	14.93	0.01	0.02	0.02	0.20	0.01	0.03	0.03	0.21	0.22	0.06	0.03	0.01	0.02
	SH2	0.17	0.06	0.21	0.00	0.03	0.03	0.29	0.03	0.02	0.02	0.20	0.04	0.03	0.05	0.02	0.01
	SH3	0.37	0.05	0.25	0.00	0.01	0.01	0.08	0.01	0.01	0.00	0.03	0.15	0.03	0.01	0.01	0.01
	SH4	0.04	0.13	0.28	0.02	0.01	0.01	0.01	0.02	0.02	0.02	0.08	0.27	0.01	0.02	0.02	0.01
	SH6	0.05	0.15	0.24	0.00	0.01	0.01	1.96	0.14	0.01	0.01	0.05	0.18	0.02	0.05	0.00	0.03
	SH7	0.03	0.12	0.15	0.00	0.01	0.00	0.02	0.03	0.01	0.01	0.06	0.15	0.00	0.04	0.01	0.01
	SH8	0.03	0.12	0.29	0.01	0.02	0.02	0.95	0.09	0.01	0.01	0.04	0.17	0.02	0.03	0.01	0.02
	SH10	0.07	0.23	0.22	0.02	0.05	0.05	0.07	0.01	0.06	0.05	0.19	0.13	0.13	0.02	0.07	0.02
	SH11	0.09	0.18	0.28	0.01	0.01	0.01	0.19	0.05	0.02	0.00	0.08	0.23	0.02	0.02	0.02	0.02

< LOD: Limit of detection.

Table S6. Concentrations of 10 styrene oligomers in sediments along the Yangtze River, China.

City	Sites	Concentration of SOs (ng g^{-1} dw)									
		SD1	**SD2**	**SD3**	**SD4**	**ST1**	**ST2**	**ST3**	**ST4**	**ST5**	**ST6**
Nanjing	NJ2	2.04	1.56	2.82	8.65	22.37	8.97	10.68	7.26	4.26	1.53
	NJ8	0.67	0.19	2.92	2.35	6.57	1.55	1.59	0.96	0.68	0.31
	NJ10	0.58	0.18	8.09	1.12	5.21	1.30	1.33	1.16	0.66	0.38
	NJ12	2.54	1.94	69.64	7.73	7.13	3.86	3.39	0.89	1.54	3.52
	NJ20	0.64	0.42	0.60	5.74	9.47	6.66	7.17	3.35	3.69	0.35
Yangzhou	YZ2	0.33	0.17	3.45	1.31	3.31	1.33	1.41	1.19	0.49	0.32
	YZ5	0.62	0.16	1.59	1.28	6.26	1.27	1.32	1.26	0.62	0.20
	YZ6	0.53	0.17	1.92	1.07	4.45	2.46	1.80	0.81	0.81	0.33
Zhenjiang	ZJ4	0.82	0.38	1.83	5.19	10.35	5.52	5.81	3.40	3.19	0.27
	ZJ5	0.69	0.42	4.20	6.16	10.14	6.15	5.60	3.33	3.61	0.38
	ZJ12	0.72	0.35	0.55	5.36	7.84	5.26	4.64	2.67	2.82	0.30
	ZJ13	0.73	0.33	0.43	4.47	9.61	5.71	3.11	5.57	3.11	0.39
	ZJ16	0.52	0.31	0.41	4.34	8.59	5.22	2.56	2.52	3.09	0.18
Taizhou	TZ1	0.58	0.32	0.45	4.26	8.05	5.52	4.84	2.54	3.19	0.28
	TZ2	0.43	0.13	3.06	0.78	4.28	1.12	0.98	1.15	0.48	0.24
	TZ3	0.77	0.41	3.62	5.10	10.04	5.43	4.81	3.24	2.77	0.27
	TZ4	0.90	1.25	5.11	14.59	17.23	12.62	11.53	7.26	7.09	0.72
	TZ5	0.88	0.53	3.64	5.09	9.98	5.66	4.95	3.35	2.84	0.38
	TZ6	0.48	0.17	1.64	0.15	4.35	3.01	0.86	4.44	0.84	0.46
	TZ7	0.69	0.68	2.73	8.05	11.67	6.93	5.83	6.13	5.15	0.45
	TZ8	0.53	0.49	2.86	5.88	12.04	7.23	6.37	4.59	3.68	0.21
Changzhou	CZ1	0.75	0.57	3.76	6.51	10.29	6.95	6.14	2.85	2.85	0.93
Wuxi	WX1	0.50	0.11	1.28	0.75	5.07	0.87	0.65	0.57	0.39	0.23
	WX2	0.41	0.11	0.67	0.73	4.58	0.84	0.69	0.72	0.33	0.19
Suzhou	SZ1	0.54	0.26	1.31	0.68	3.96	1.40	1.11	1.05	0.89	0.22
	SZ2	0.64	0.70	1.70	5.62	17.84	9.94	8.27	5.45	5.41	0.33
	SZ3	0.35	0.06	0.38	0.43	3.79	0.76	0.70	0.31	0.22	0.42
	SZ4	0.54	0.16	1.70	0.72	5.72	1.99	1.12	0.77	0.45	0.22
	SZ5	0.27	0.05	0.29	0.28	3.46	0.61	0.62	0.49	0.22	0.02
	SZ6	0.55	0.47	2.76	5.59	9.33	5.37	4.88	2.75	3.29	0.37
	SZ8	1.67	0.83	3.63	6.10	42.63	14.20	9.01	8.46	7.38	0.20
	SZ9	0.42	0.20	0.19	2.72	4.82	3.14	4.52	1.97	1.47	0.21
	SZ10	0.94	0.47	2.62	4.95	11.63	4.39	4.48	2.61	2.52	0.09
Nantong	NT1	0.68	0.26	10.24	5.43	8.77	7.09	5.66	5.47	2.64	0.05
	NT2	0.42	0.16	1.11	1.76	2.69	1.52	0.92	1.68	0.39	0.04
	NT3	0.76	0.31	4.60	2.17	10.25	6.45	1.83	8.30	0.93	0.30

	NT4	0.52	0.25	0.90	1.85	3.58	9.04	1.53	14.31	0.87	0.29
	NT5	0.69	0.09	2.77	2.76	6.55	5.43	7.39	3.52	2.65	0.42
	NT6	4.39	0.53	2.65	27.62	32.50	27.71	49.59	15.91	15.56	0.98
	NT7	0.51	0.35	2.57	4.99	11.32	9.39	12.04	9.17	4.79	0.20
	NT8	0.52	0.26	0.86	3.11	4.84	2.37	3.26	1.35	1.24	0.20
	NT9	0.34	0.09	0.21	1.10	3.36	1.03	1.28	0.74	0.49	0.29
	NT10	0.41	0.17	1.47	1.58	3.00	1.28	1.08	0.83	0.40	0.07
	NT11	0.29	0.13	0.82	1.29	2.73	1.32	1.48	1.64	0.73	0.25
	NT12	0.70	0.31	0.62	4.40	8.25	3.74	3.04	1.61	2.11	0.29
	NT13	0.54	0.20	0.43	2.93	5.57	2.25	2.04	0.99	1.24	0.23
	NT14	0.38	0.09	0.24	1.41	2.83	0.73	1.01	0.36	0.36	0.17
Shanghai	SH1	0.37	0.08	0.27	0.67	2.56	0.85	0.98	0.58	0.37	0.13
	SH2	0.45	0.16	0.16	1.36	4.79	1.17	1.51	0.60	0.46	0.27
	SH3	0.27	0.11	3.47	0.84	2.21	4.27	0.80	5.50	0.46	0.20
	SH4	0.53	0.23	11.63	1.65	3.26	13.48	1.37	18.15	1.15	0.43
	SH6	0.25	0.08	0.19	0.40	2.08	0.83	0.79	0.57	0.31	0.20
	SH7	0.40	0.11	1.26	1.27	2.84	0.69	0.75	0.82	0.44	0.35
	SH8	0.33	0.05	0.15	0.64	2.88	0.81	0.95	0.62	0.36	0.12
	SH10	0.40	0.08	0.26	0.93	5.11	0.81	0.59	0.72	0.23	0.07
	SH11	0.30	0.10	0.30	0.58	4.56	1.49	0.86	0.82	0.87	0.03

< LOD: Limit of detection.

Table S7. Concentrations of 6 alkylphenols in sediments along the Yangtze River, China.

City	Sites	Concentration of APs (ng g^{-1} dw)					
		t-OP	NPs	t-OP1EO	NP1EOs	t-OP2EO	NP2EOs
Nanjing	NJ2	2.04	1.56	2.82	8.65	22.37	8.97
	NJ8	0.67	0.19	2.92	2.35	6.57	1.55
	NJ10	0.58	0.18	8.09	1.12	5.21	1.30
	NJ12	2.54	1.94	69.64	7.73	7.13	3.86
	NJ20	0.64	0.42	0.60	5.74	9.47	6.66
Yangzhou	YZ2	0.33	0.17	3.45	1.31	3.31	1.33
	YZ5	0.62	0.16	1.59	1.28	6.26	1.27
	YZ6	0.53	0.17	1.92	1.07	4.45	2.46
Zhenjiang	ZJ4	0.82	0.38	1.83	5.19	10.35	5.52
	ZJ5	0.69	0.42	4.20	6.16	10.14	6.15
	ZJ12	0.72	0.35	0.55	5.36	7.84	5.26
	ZJ13	0.73	0.33	0.43	4.47	9.61	5.71
	ZJ16	0.52	0.31	0.41	4.34	8.59	5.22
Taizhou	TZ1	0.58	0.32	0.45	4.26	8.05	5.52
	TZ2	0.43	0.13	3.06	0.78	4.28	1.12
	TZ3	0.77	0.41	3.62	5.10	10.04	5.43
	TZ4	0.90	1.25	5.11	14.59	17.23	12.62
	TZ5	0.88	0.53	3.64	5.09	9.98	5.66
	TZ6	0.48	0.17	1.64	0.15	4.35	3.01
	TZ7	0.69	0.68	2.73	8.05	11.67	6.93
	TZ8	0.53	0.49	2.86	5.88	12.04	7.23
Changzhou	CZ1	0.75	0.57	3.76	6.51	10.29	6.95
Wuxi	WX1	0.50	0.11	1.28	0.75	5.07	0.87
	WX2	0.41	0.11	0.67	0.73	4.58	0.84
Suzhou	SZ1	0.54	0.26	1.31	0.68	3.96	1.40
	SZ2	0.64	0.70	1.70	5.62	17.84	9.94
	SZ3	0.35	0.06	0.38	0.43	3.79	0.76
	SZ4	0.54	0.16	1.70	0.72	5.72	1.99
	SZ5	0.27	0.05	0.29	0.28	3.46	0.61
	SZ6	0.55	0.47	2.76	5.59	9.33	5.37
	SZ8	1.67	0.83	3.63	6.10	42.63	14.20
	SZ9	0.42	0.20	0.19	2.72	4.82	3.14
	SZ10	0.94	0.47	2.62	4.95	11.63	4.39
Nantong	NT1	0.68	0.26	10.24	5.43	8.77	7.09
	NT2	0.42	0.16	1.11	1.76	2.69	1.52
	NT3	0.76	0.31	4.60	2.17	10.25	6.45

	NT4	0.52	0.25	0.90	1.85	3.58	9.04
	NT5	0.69	0.09	2.77	2.76	6.55	5.43
	NT6	4.39	0.53	2.65	27.62	32.50	27.71
	NT7	0.51	0.35	2.57	4.99	11.32	9.39
	NT8	0.52	0.26	0.86	3.11	4.84	2.37
	NT9	0.34	0.09	0.21	1.10	3.36	1.03
	NT10	0.41	0.17	1.47	1.58	3.00	1.28
	NT11	0.29	0.13	0.82	1.29	2.73	1.32
	NT12	0.70	0.31	0.62	4.40	8.25	3.74
	NT13	0.54	0.20	0.43	2.93	5.57	2.25
	NT14	0.38	0.09	0.24	1.41	2.83	0.73
Shanghai	SH1	0.37	0.08	0.27	0.67	2.56	0.85
	SH2	0.45	0.16	0.16	1.36	4.79	1.17
	SH3	0.27	0.11	3.47	0.84	2.21	4.27
	SH4	0.53	0.23	11.63	1.65	3.26	13.48
	SH6	0.25	0.08	0.19	0.40	2.08	0.83
	SH7	0.40	0.11	1.26	1.27	2.84	0.69
	SH8	0.33	0.05	0.15	0.64	2.88	0.81
	SH10	0.40	0.08	0.26	0.93	5.11	0.81
	SH11	0.30	0.10	0.30	0.58	4.56	1.49

< LOD: Limit of detection.

Table S8. Concentrations of 15 polyhalogenated carbazoles in sediments along the Yangtze River, China.

City	Sites	Concentration of 15 PHCZs (ng g^{-1} dw)														
		1-BCZ	2-CCZ	3-CCZ	4-BCZ	2-BCZ	3-BCZ	1,3,6,8-TCCZ	1,3,6,9-CZ	2,7-DBCZ	3,6-DBCZ	18-B-36CCZ	3-B-9-PCZ	1,3,6-TBCZ	1,3,6,8-TBCZ	3,6-D-9PCZ
Nanjing	NJ2	0.68	0.02	6.55	0.26	0.10	0.36	0.14	1.56	0.37	1.04	0.68	0.00	2.33	1.34	0.02
	NJ8	0.67	0.05	5.37	0.45	0.09	0.82	0.16	1.23	0.61	0.73	0.82	0.00	0.70	0.87	0.06
	NJ10	0.94	0.11	3.94	0.54	0.37	0.89	0.27	1.16	0.40	1.39	0.65	0.01	0.93	1.62	0.09
	NJ12	8.36	0.13	53.97	1.73	2.92	11.29	0.35	510	1.34	7.24	0.26	6.96	0.13	0.04	0.02
	NJ20	0.66	0.08	2.57	0.05	0.23	0.34	0.16	0.72	0.41	0.80	0.49	0.01	0.26	0.92	0.17
Yangzhou	YZ2	0.60	0.06	3.81	0.40	0.48	0.40	0.17	1.32	0.61	1.83	0.51	0.01	0.99	1.15	0.10
	YZ5	1.97	0.09	5.44	0.27	0.24	1.08	0.25	1.51	0.85	2.45	0.73	0.02	1.11	1.47	0.06
	YZ6	2.37	0.18	2.64	1.36	0.69	1.09	0.87	0.71	0.39	2.07	0.49	0.01	1.01	1.07	0.17
Zhenjiang	ZJ4	1.97	0.08	5.23	0.42	0.34	1.22	0.34	0.95	0.24	1.11	0.67	0.02	1.04	0.84	0.11
	ZJ5	1.52	0.60	3.89	0.74	0.64	1.21	0.87	2.79	3.29	3.49	1.90	0.96	3.37	3.27	2.33
	ZJ12	0.70	0.05	4.72	0.32	0.24	0.64	0.19	1.13	0.55	1.28	0.60	0.00	0.67	1.07	0.05
	ZJ13	0.36	0.12	4.23	6.84	0.80	16.47	0.16	1.30	1.33	2.69	0.82	0.01	1.54	2.18	0.17
	ZJ16	0.84	0.11	5.65	0.62	0.23	1.48	0.20	1.33	1.15	1.55	0.82	0.03	0.94	1.72	0.38
Taizhou	TZ1	1.76	0.17	8.08	0.44	0.61	0.64	0.59	2.08	1.37	11.91	1.26	0.03	1.83	2.81	0.42
	TZ2	1.29	0.01	3.23	0.17	0.07	0.37	0.09	5.65	0.08	0.57	3.12	0.00	0.47	1.08	0.05
	TZ3	1.67	0.10	6.14	0.53	0.63	1.53	0.30	1.69	0.92	3.63	0.96	1.63	1.78	2.58	0.49
	TZ4	1.66	0.06	6.13	0.29	0.60	0.61	0.25	1.43	0.16	2.32	0.89	0.19	1.04	2.13	0.17
	TZ5	1.05	0.54	4.63	1.90	0.84	1.59	0.63	2.91	4.32	4.73	1.94	1.24	3.55	3.21	2.21
	TZ6	1.28	0.08	6.77	1.02	0.08	0.15	0.19	1.38	1.23	2.02	0.94	0.03	1.10	1.78	0.09
	TZ7	2.19	0.12	6.60	0.64	0.52	0.53	0.26	1.62	0.47	2.28	0.96	0.00	1.14	2.39	0.08
	TZ8	1.38	0.08	10.32	1.74	0.85	1.30	0.28	1.62	0.58	2.03	0.91	0.13	1.10	2.28	0.09
Changzhou	CZ1	1.40	0.17	4.93	1.32	3.92	1.01	0.16	1.59	0.93	3.28	0.74	0.01	1.46	2.03	0.10
Wuxi	WX1	1.27	0.07	3.86	0.39	0.39	0.41	0.16	0.93	0.14	0.66	0.56	0.00	0.58	1.33	0.05
	WX2	1.41	0.04	0.44	0.35	0.55	0.53	0.01	0.08	0.02	0.22	0.10	0.00	0.10	0.06	0.06
Suzhou	SZ1	6.05	0.06	0.27	0.63	0.68	1.33	0.07	0.33	0.19	0.39	0.22	0.02	0.05	0.35	0.10
	SZ2	2.53	0.10	9.92	0.68	0.25	1.38	0.36	4.21	0.76	4.57	1.02	0.03	2.29	2.85	0.10
	SZ3	0.65	0.04	0.25	5.67	0.09	13.00	0.01	0.18	0.06	0.19	0.08	0.00	0.11	0.06	0.03
	SZ4	0.69	0.07	0.70	0.33	0.09	0.32	0.04	0.21	0.09	0.35	0.12	0.01	0.07	0.27	0.07
	SZ5	1.06	0.11	3.19	0.42	0.56	0.38	0.16	0.88	0.30	1.45	0.58	0.01	0.56	0.99	0.07
	SZ6	2.79	0.21	3.71	0.78	0.15	0.35	0.24	1.23	0.54	1.57	0.69	0.04	0.97	0.98	0.17
	SZ8	5.11	0.20	6.01	0.39	0.34	2.37	0.54	2.44	0.63	3.29	0.94	0.05	2.69	3.74	0.10
	SZ9	3.94	0.12	2.38	0.43	0.36	0.36	0.17	0.60	0.19	1.10	0.28	0.04	0.55	2.68	0.09
	SZ10	4.61	0.12	2.33	0.19	0.27	1.07	0.36	0.96	0.27	2.36	0.81	0.02	1.21	2.10	0.08
Nantong	NT1	1.42	0.21	4.36	0.54	0.78	0.54	0.23	1.01	0.66	1.86	0.70	6.85	0.93	1.50	0.11
	NT2	1.08	0.07	4.37	0.46	0.21	2.15	0.15	1.05	0.49	2.09	0.55	0.58	0.76	1.05	0.05
	NT3	1.95	0.15	6.28	1.03	1.91	0.84	0.38	2.05	1.32	2.73	0.87	0.42	1.60	2.18	0.07

	NT4	1.20	0.06	2.29	0.40	0.50	1.08	0.12	0.45	0.31	130	0.17	0.38	0.44	0.79	0.06
	NT5	1.98	0.05	1.88	0.30	0.23	1.67	1.23	1.48	0.11	1.36	0.59	0.01	0.98	1.21	0.06
	NT6	1.56	0.05	1.29	42.75	0.94	80.69	0.07	0.81	0.30	0.84	0.27	0.04	2.19	0.47	0.05
	NT7	3.90	0.15	5.37	0.42	0.50	3.71	0.37	1.36	0.87	2.53	0.80	0.31	1.36	3.34	0.07
	NT8	1.28	0.10	2.30	0.37	3.02	0.27	0.21	0.67	0.08	1.37	0.42	0.01	1.02	6.74	0.03
	NT9	6.14	0.38	2.13	0.35	0.14	0.74	0.18	0.72	0.07	1.50	0.39	0.01	0.98	6.71	0.04
	NT10	1.67	0.15	3.84	0.51	0.77	0.79	0.37	1.49	0.17	2.98	0.90	0.04	2.04	12.02	0.01
	NT11	0.95	0.12	3.64	0.30	0.26	0.97	0.46	1.99	0.40	4.97	1.02	0.03	3.92	7.13	0.04
	NT12	0.75	0.03	0.82	0.16	0.11	0.35	0.13	0.23	0.04	0.49	0.30	0.01	0.24	1.03	0.04
	NT13	1.29	0.02	0.21	0.25	0.24	0.34	0.02	0.14	0.02	0.14	0.14	0.00	0.07	0.11	0.01
	NT14	0.43	0.03	0.36	0.44	0.23	0.15	0.05	0.19	0.04	0.26	0.24	0.00	0.05	0.08	0.05
Shanghai	SH1	2.46	0.81	3.99	0.57	0.09	0.32	0.45	1.24	0.14	3.33	1.04	0.03	2.45	11	0.05
	SH2	1.04	0.06	1.83	0.17	0.15	0.55	0.18	1.43	0.06	1.31	0.43	0.02	0.70	1.49	0.04
	SH3	1.39	0.08	2.77	0.55	0.13	1.03	0.23	0.84	0.13	2.30	0.61	0.02	1.31	8.61	0.05
	SH4	3.10	0.18	4.59	1.07	0.42	0.90	0.37	1.41	0.45	3.04	0.78	0.16	2.13	6.49	0.10
	SH6	3.34	0.10	4.43	0.17	0.33	2.43	0.45	3.78	0.13	6.97	2.81	0.02	3.98	7.87	0.02
	SH7	0.60	0.07	2.15	0.79	0.23	0.44	0.21	0.61	0.12	1.40	0.40	0.02	0.70	2.51	0.03
	SH8	0.82	0.07	2.79	0.33	0.18	0.62	0.26	0.86	0.11	2.91	0.54	0.01	0.95	4.19	0.02
	SH10	0.68	0.03	0.46	0.54	0.41	0.76	0.05	0.26	0.00	0.38	0.18	0.01	0.38	1.10	0.02
	SH11	1.85	0.03	1.02	0.54	0.39	0.67	0.10	6.44	0.10	5.37	8.92	0.01	16.54	130	0.04

< LOD: Limit of detection.

Table S9. Predicted no-effect concentration (PNEC) of 63 PTSs using ecological structure-activity relationships (ECOSAR) model.

Compounds	Organism	Endpoint	Duration	Value ($mg\ L^{-1}$)	Assessment factor	Log K_{OW}	PNEC (Sediment, $ng\ g^{-1}$)
Polychlorinated biphenyl (PCBs)							
2,4'-Dichlorobiphenyl	Green Algae	EC50	96h	0.604	1000	5.09	561
2,4,4'-Trichlorobiphenyl	Green Algae	EC50	96h	0.25	1000	5.62	257
2,2',5,5'-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	6.09	112
2,2',4,5'-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	6.22	115
2,2',3,5'-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	5.81	107
3,4,4'-Trichlorobiphenyl	Green Algae	EC50	96h	0.25	1000	5.9	269
2,4,4',5-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	6.67	123
2,3',4',5-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	6.23	115
2,3',4,4'-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	6.31	116
2,3,4,4'-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	5.84	107
2,2',4,5,5'-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	6.8	50.9
2,2',4,4',5-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	7.21	54.0
2,2',3,4,5'-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	6.85	51.3
3,3',4,4'-Tetrachlorobiphenyl	Green Algae	EC50	96h	0.101	1000	6.63	122
2,2',3,3',4-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	6.68	50.0
2,3',4,4',5-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	7.12	53.3
2,3,4,4',5-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	6.98	52.3
2,2',4,4',5,5'-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7.75	22.6
2,3,3',4,4'-Pentachlorobiphenyl	Green Algae	EC50	96h	0.041	1000	6.79	50.8
2,2',3,3',5,6,6'-Heptachlorobiphenyl	Green Algae	EC50	96h	0.0063	1000	8.27	9.51
2,2',3,4,4',5'-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7.44	21.7
2,3,3',4,4',6-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7.62	22.3
3,3',4,4',5-Pentachlorobiphenyl	Green Algae	EC50	96h	0.41	1000	6.98	523
2,3,4,4',5,6-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7.31	21.4
2,2',3,4',5,5',6-Heptachlorobiphenyl	Green Algae	EC50	96h	0.0063	1000	8.27	9.51
2,2',3,4,4',5',6-Heptachlorobiphenyl	Green Algae	EC50	96h	0.0063	1000	8.27	9.51
2,2',3,3',4,4'-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7..31	21.4
2,3,3',4,4',5-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7.6	22.2
2,2',3,4,4',5,5'-Heptachlorobiphenyl	Green Algae	EC50	96h	0.0063	1000	8.27	9.51
3,3',4,4',5,5'-Hexachlorobiphenyl	Green Algae	EC50	96h	0.016	1000	7.41	21.7
2,2',3,3',4,4',5-Heptachlorobiphenyl	Green Algae	EC50	96h	0.0063	1000	8.27	9.51
2,3,3',4,4',5,5'-Heptachlorobiphenyl	Green Algae	EC50	96h	0.0063	1000	8.27	9.51
Styrene oligomers (SOs)							
1,3-Diphenylpropane	Green Algae	EC50	96h	0.396	1000	3.43	0.72
cis-1,2-Diphenylcyclobutane	Green Algae	EC50	96h	0.291	1000	5.46	1.15

2,4-Diphenyl-1-butene	Green Algae	EC50	96h	0.218	1000	5.64	1.18
trans-1,2-Diphenylcyclobutane	Green Algae	EC50	96h	0.291	1000	5.46	1.15
2,4,6-Triphenyl-1-hexene	Green Algae	EC50	96h	0.0051	1000	8.26	1.73
1e-Phenyl-4e-(1-phenylethyl)-tetralin	Green Algae	EC50	96h	0.014	1000	7.62	1.60
1a-Phenyl-4e-(1-phenylethyl)-tetralin	Green Algae	EC50	96h	0.014	1000	7.62	1.60
1a-Phenyl-4a-(1-phenylethyl)-tetralin	Green Algae	EC50	96h	0.014	1000	7.62	1.60
1e-Phenyl-4a-(1-phenylethyl)-tetralin	Green Algae	EC50	96h	0.014	1000	7.62	1.60
1,3,5-Triphenylcyclohexane	Green Algae	EC50	96h	0.0067	1000	8.08	1.70
Alkylphenols (APs)							
4-*tert*-Octylphenol	Green Algae	EC50	96h	0.387	1000	0.387	5.28
4-*tert*-Octylphenol monoethoxylate	Green Algae	EC50	96h	0.907	1000	0.907	4.86
4-*tert*-Octylphenol diethoxylate	Green Algae	EC50	96h	1.65	1000	1.65	4.59
Nonylphenols	Green Algae	EC50	96h	0.189	1000	0.189	5.77
Nonylphenol monoethoxylates	Green Algae	EC50	96h	0.307	1000	0.307	5.58
Nonylphenol diethoxylates	Green Algae	EC50	96h	0.555	1000	0.555	5.30
Polyhalogenated carbazoles (PHCZs)							
1-Bromocarbazole	Green Algae	EC50	96h	2.91	1000	2.91	4.12
2-Chlorocarbazole	Green Algae	EC50	96h	3.53	1000	3.53	3.88
3-Chlorocarbazole	Green Algae	EC50	96h	3.53	1000	3.53	3.88
4-Bromocarbazole	Green Algae	EC50	96h	2.91	1000	2.91	4.12
2-Bromocarbazole	Green Algae	EC50	96h	2.91	1000	2.91	4.12
3-Bromocarbazole	Green Algae	EC50	96h	2.91	1000	2.91	4.12
1,3,6,8-Tetrachloro-9H-carbazole	Green Algae	EC50	96h	0.245	1000	0.245	5.80
1-Bromo-3,6-dichloro-9H-carbazole	Green Algae	EC50	96h	0.477	1000	0.477	5.40
2,7-Dibromocarbazole	Green Algae	EC50	96h	0.93	1000	0.93	5.01
3,6-Dibromocarbazole	Green Algae	EC50	96h	0.93	1000	0.93	5.01
1,8-Dibromo-3,6-dichloro-9H-carbazole	Green Algae	EC50	96h	0.145	1000	0.145	6.30
3-Bromo-9-phenylcarbazole	Green Algae	EC50	96h	0.229	1000	0.229	5.88
1,3,6-Tribromocarbazole	Green Algae	EC50	96h	0.28	1000	0.28	5.90
1,3,6,8-Tetrabromocarbazole	Green Algae	EC50	96h	0.081	1000	0.081	6.79
3,6-Dibromo-9-phenylcarbazole	Green Algae	EC50	96h	0.069	1000	0.069	6.77

Supplementary Figures

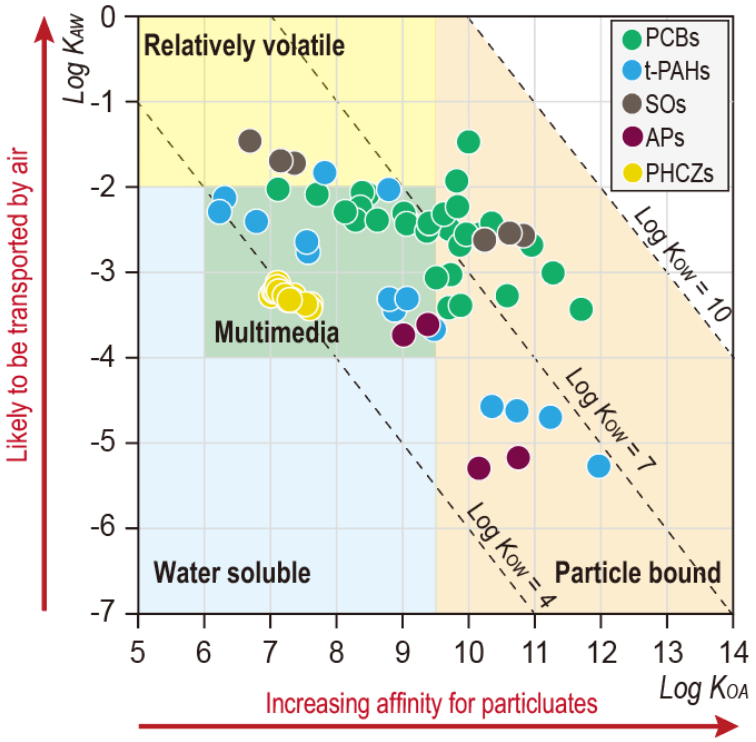

Fig. S1. Chemical space map of persistent toxic substances, including 32 PCBs, 15 traditional PAHs, 10 SOs, 6 APs, and 15 PHCZs. Distribution coefficients, such as log K_{OA}, log K_{AW}, and log K_{OW} of PTSs were obtained from ChemSpider (https://www.chemspider.com/) and Jin et al. (2021).

Jin, H., Zhao, N., Hu, H., Liu, W., Zhao, M., 2021. Occurrence and partitioning of polyhalogenated carbazoles in seawater and sediment from East China Sea. Water Res. 190, 116717. https://doi.org/10.1016/j.watres.2020.116717.

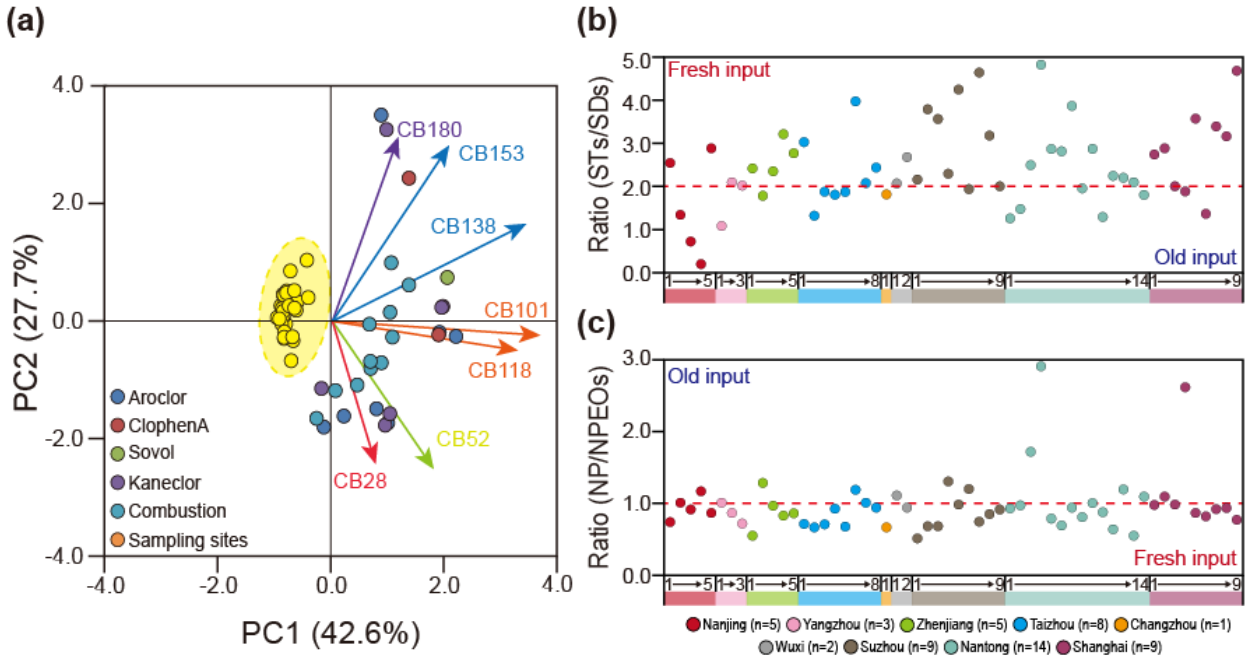

Fig. S2. (a) Source identification of sedimentary PCBs using principal component analysis. Assessment of fresh inputs of **(b)** SOs and **(c)** APs in sediments along the Yangtze River, China.