Supporting information (SI)

Occurrence, sources, and risks of short-, medium-, and long-chain chlorinated paraffins in sediments from an e-waste recycling area in China

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This supplementary document contains additional but necessary details of sampling, sample analysis, original data, statistical analysis results, risk calculation results, and related references. It comprises 24 pages, 5 sections, 10 figures, and 6 tables in total.

SI — Sample Collection

Figure S1. Geographical locations of the Lian River basin, Puning City, and Shantou City, China.

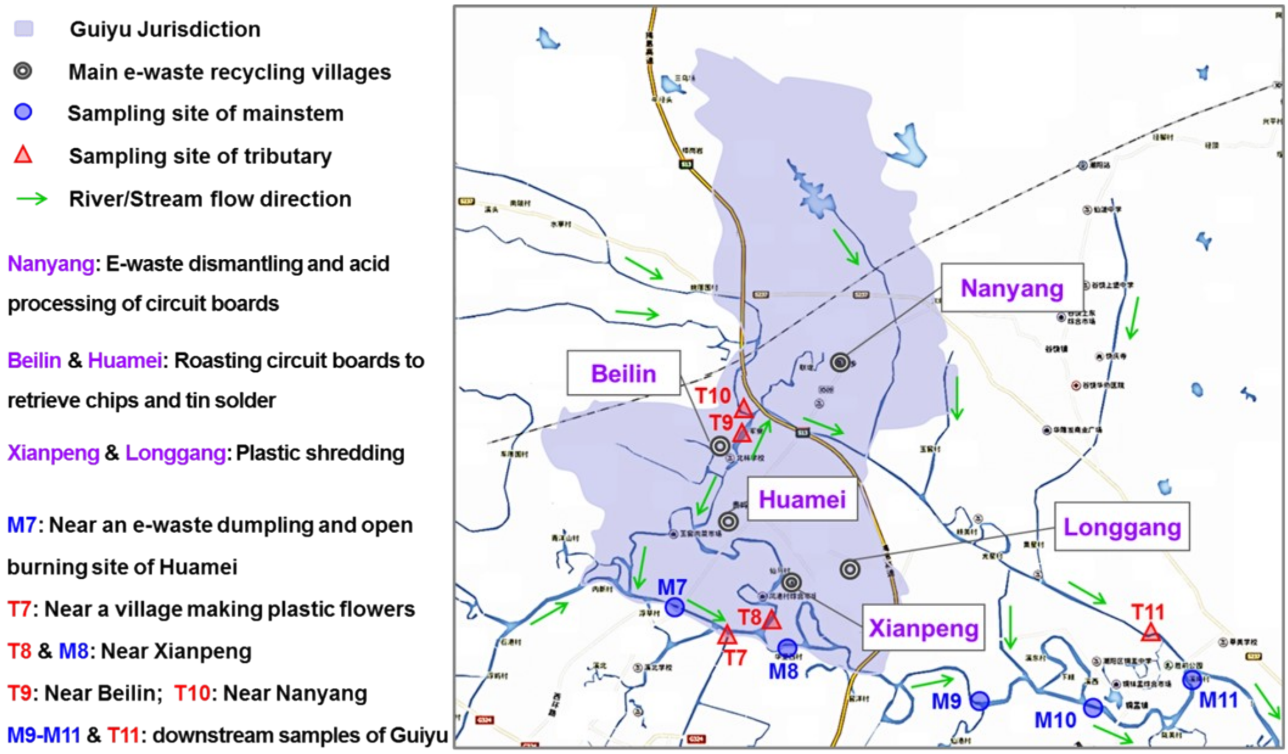

Figure S2. Major villages within the Guiyu e-waste recycling zone, e-wastes handled and associated recycling activities, river/stream flow directions and our sediment sampling sites (which have been documented in our previous publication Li et al., 2019).

SI — Sample Analysis

Separation and analysis of all chlorinated paraffin (CP) congeners/homologues were conducted using a Thermo Ultimate 3000 ultra-performance liquid chromatography (UPLC) system coupled to a Q-Exactive Orbitrap mass spectrometer (MS; Thermo Fisher Scientific, USA). Chromatographic separation was performed on a Thermo Scientific™ Accucore™ C18 column (2.1 × 100 mm, 2.6 μm), maintained at 40 °C. The mobile phase consisted of (A) water and (B) acetonitrile, with 0.05 mmol L^{-1} tetramethylammonium chloride (TMAC) added to acetonitrile to enhance CP ionization. A flow rate of 0.3 mL min^{-1} was used for elution. The gradient program was as follows: initiated from 30% B (held for 2 min), ramped to 70% B over 3 minutes, further increased to 100% B in1 minute (held for 4 minutes), then returned to 30% B in 1 minute (stabilized for 3 minutes). Detailed gradient conditions are provided in Table S1.

The optimized MS parameters for accurate detection and quantification of CPs were as follows: Ionization mode: Negative electrospray ionization (ESI^-); Capillary temperature: 275 °C; Spray voltage: 2.5 kV; Auxiliary gas heater temperature: 300 °C; Sheath gas flow rate: 46 (arbitrary units); Auxiliary gas flow rate: 5 (arbitrary units); Sweep gas: Disabled; Detector: Orbitrap mass analyzed (resolution: 70,000 FWHM); Scan range: 100–1200 m/z; Maximum injection time: 200 ms; Automated gain control (AGC) target: 1.0×10^6; S-lens RF level: 55 V. Ion-monitoring followed our previously established method (Huang et al., 2021), which were based on $[M+Cl]^-$ adducts of individual CP congeners with a mass tolerance of 5 ppm. Quantitative and qualitative ions for specific CP compounds are detailed in Table S2.

Table S1. Gradient elution program for the liquid chromatographic separation of CPs.

Time (min)	A (%)	B (%)	Flow rate (mL min^{-1})
0	70	30	0.3
2	70	30	0.3
5	30	70	0.3
6	0	100	0.3
10	0	100	0.3
11	70	30	0.3
14	70	30	0.3

Table S2. Molecular Weight (MW), quantitative and qualitative ions (m/z), and method detection limits (MDLs, ng g^{-1}) for specific congeners/homologues of short-chain CPs (SCCPs), medium-chain CPs (MCCPs), and long-chain CPs (LCCPs).

CPs	MW	Quantitative Ion	MDLs	CPs	MW	Quantitative Ion	MDLs
$C_{10}H_{13}Cl_9$	452.264	486.7849	0.15	$C_{17}H_{28}Cl_8$	516.011	550.93342	0.10
$C_{10}H_{14}Cl_8$	417.822	452.82387	0.15	$C_{17}H_{29}Cl_7$	481.569	516.9724	0.05
$C_{10}H_{15}Cl_7$	383.38	418.86285	0.15	$C_{17}H_{30}Cl_6$	447.127	481.01432	0.05
$C_{10}H_{16}Cl_6$	348.938	382.90477	0.15	$C_{17}H_{31}Cl_5$	412.685	447.05329	0.05
$C_{10}H_{17}Cl_5$	314.496	348.94374	0.15	$C_{17}H_{32}Cl_4$	378.243	413.09226	0.05
$C_{10}H_{18}Cl_4$	280.054	314.98271	0.10	$C_{18}H_{27}Cl_{11}$	633.364	668.82921	0.20
$C_{11}H_{13}Cl_{11}$	535.175	570.71966	0.15	$C_{18}H_{28}Cl_{10}$	598.922	632.87113	0.20
$C_{11}H_{14}Cl_{10}$	500.733	534.76158	0.15	$C_{18}H_{29}Cl_9$	564.48	598.9101	0.20
$C_{11}H_{15}Cl_9$	466.291	500.80055	0.15	$C_{18}H_{30}Cl_8$	530.038	564.94907	0.20
$C_{11}H_{16}Cl_8$	431.849	466.83952	0.15	$C_{18}H_{31}Cl_7$	495.596	530.98805	0.20
$C_{11}H_{17}Cl_7$	397.407	432.8785	0.15	$C_{18}H_{32}Cl_6$	461.154	495.02997	0.20
$C_{11}H_{18}Cl_6$	362.965	396.92042	0.15	$C_{18}H_{33}Cl_5$	426.712	461.06894	0.15
$C_{11}H_{19}Cl_5$	328.523	362.95939	0.15	$C_{18}H_{34}Cl_4$	392.27	427.10791	0.15
$C_{11}H_{20}Cl_4$	294.081	328.99836	0.10	$C_{19}H_{29}Cl_{11}$	647.391	682.84486	0.20
$C_{12}H_{14}Cl_{12}$	583.644	618.69633	0.15	$C_{19}H_{30}Cl_{10}$	612.949	646.88678	0.20
$C_{12}H_{15}Cl_{11}$	549.202	584.73531	0.15	$C_{19}H_{31}Cl_9$	578.507	612.92575	0.20
$C_{12}H_{16}Cl_{10}$	514.76	548.77723	0.15	$C_{19}H_{32}Cl_8$	544.065	578.96472	0.20
$C_{12}H_{17}Cl_9$	480.318	514.8162	0.15	$C_{19}H_{33}Cl_7$	509.623	545.0037	0.20
$C_{12}H_{18}Cl_8$	445.876	480.85517	0.15	$C_{19}H_{34}Cl_6$	475.181	509.04562	0.20
$C_{12}H_{19}Cl_7$	411.434	446.89415	0.15	$C_{19}H_{35}Cl_5$	440.739	475.08459	0.15
$C_{12}H_{20}Cl_6$	376.992	410.93607	0.15	$C_{19}H_{36}Cl_4$	406.297	441.12356	0.15
$C_{12}H_{21}Cl_5$	342.55	376.97504	0.15	$C_{20}H_{31}Cl_{11}$	661.418	696.86051	0.20
$C_{12}H_{22}Cl_4$	308.108	343.01401	0.10	$C_{20}H_{32}Cl_{10}$	626.976	660.90243	0.20
$C_{13}H_{16}Cl_{12}$	597.671	632.71198	0.15	$C_{20}H_{33}Cl_9$	592.534	626.9414	0.20
$C_{13}H_{17}Cl_{11}$	563.229	598.75096	0.15	$C_{20}H_{34}Cl_8$	558.092	592.98037	0.20
$C_{13}H_{18}Cl_{10}$	528.787	562.79288	0.15	$C_{20}H_{35}Cl_7$	523.65	559.01935	0.20
$C_{13}H_{19}Cl_9$	494.345	528.83185	0.15	$C_{20}H_{36}Cl_6$	489.208	523.06127	0.20
$C_{13}H_{20}Cl_8$	459.903	494.87082	0.15	$C_{20}H_{37}Cl_5$	454.766	489.10024	0.15
$C_{13}H_{21}Cl_7$	425.461	460.9098	0.15	$C_{20}H_{38}Cl_4$	420.324	455.13921	0.15

$C_{13}H_{22}Cl_6$	391.019	424.95172	0.15	$C_{21}H_{33}Cl_{11}$	675.445	710.87616	0.20
$C_{13}H_{23}Cl_5$	356.577	390.99069	0.10	$C_{21}H_{34}Cl_{10}$	641.003	670.92398	0.20
$C_{13}H_{24}Cl_4$	322.135	357.02966	0.10	$C_{21}H_{35}Cl_9$	606.561	636.96295	0.20
$C_{14}H_{19}Cl_{11}$	577.256	612.76661	0.10	$C_{21}H_{36}Cl_8$	572.119	603.00192	0.20
$C_{14}H_{20}Cl_{10}$	542.814	576.80853	0.10	$C_{21}H_{37}Cl_7$	537.677	569.0409	0.20
$C_{14}H_{21}Cl_9$	508.372	542.8475	0.10	$C_{21}H_{38}Cl_6$	503.235	535.07987	0.15
$C_{14}H_{22}Cl_8$	473.93	508.88647	0.10	$C_{21}H_{39}Cl_5$	468.793	501.11884	0.15
$C_{14}H_{23}Cl_7$	439.488	474.92545	0.10	$C_{21}H_{40}Cl_4$	434.351	469.15486	0.15
$C_{14}H_{24}Cl_6$	405.046	438.96737	0.05	$C_{22}H_{39}Cl_7$	551.704	583.05655	0.20
$C_{14}H_{25}Cl_5$	370.604	405.00634	0.05	$C_{22}H_{40}Cl_6$	517.262	549.09552	0.15
$C_{14}H_{26}Cl_4$	336.162	371.04531	0.05	$C_{22}H_{41}Cl_5$	482.82	515.13449	0.15
$C_{15}H_{20}Cl_{12}$	625.725	660.74328	0.10	$C_{22}H_{42}Cl_4$	448.378	483.17051	0.15
$C_{15}H_{21}Cl_{11}$	591.283	626.78226	0.10	$C_{23}H_{40}Cl_8$	600.173	631.03322	0.20
$C_{15}H_{22}Cl_{10}$	556.841	590.82418	0.10	$C_{23}H_{41}Cl_7$	565.731	597.0722	0.20
$C_{15}H_{23}Cl_9$	522.399	556.86315	0.10	$C_{23}H_{42}Cl_6$	531.289	563.11117	0.15
$C_{15}H_{24}Cl_8$	487.957	522.90212	0.10	$C_{23}H_{43}Cl_5$	496.847	529.15014	0.15
$C_{15}H_{25}Cl_7$	453.515	488.9411	0.10	$C_{23}H_{44}Cl_4$	462.405	497.18616	0.15
$C_{15}H_{26}Cl_6$	419.073	452.98302	0.05	$C_{24}H_{42}Cl_8$	614.2	645.04887	0.20
$C_{15}H_{27}Cl_5$	384.631	419.02199	0.05	$C_{24}H_{43}Cl_7$	579.758	611.08785	0.20
$C_{15}H_{28}Cl_4$	350.189	385.06096	0.05	$C_{24}H_{44}Cl_6$	545.316	577.12682	0.15
$C_{16}H_{22}Cl_{12}$	639.752	674.75893	0.10	$C_{24}H_{45}Cl_5$	510.874	543.16579	0.15
$C_{16}H_{23}Cl_{11}$	605.31	640.79791	0.10	$C_{24}H_{46}Cl_4$	476.432	511.20181	0.15
$C_{16}H_{24}Cl_{10}$	570.868	604.83983	0.10	$C_{25}H_{40}Cl_{12}$	765.995	800.89978	0.20
$C_{16}H_{25}Cl_9$	536.426	570.8788	0.10	$C_{25}H_{41}Cl_{11}$	731.553	766.93876	0.20
$C_{16}H_{26}Cl_8$	501.984	536.91777	0.10	$C_{25}H_{44}Cl_8$	628.227	659.06452	0.20
$C_{16}H_{27}Cl_7$	467.542	502.95675	0.05	$C_{25}H_{45}Cl_7$	593.785	625.1035	0.15
$C_{16}H_{28}Cl_6$	433.1	466.99867	0.05	$C_{25}H_{46}Cl_6$	559.343	591.14247	0.15
$C_{16}H_{29}Cl_5$	398.658	433.03764	0.05	$C_{25}H_{47}Cl_5$	524.901	557.18144	0.15
$C_{16}H_{30}Cl_4$	364.216	399.07661	0.05	$C_{25}H_{48}Cl_4$	490.459	525.21746	0.15
$C_{17}H_{24}Cl_{12}$	653.779	688.77458	0.10	$C_{26}H_{47}Cl_7$	607.812	639.11915	0.15
$C_{17}H_{25}Cl_{11}$	619.337	654.81356	0.10	$C_{26}H_{48}Cl_6$	573.37	605.15812	0.15
$C_{17}H_{26}Cl_{10}$	584.895	618.85548	0.10	$C_{26}H_{49}Cl_5$	538.928	571.19709	0.15
$C_{17}H_{27}Cl_9$	550.453	584.89445	0.10	$C_{26}H_{50}Cl_4$	504.486	539.23311	0.15

CP Quantification and Data Processing

Following the methodological framework of Bogdal et al. (2015)(**Fig. S3**), a deconvolution-based quantification model was applied to quantify CPs, as described in our previous work (Huang et al., 2021).

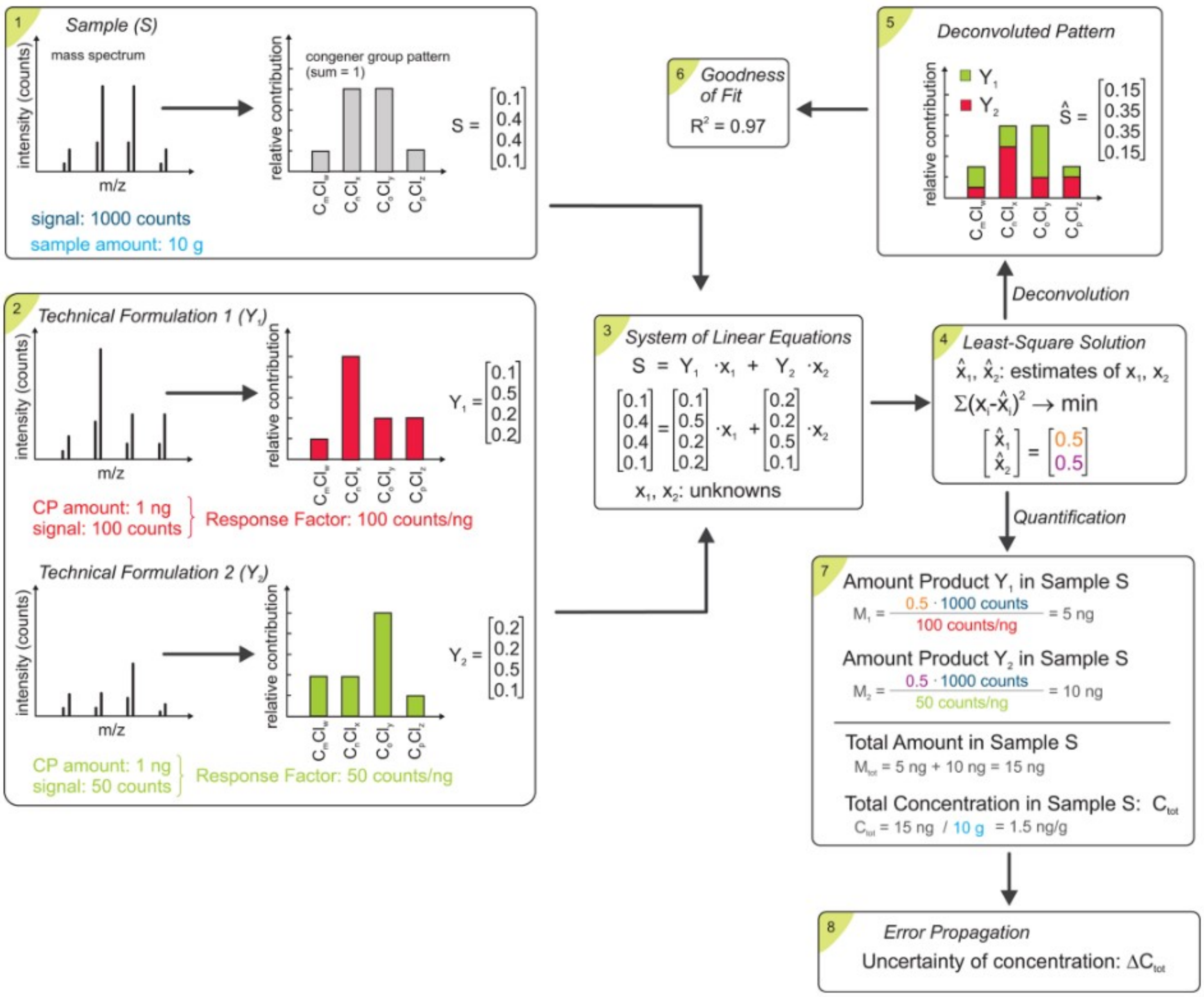

Figure S3. Data processing flowchart of the deconvolution-based quantification model for CPs using Orbitrap HRMS data (adapted from Bogdal et al., 2015).

This approach mathematically deconvolves overlapping chromatographic signals into distinct carbon-chain components using predefined homologue patterns and instrument response functions. By constructing a linear matrix from the homologue distributions of samples and standards, the contributions of each standard to the sample signal can be solved, enabling accurate CP quantification.

Quantification was performed using calibration mixtures that included three SCCP (Cl%: 51.5%, 55.5%, and 63%), three MCCP (Cl%: 42%, 52%, and 57%), and two LCCP mixtures (Cl%: 36% and 49%), each at a concentration of 5 ppm. Taking SCCPs as an example, 36 congener peaks ($C_{10-13}Cl_{4-12}$) were integrated to obtain their relative abundances (**Eqs. S1-S3**). The sample's congener profile was modeled as a linear combination of the three SCCP calibration profiles through a system of linear equations (**Eq. S4**). Coefficients were determined using MATLAB's non-negative least-squares algorithm (lsqnonneg), normalized (**Eq. S5**), and applied to weight the calibration mixtures for calculating SCCP mass (**Eq. S6**).

$$y_{i,j} = \frac{A_{i,j}}{\sum_{i=1}^{32} A_{i,j}} = \frac{A_{i,j}}{A_{j,tot}^{SCCPs}} \quad (Eq. S1)$$

$$R_j = \frac{A_{i,j}}{M_j^{SCCPs}} \quad (Eq. S2)$$

$$S_i = \frac{A_{s,i}}{\sum_{i=1}^{32} A_{s,i}} = \frac{A_{s,i}}{A_{s,tot}^{SCCPs}} \quad (Eq. S3)$$

$$S_i = \sum_{j}^{n} y_{j,i} \times x_j \rightarrow \begin{cases} s_1 = y_{1,1} \times x_1 + y_{2,1} \times x_2 + y_{3,1} \times x_3 \\ \vdots \\ s_{24} = y_{1,32} \times x_1 + y_{2,32} \times x_2 + y_{3,32} \times x_3 \end{cases} \quad (Eq. S4)$$

$$x_j^{'} = \frac{x_j}{\sum_{j=1}^{n} x_j} \quad (Eq. S5)$$

$$M_{tot}^{SCCPs} = \sum_{j=1}^{n} M_{j}^{SCCPs} = \sum_{j=1}^{n} \left(\frac{A_{s,tot}^{SCCPs} \times x_j^{'}}{R_j} \right) \quad (Eq. S6)$$

In **Eqs. S1-S6**, $A_{j,tot}^{SCCPs}$ denotes the sum of the peak areas of the 32 homologs, *i* and *j* represent the number of homologs and the number of standard samples used, respectively. In this paper, *i*=1–32 and *j*=1–3. Meanwhile, the response factor R_j is calculated using $A_{i,j}$ and the injected mass M_{j}^{SCCPs}. The method for determining the homolog proportion S_i of SCCPs in the sample is similar to that of the standard sample. The lsqnonneg function in Matlab is used to solve for the n unknowns x_j in the linear equations S_i via the least squares method, and simultaneously normalize them to obtain x_j. Thus, the injected mass M_{tot}^{SCCPs} of SCCPs in the sample is calculated using M_{j}^{SCCPs} composed of n standard substances.

Instrumental Analysis of ^{13}C-PCBs

Surrogate standards ($^{13}C_{12}$-PCB-141 and $^{13}C_{12}$-PCB-208) were analyzed together with polybrominated diphenyl ethers (PBDEs) (Song et al., 2020), using an Agilent 7890A gas chromatograph coupled with an Agilent 5975C mass spectrograph (GC-MS) in negative chemical ionization (NCI) mode. Chromatographic separation was performed on a 30-m HP-5 MS column (250 μm i.d., 0.25-μm film thickness). The GC oven temperature program was as follows: initial temperature was set at 110 °C and held for 1.0 min; increased to 180 °C at a rate of 8 °C min^{-1} and held for 1.0 min; then raised to 240 °C at 2 °C min^{-1} and held for 5.0 min; further increased to 280 °C at 2 °C min^{-1} and held for 15 min; and finally ramped to 300 °C at 10 °C min^{-1} and held for 12 min. The injection port and transfer line temperatures were set at 280 °C and 300 °C, respectively. The ion source temperature was maintained at 200 °C. An injection volume of 1 μL was used for both samples and standards. The monitored ions (m/z) were 372.0 and 374.0 for

$^{13}C_{12}$-PCB-141, 473.7 and 475.7 for $^{13}C_{12}$-PCB-208, and 262.8 and 264.8 for the internal standard, decachlorodiphenyl ether. The recoveries of spiked $^{13}C_{12}$-PCBs in Lian River sediment samples are presented in **Table S3**.

SI — Original Data

Table S3. Concentrations (ng g^{-1}, dry weight (dw)) of specific CP homologues (C_{10}–C_{26}), CP classes and triclosan (TCS), along with total organic carbon (TOC, %) content, recoveries of ^{13}C-PCBs (R, %), and total concentrations (ng g^{-1}, dw) of CPs, brominated flame retardants (BFRs)[1], organophosphate esters (OPEs)[2], and Dechlorane plus (DPs)[3] in the mainstem and tributary sediments of the Lian River, China.

Site	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12	M13	M14
C_{10}	4.68	17.9	12.0	18.3	45.7	832	975	9.05	14.5	139	35.9	13.4	16.5	37.3
C_{11}	10.2	36.0	28.2	47.7	117	945	1140	20.8	31.6	208	86.7	34.5	33.6	248
C_{12}	8.51	39.9	38.6	56.6	141	582	667	31.0	40.2	146	93.8	43.3	31.5	130
C_{13}	13.0	65.6	74.5	91.2	199	972	1210	65.7	75.2	241	140	86.6	57.0	177
ΣSCCPs	36.4	159	153	214	503	3330	3990	127	161	735	356	178	139	591
C_{14}	25.2	104	227	231	402	1020	1410	219	145	313	309	206	180	51.9
C_{15}	9.99	53.3	94.1	118	177	362	635	99.4	60.0	122	119	87.0	85.3	23.1
C_{16}	5.43	37.0	63.9	62.5	112	158	362	62.3	40.5	67.5	71.9	51.9	54.8	16.1
C_{17}	4.12	29.8	58.0	58.3	105	105	296	52.9	33.4	54.0	59.6	44.4	48.0	12.9
ΣMCCPs	44.8	224	443	470	794	1650	2700	433	279	556	560	389	368	104
C_{18}	3.69	25.9	63.4	80.5	149	104	326	53.6	35.6	57.2	60.2	48.5	49.6	12.8
C_{19}	2.37	14.7	40.3	64.0	121	55.2	201	37.0	27.3	32.1	34.9	28.9	33.2	8.09
C_{20}	1.83	11.2	32.6	55.9	101	31.0	128	37.0	26.1	19.7	23.0	22.0	29.1	5.42
C_{21}	0.305	3.03	8.47	14.8	23.3	0.806	28.0	9.98	8.38	3.68	1.92	6.20	11.1	1.06
C_{22}	0.151	1.56	2.94	4.83	2.64	n.d	1.84	4.16	3.61	n.d	n.d	2.48	6.49	0.165
C_{23}	0.246	2.62	3.40	7.87	n.d	0.0218	n.d	3.82	5.13	n.d	n.d	4.15	8.60	0.741

C_{24}		0.104	2.18	1.34	3.46	0.224	n.d	0.877	2.72	2.03	n.d	n.d	3.50	4.56	n.d
C_{25}		0.199	3.52	4.83	9.37	9.99	n.d	7.61	5.11	3.95	1.58	2.57	5.66	5.90	0.546
C_{26}		0.00406	0.700	0.0469	0.532	0.118	n.d	n.d	n.d	0.703	n.d	n.d	n.d	n.d	0.0356
ΣLCCPs		8.90	65.4	157	241	407	191	693	153	113	114	123	121	149	28.9
ΣCPs		90.0	449	754	925	1700	5170	7390	713	553	1410	1040	688	655	724
TCS		2.18	25.0	76.8	322	83.2	386	181	17.3	35.3	99.6	25.8	21.8	10.5	113
TOC		1.46	0.999	5.00	6.65	9.79	16.4	18.6	4.77	2.23	8.40	8.82	3.93	4.90	10.0
R	**^{13}C-PCB-141**	90.0	73.9	75.8	82.7	78.0	70.6	62.6	78.2	84.6	71.6	140	68.1	81.7	70.9
	^{13}C-PCB-208	95.5	84.7	68.9	84.4	80.4	84.1	83.2	81.3	85.1	92.7	90.9	64.7	77.1	72.3
ΣBFRs		4.56	31.0	99.9	135	106	479	337000	16700	521	4100	2130	1160	1900	501
ΣOPEs		91.3	300	295	749	1880	7110	2190000	42900	2470	16300	16700	8470	9580	2530
ΣDPs		0.417	3.60	9.06	2.72	21.9	623	3740	255	24.1	325	387	96.5	153	48.0
Site		**M15**	**T1**	**T2**	**T3**	**T4**	**T5**	**T6**	**T7**	**T8**	**T9**	**T10**	**T12**	**T13**	**T11**
C_{10}		43.2	60.0	6.35	55.9	8.23	90.9	14.1	9.10	98.2	301	13.5	88.8	131	50.7
C_{11}		274	163	17.3	99.0	18.9	217	16.1	26.9	270	744	34.2	94.0	222	100
C_{12}		148	171	27.3	69.8	23.0	242	14.5	39.6	302	754	60.7	54.9	171	99.2
C_{13}		202	241	52.0	102	37.0	285	24.4	70.8	266	957	179	98.0	297	168
ΣSCCPs		668	636	103	326	87.1	834	69.1	146	936	2760	287	336	820	418
C_{14}		111	636	163	163	116	749	42.5	235	665	2560	322	89.3	385	319
C_{15}		52.8	196	67.6	61.8	58.1	320	18.5	96.0	306	1370	208	37.3	156	144
C_{16}		34.0	120	42.7	32.3	28.3	194	11.4	64.2	246	1100	186	20.6	89.4	99.8
C_{17}		27.5	110	38.3	24.0	21.4	166	9.02	59.0	214	966	169	17.2	69.6	88.3
ΣMCCPs		225	1060	312	281	224	1430	81.4	454	1430	5990	885	164	700	651
C_{18}		28.5	121	39.4	21.4	20.6	157	10.9	69.4	167	599	160	24.6	73.1	93.3
C_{19}		17.6	93.4	25.9	11.6	12.4	97.4	8.34	43.0	87.0	310	98.6	16.1	38.3	53.0
C_{20}		11.8	93.2	22.2	7.22	9.67	83.6	6.41	37.7	57.2	220	80.7	10.5	21.0	35.8
C_{21}		2.62	35.4	6.23	1.22	2.61	83.7	1.36	9.35	9.60	54.9	25.4	1.81	3.40	8.83
C_{22}		1.35	22.7	3.28	0.332	0.923	16.3	0.301	4.17	n.d	6.45	14.7	0.142	0.297	n.d

C$_{23}$		2.36	33.6	4.87	0.501	1.61	27.2	0.483	4.66	n.d	9.02	18.6	0.155	n.d	n.d
C$_{24}$		1.02	28.7	2.26	0.291	1.26	27.0	0.314	2.71	n.d	5.20	13.9	0.110	n.d	n.d
C$_{25}$		0.547	35.2	4.64	0.449	1.57	38.1	0.605	5.88	n.d	25.9	15.4	0.663	1.80	3.92
C$_{26}$		0.423	11.8	n.d	0.0148	0.266	12.6	n.d	n.d	n.d	0.00896	2.25	n.d	n.d	n.d
ΣLCCPs		66.3	475	109	43.0	50.9	542	28.7	177	321	1230	430	54.0	138	195
ΣCPs		959	2170	523	650	362	2810	179	777	2690	9980	1600	554	1660	1260
TCS		12.1	354	32.3	34.3	16.4	393	8.12	57.0	18.0	196	7.66	29.6	53.1	127
TOC		12.4	5.80	3.35	9.52	2.31	10.4	2.26	5.55	9.58	34.9	4.39	9.67	20.6	5.63
R	**^{13}C-PCB-141**	89.3	84.9	82.8	76.4	118	60.5	88.2	65.6	105	76.5	77.3	76.8	72.2	69.1
	^{13}C-PCB-208	88.7	98.1	90.7	92.8	74.4	72.4	70.9	98.1	64.7	86.3	76.2	82.9	84.8	74.6
ΣBFRs		n.d	86.1	106	104	36.5	863	n.d	6560	24700	47600	40600	6700	410	3280
ΣOPEs		428	289	415	571	557	23400	7090	8990	41800	161000	156000	27300	1680	2920
ΣDPs		1.42	7.49	8.89	206	3.81	438	12.0	595	1920	2710	782	1040	175	64.3

[1] BFRs comprised 12 polybrominated diphenyl ether (PBDE) congeners, 3 hexabromocyclododecane (HBCD) isomers, decabromodiphenyl ethane (DBDPE), 1,2-bis(2,4,6,-tribromophenoxy)ethane (BTBPE), bis(2-ethylhexyl) 3,4,5,6-tetrabromophthalate (TBPH) and and 2-ethylhexyl-2,3,4,5-tetrabromobenzoate (TBB). Data were derived from our previous study (Li et al., 2019).

[2] OPEs included 25 congeners: 9 alkyl-substituted, 10 aryl-substituted, and 6 halogenated OPEs. Data were obtained from our prior research (Liu et al., 2023).

[3] DPs consisted of two isomers (*syn-* and *anti*-DPs); these data are unpublished.

SI —Data Analysis and Results

Correlation Analysis

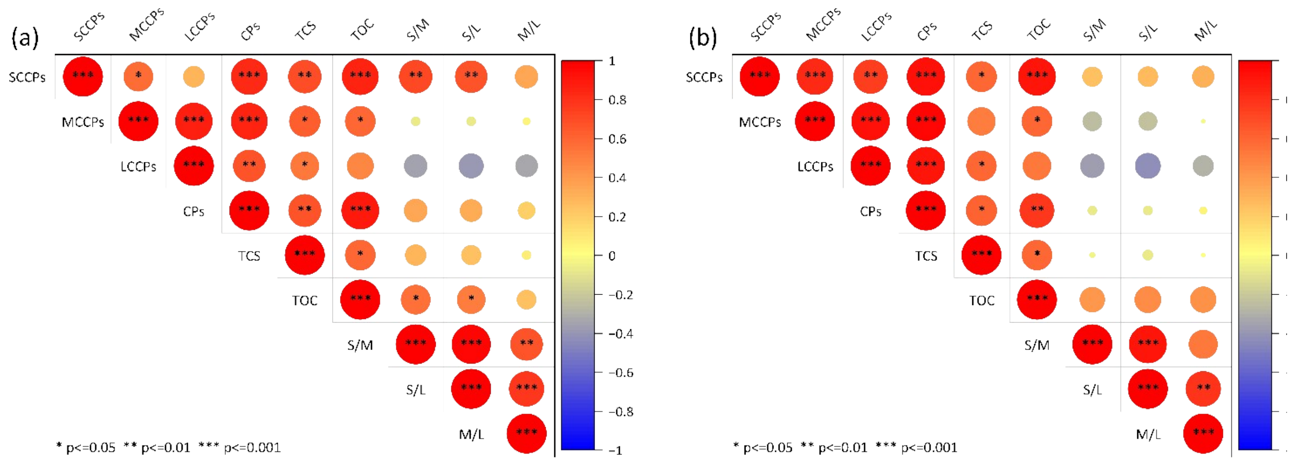

Figure S4. Spearman correlation analysis results between the concentrations of three CP classes (S: SCCPs; M: MCCPs; L: LCCPs), TOC, TCS, S/M, S/L, and M/L in mainstem (a) and tributary (b) sediments of the Lian River.

Compositions Analysis

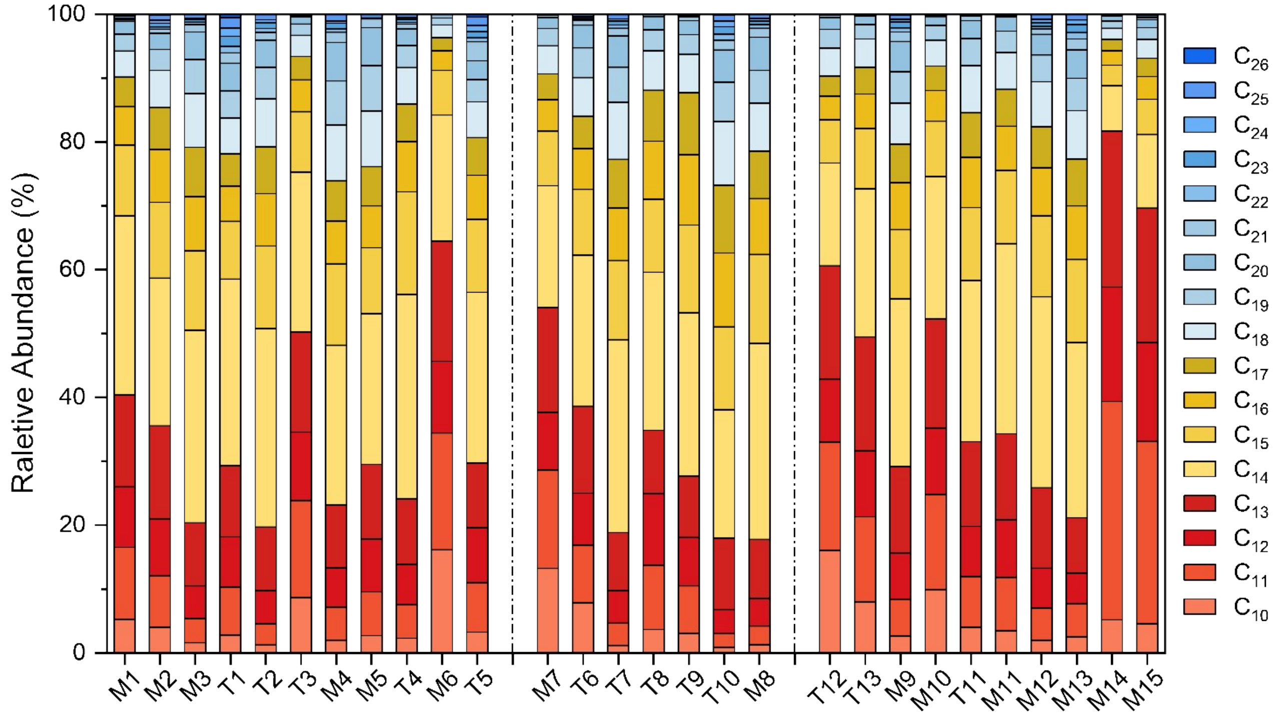

Figure S5. Relative percentages of CP homologues with different carbon-chain lengths ($C_{10–26}$) in the mainstem and tributary sediments of the Lian River (Data were normalized to total concentrations of CPs).

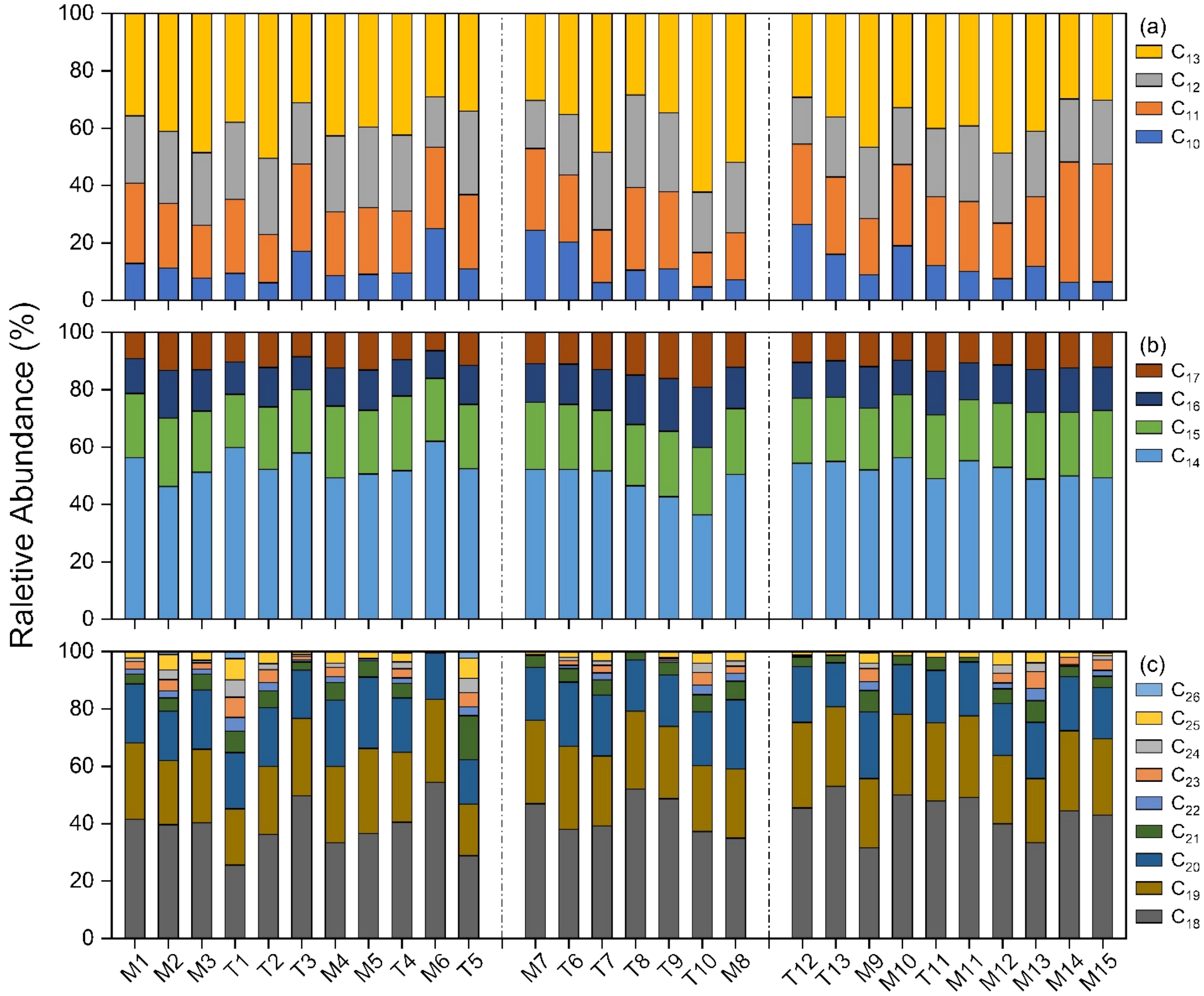

Figure S6. Homologue distribution profiles of (a) SCCP ($C_{10–14}$), (b) MCCP ($C_{14–17}$), and (c) LCCP ($C_{18–26}$) in the mainstem and tributary sediments of the Lian River (Data were normalized to the total concentrations of SCCPs, MCCPs, and LCCPs, respectively).

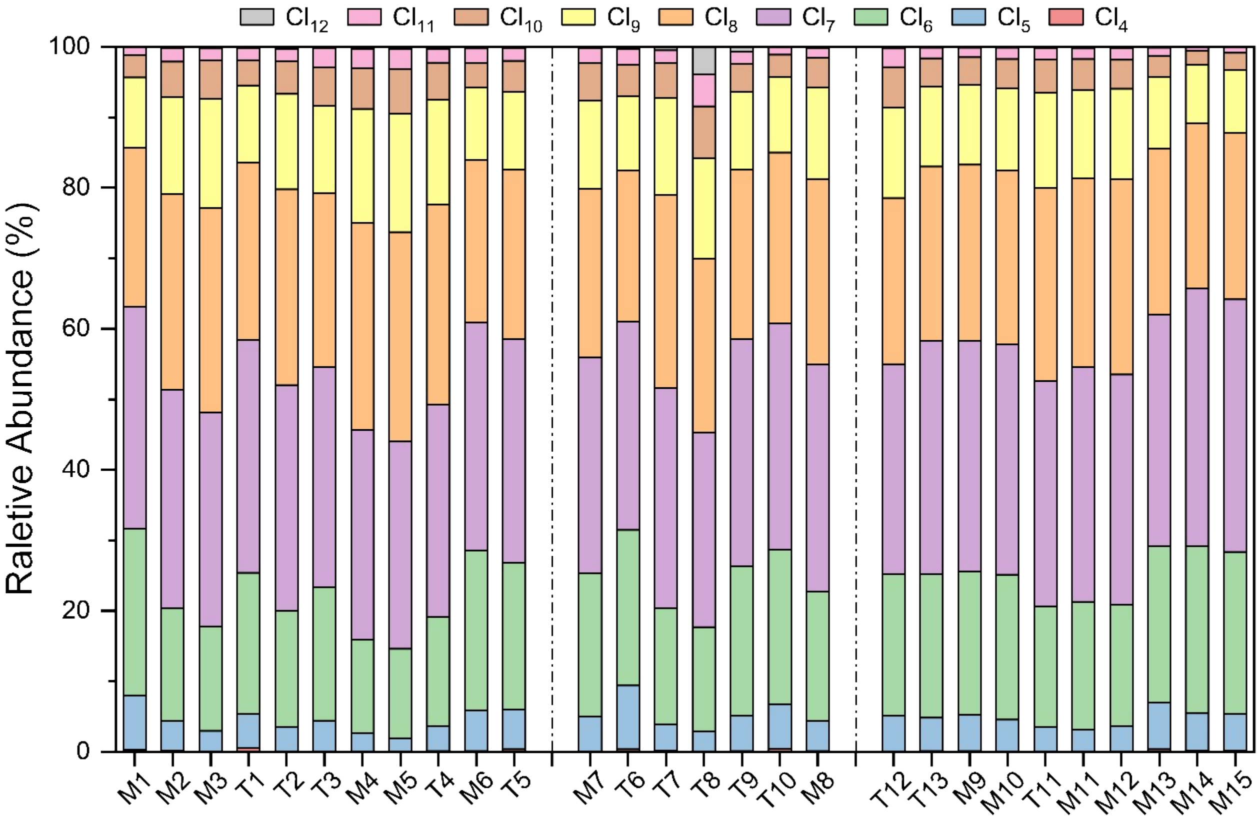

Figure S7. Relative contributions of CP homologues with different chlorine numbers (Cl_{5-11}) to total CP concentrations in sediments from the Lian River (Data were normalized to total concentrations of CPs).

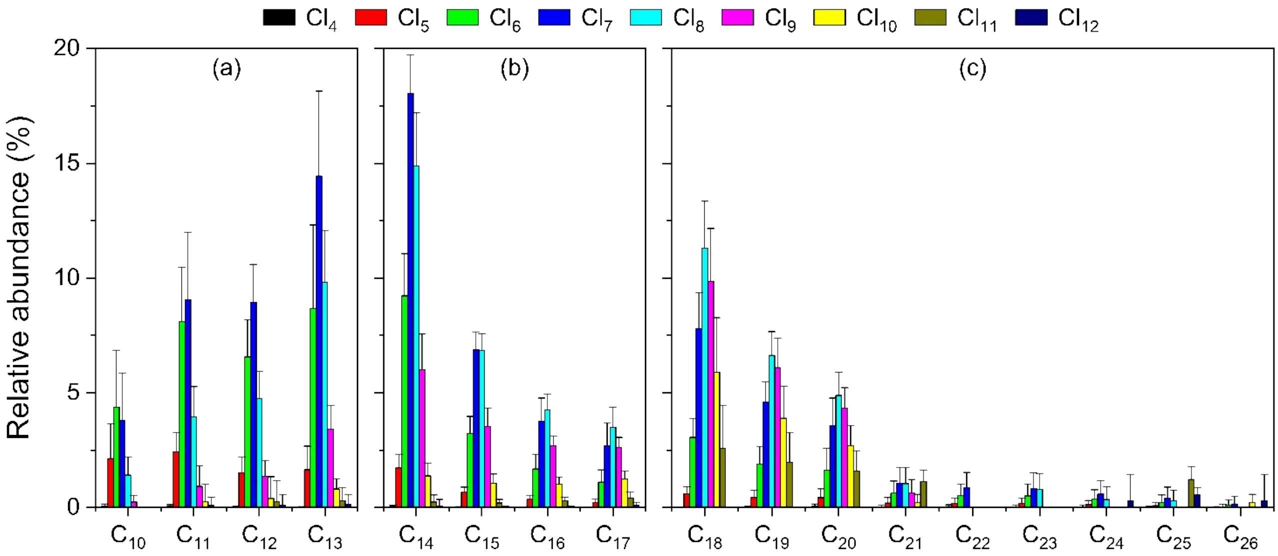

Figure S8. Relative contributions of CP homologues with different chlorine numbers ($Cl_{5–11}$) to (a) SCCPs, (b) MCCPs, and (c) LCCPs in sediments from the Lian River (Data were normalized to the total concentrations of SCCPs, MCCPs, and LCCPs, respectively).

Principal Component Analysis-Multiple Linear Regression (PCA-MLR)

Table S4. Principal component analysis (PCA) results of CP concentrations in sediments from the Lian River.

Factor loads on CP homologues and the total variance				**Factor scores on specific sampling sites**			
Congeners	**Components**			**Samples**	**Components**		
	F1	**F2**	**F3**		**F1**	**F2**	**F3**
C_{10}	0.207	-0.089	0.962	**M1**	-0.537	-0.504	-0.456
C_{11}	0.413	-0.054	0.904	**M2**	-0.428	-0.249	-0.373
C_{12}	0.640	0.032	0.754	**M3**	-0.081	-0.238	-0.553
C_{13}	0.521	0.007	0.851	**T1**	-0.435	3.356	0.270
C_{14}	0.846	0.151	0.493	**T2**	-0.269	-0.162	-0.524
C_{15}	0.913	0.102	0.380	**T3**	-0.465	-0.488	-0.168
C_{16}	0.958	0.085	0.234	**M4**	0.028	0.132	-0.546
C_{17}	0.967	0.094	0.194	**M5**	0.643	-0.237	-0.523
C_{18}	0.931	0.158	0.317	**T4**	-0.408	-0.383	-0.453
C_{19}	0.894	0.229	0.329	**M6**	-0.792	-0.455	3.370
C_{20}	0.872	0.351	0.238	**T5**	-0.018	3.283	0.324
C_{21}	0.542	0.751	0.113	**M7**	0.714	-0.277	3.373
C_{22}	0.144	0.952	-0.079	**T6**	-0.489	-0.480	-0.442
C_{23}	0.105	0.973	-0.084	**T7**	-0.061	-0.112	-0.575
C_{24}	0.058	0.994	-0.018	**T8**	0.666	-0.668	-0.043
C_{25}	0.416	0.900	0.011	**T9**	4.704	-0.135	-0.056
C_{26}	-0.061	0.968	0.055	**T10**	0.384	1.193	-0.675
Total variance	59.816%	28.760%	8.179%	**M8**	-0.103	-0.132	-0.574
				T12	-0.503	-0.488	-0.136
				T13	-0.212	-0.513	0.245
				M9	-0.319	-0.091	-0.432
				M10	-0.315	-0.504	0.211
				T11	0.090	-0.497	-0.340
				M11	-0.125	-0.534	-0.296
				M12	-0.236	-0.163	-0.454
				M13	-0.237	0.142	-0.512
				M14	-0.633	-0.463	0.143
				M15	-0.561	-0.335	0.197

Table S5. Multiple linear regression (MLR) coefficients for the three PCA-derived factors explaining CP concentrations in Lian River sediments.

Model		Coefficients[1]			*t*	Sig.[2]	Collinearity Statistics	
		Unstandardized Coefficients		Standardized Coefficients				
		β	Std. Erro	*β*			Tolerance	VIF
CPs	**Constant**	-3.70E-17	0.01	□	0	1	□	□
	PCA-F1	0.774	0.01	0.774	77.967	0	1	1
	PCA-F2	0.094	0.01	0.094	9.474	0	1	1
	PCA-F3	0.624	0.01	0.624	62.862	0	1	1

[1] Dependent Variable: Zscore(Σ17CPs) ; Independent variables: factor score of PCA-F1, PCA-F2, and PCA-F3 for CPs.

[2] Statistical significance was defined as $p<0.05$; insignificant correlations ($p>0.05$) indicate no meaningful relationship between independent and dependent variables.

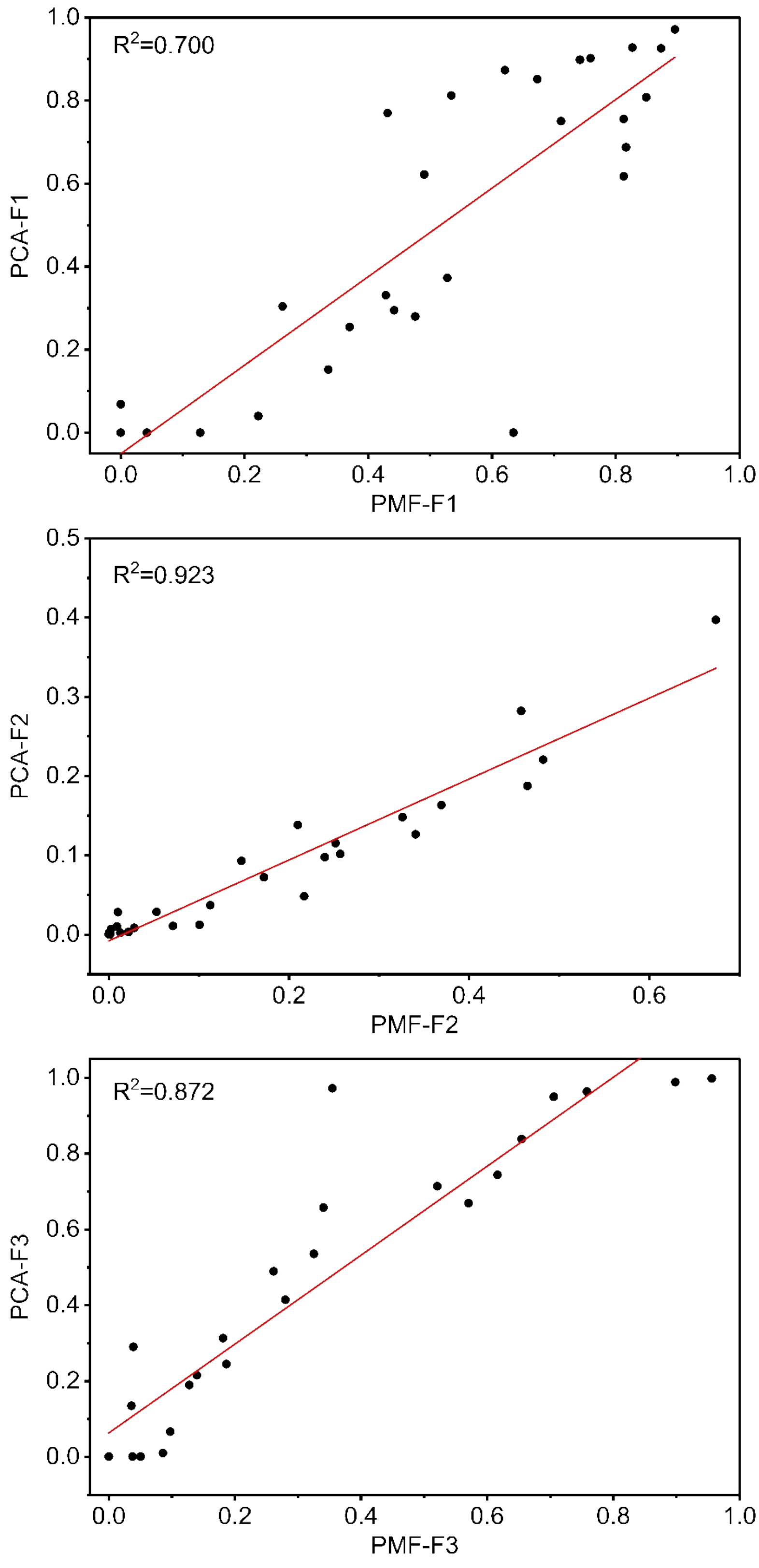

Figure S9. Correlations between matched PCA-derived and PMF-resolved factor contributions to CPs in Lian River sediments.

Risk Calculation Results

Table S6. Hazard quotients (HQs) of CPs in sediments from the Lian River.

Sites	UNEP-based HQ[1]				ECCC-derived HQ[2]			
	SCCPs	MCCPs	C_{18-26} LCCPs	Total CPs	SCCPs	MCCPs	C_{18-20} LCCPs	Total CPs
M1	0.00649	0.00344	0.00000538	0.00994	0.0138	0.00567	0.0000609	0.0195
M2	0.0285	0.0172	0.0000361	0.0457	0.0887	0.0415	0.000655	0.131
M3	0.0274	0.0341	0.0000933	0.0616	0.0171	0.0164	0.000315	0.0338
T1	0.114	0.0817	0.000225	0.195	0.0609	0.0339	0.000820	0.0957
T2	0.0184	0.0240	0.0000608	0.0424	0.0171	0.0172	0.000325	0.0346
T3	0.0583	0.0216	0.0000272	0.0799	0.0190	0.00546	0.0000452	0.0245
M4	0.0382	0.0361	0.000138	0.0745	0.0179	0.0131	0.000362	0.0313
M5	0.0898	0.0611	0.000251	0.151	0.0285	0.0150	0.000416	0.0440
T4	0.0156	0.0172	0.0000294	0.0328	0.0210	0.0179	0.000220	0.0391
M6	0.595	0.127	0.000127	0.722	0.113	0.0186	0.000117	0.132
T5	0.149	0.110	0.000249	0.259	0.0445	0.0254	0.000521	0.0704
M7	0.713	0.208	0.000441	0.921	0.119	0.0269	0.000373	0.147
T6	0.0123	0.00626	0.0000175	0.0186	0.0170	0.00668	0.000127	0.0238
T7	0.0261	0.0349	0.000103	0.0612	0.0146	0.0151	0.000318	0.0301
T8	0.167	0.110	0.000209	0.277	0.0543	0.0277	0.000335	0.0823
T9	0.492	0.461	0.000764	0.954	0.0438	0.0318	0.000352	0.0759
T10	0.0513	0.0681	0.000237	0.120	0.0363	0.0374	0.000979	0.0747
M8	0.0226	0.0333	0.0000880	0.0560	0.0147	0.0168	0.000321	0.0319
T12	0.0599	0.0126	0.0000344	0.0726	0.00904	0.00148	0.0000262	0.0105
T13	0.146	0.0539	0.0000889	0.200	0.0809	0.0230	0.000245	0.104
M9	0.0288	0.0215	0.0000621	0.0503	0.0402	0.0232	0.000506	0.0639
M10	0.131	0.0428	0.0000732	0.174	0.0486	0.0123	0.000136	0.0610
T11	0.0746	0.0501	0.000123	0.125	0.0240	0.0125	0.000202	0.0367
M11	0.0636	0.0431	0.0000793	0.107	0.0224	0.0118	0.000139	0.0343
M12	0.0318	0.0299	0.0000688	0.0618	0.0252	0.0184	0.000309	0.0438
M13	0.0247	0.0283	0.0000789	0.0531	0.0157	0.0139	0.000303	0.0299
M14	0.106	0.00800	0.0000178	0.114	0.0328	0.00192	0.0000288	0.0348
M15	0.119	0.0173	0.0000396	0.137	0.0299	0.00336	0.0000535	0.0333

[1] HQ values were calculated using predicted non-effect concentrations (PNECs) specified by the United Nations Environment Programme (UNEP, 2011).

[2] HQ values were calculated following the assessment guidelines established by Environment and Climate Change Canada (ECCC, 2016).

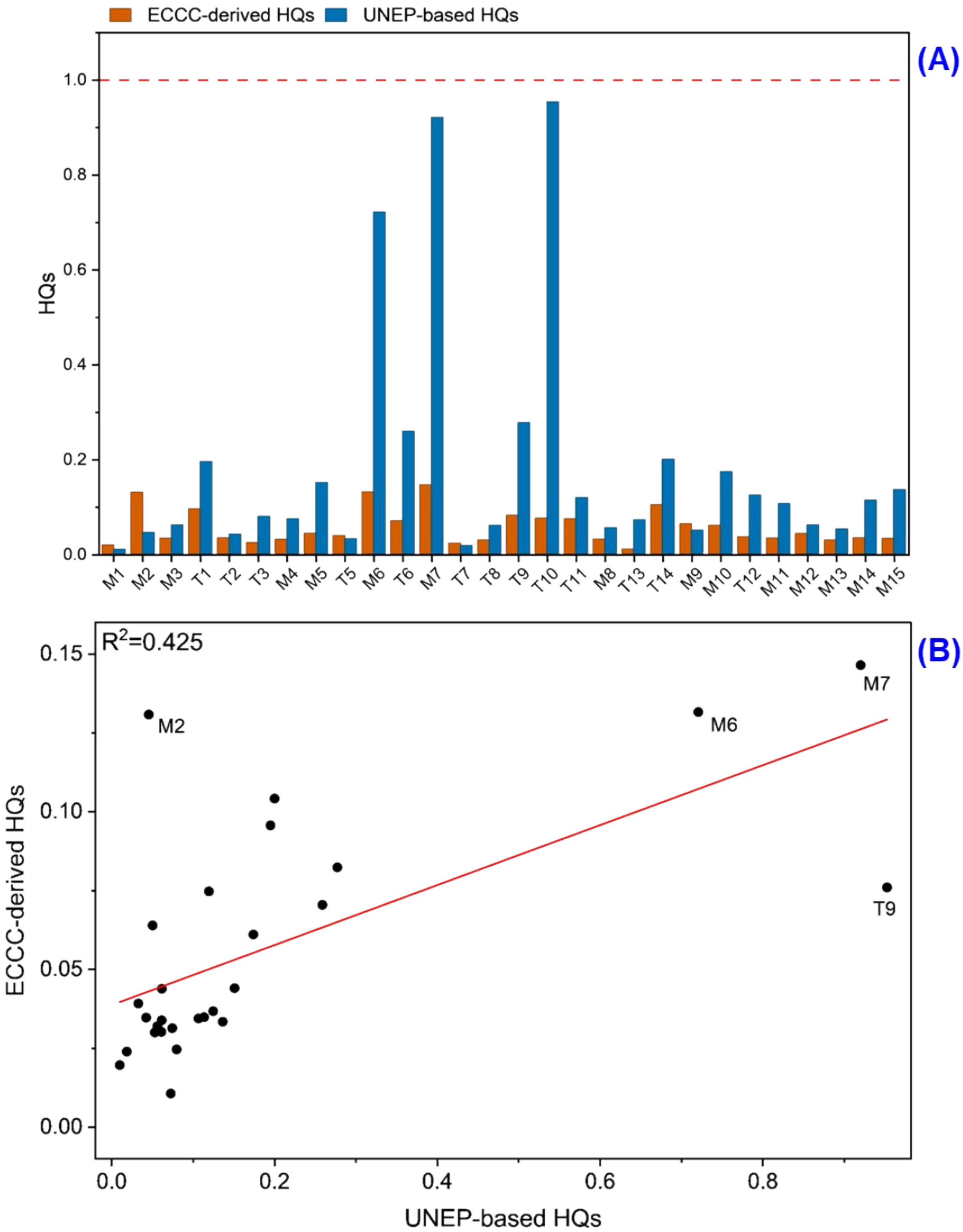

Figure S10. Comparison (A) and correlation (B) between ECCC-derived and UNEP-based HQs of CPs in specific sediments of the Lian River.

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