

## Supplemental Material

### **Organophosphate esters in sediment from Taihu Lake, China: Bridging the gap between riverine sources and Lake sinks**

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**Table S1. Physicochemical properties of OPEs**

	compounds	abbreviations	formula	molecular weight	CAS	log $K_{ow}$	solubility (25°C, mg/L)	vapour pressure (25°C, mm Hg)
<b>alkyl-OPEs</b>	trimethyl phosphate	TEP	C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P	182.16	78-40-0	0.80	5.00×10 <sup>5</sup>	0.29
	tripropyl phosphate	TPrP	C <sub>9</sub> H <sub>21</sub> O <sub>4</sub> P	224.23	513-08-6	2.67	827	2.9×10 <sup>-2</sup>
	tributyl phosphate	TnBP	C <sub>21</sub> H <sub>27</sub> O <sub>4</sub> P	266.32	126-73-8	5.29	3.72	1.3×10 <sup>-2</sup>
	tris(2-butoxyethyl) phosphate	TBEP	C <sub>18</sub> H <sub>39</sub> O <sub>7</sub> P	398.47	78-51-3	3.65	1.2×10 <sup>3</sup>	2.1×10 <sup>-7</sup>
	tri(2-ethylhexyl) phosphate	TEHP	C <sub>24</sub> H <sub>51</sub> O <sub>4</sub> P	434.63	78-42-2	9.49	2.0×10 <sup>-6</sup>	9.6×10 <sup>-5</sup>
<b>Cl-OPEs</b>	tris(2-chloroethyl) phosphate	TCEP	C <sub>6</sub> H <sub>12</sub> Cl <sub>3</sub> O <sub>4</sub> P	285.49	115-96-8	1.44	7×10 <sup>3</sup>	1.1×10 <sup>-4</sup>
	tris(1-chloro-2-propyl) phosphate	TCPP	C <sub>9</sub> H <sub>18</sub> Cl <sub>3</sub> O <sub>4</sub> P	327.57	13674-84-5	2.59	1.6×10 <sup>3</sup>	0.75
	tri(dichloropropyl) phosphate	TDCP	C <sub>9</sub> H <sub>15</sub> Cl <sub>6</sub> O <sub>4</sub> P	430.90	13674-87-8	3.8	1.50	7.4×10 <sup>-8</sup>
<b>aryl-OPEs</b>	triphenyl phosphate	TPhP	C <sub>18</sub> H <sub>18</sub> O <sub>4</sub> P	326.28	115-86-6	4.59	1.9	1.2×10 <sup>-6</sup>
	tricresyl phosphate	TCP	C <sub>21</sub> H <sub>21</sub> O <sub>4</sub> P	368.37	1330-78-5	5.11	1.84×10 <sup>-2</sup>	1.4×10 <sup>-7</sup>
	2-ethylhexyl diphenyl phosphate	EHDPP	C <sub>20</sub> H <sub>27</sub> O <sub>4</sub> P	265.41	1241-94-7	6.64	1.9	3.34×10 <sup>-5</sup>

**Table S2. The coordinates of sampling sites**

<b>Number</b>	<b>Site</b>	<b>Coordinate</b>	
R1	Xuguang River	N:31°18'2"	E:120°21'13"
R2	Xujiang River	N:31°13'14"	E:120°27'48"
R3	Tiao Rivulet	N:30°56'30"	E:120°20'22"
R4	Tiao Rivulet (Daqian Lough)	N:30°55'49"	E:120°11'26"
R5	Huanqing Lough	N:30°56'25"	E:120°7'26"
R6	Tiao Rivulet (Xiaomei Lough)	N:30°57'26"	E:120°6'13"
R7	Yangjiapu Bridge	N:31°1'11"	E:120°0'42"
R8	He Rivulet (Daxing Lough)	N:31°2'4"	E:119°59'16"
R9	He Rivulet (Xin Lough)	N:31°3'18"	E:119°58'56"
R10	Wuxi Lough	N:31°13'47"	E:119°53'33"
R11	Dapu River	N:31°18'38"	E:119°55'54"
R12	Wuyi Canal	N: 31°21'0"	E:119°57'26"
R13	Hengtang River	N: 31°25'55"	E:120°1'45"
R14	Wuxi Bridge	N:31°27'7"	E:120°0'31"
R15	Taige Canal	N:31°28'59"	E:120°2'32"
R16	Wujin Lough	N:31°30'8"	E:120°7'22"
R17	Li River	N:31°27'49"	E:120°22'59"
R18	Wangyu River	N:31°26'46"	E:120°24'13"
L1	——	N 31°1'8"	E 120°26'9"
L2	——	N 30°59'32"	E 120°12'24"
L3	——	N 31°10'23"	E 120°1'10"
L4	——	N 31°26'32"	E 120°2'12"
L5	——	N 31°29'10"	E 120°10'28"
L6	——	N 31°25'38"	E 120°21'59"
C1	——	N 31°5'44"	E 120°3'52"
C2	——	N 31°22'54"	E 120°1'52"

**Table S3. LOD and spiked recoveries of 11 OPEs**

compound name	LOD (ng/g)	Recoveries (n=3, %)
TEP	0.37	80.05±8.49
TPrP	0.94	89.55±2.27
TnBP	0.19	86.96±3.26
TCEP	0.31	90.84±6.09
TCPP	0.23	53.10±6.32
TDCP	0.71	149.69±20.57
TBEP	0.86	132.19±30.07
TPhP	0.13	89.25±3.29
EHDPP	0.12	61.31±14.38
TEHP	0.07	55.5±3.54
TCP	1.42	95.05±19.22

**Table S4. Result of Mann-Whitney U test**

compound name	<i>p</i> values of concentration		<i>p</i> values of percentage	
	between river and lake	among different region	between river and lake	among different region
TnBP	0.095	0.110	<b>0.004</b>	0.093
TCEP	0.118	<b>0.010</b>	<b>0.004</b>	0.089
TCPP	0.091	<b>0.021</b>	0.721	0.634
TBEP	<b>0.000</b>	0.218	0.224	0.107
TPhP	0.655	0.061	<b>0.007</b>	0.258
EHDPP	0.269	0.576	0.378	0.550
TCP	<b>0.049</b>	0.081	0.177	0.100
ΣOPEs	0.208	<b>0.036</b>	—	—

**Table S5. Available log<sub>k<sub>d,s</sub></sub> of OPEs calculated from Taihu Lake**

OPEs	log <sub>k<sub>d,s</sub></sub> (L/kg)				number of values
	Min	Max	Mean	Median	
TEP	—	1.56	—	—	1
TBEP	1.94	5	4.07	3.23	18
TPhP	2.5	3.72	3.25	3.11	12
TCEP	1	2.56	2.11	1.94	25
TCPP	0.85	2.39	1.96	1.95	25

**Table S6. *foc* of sediment samples in Taihu Lake**

Site	<i>foc</i> (%)	Site	<i>foc</i> (%)
R1	5.59	R13	4.74
R2	4.68	R14	5.26
R3	4.18	R15	4.87
R4	2.94	R16	4.86
R5	3.28	R17	5.44
R6	1.62	R18	4.17
R7	3.33	L1	6.20
R8	1.87	L2	3.15
R9	3.52	L3	2.74
R10	2.82	L4	5.64
R11	3.48	L5	3.90
R12	3.56	L6	3.89

**Table S7. Spearman correlation of individual OPEs between  $k_{d,s}$  and *foc***

	TPhP	TCEP	TCPP	TBEP
<i>foc</i>	.539	<b>.490*</b>	.248	-.074

Note: \*\* Correlation is significant at the 0.1 level (2-tailed). \* Correlation is significant at the 0.05 level (2-tailed)

**Table S8. Available  $\log k_{oc}$  of OPEs calculated from Taihu Lake**

OPEs	$\log k_{oc}$ (L/kg)				number of values
	Min	Max	Mean	Median	
TEP	—	3.05	—	—	1
TBEP	3.42	6.55	4.74	4.65	18
TPhP	3.96	5.00	4.51	4.48	12
TCEP	2.50	4.06	3.32	3.30	25
TCPP	2.28	3.84	3.28	3.30	25

**Table S9. PNEC values of OPEs<sup>[1-4]</sup>**

compound	L(E)C50 /mg/L		
	fish	crusacean	algae
TEP	2140	350	900
TnBP	20	11	34
TBEP	13	75	—
TEHP	—	0.74	—
TCEP	90	330	51
TCPP	30	91	45
TDCP	5.1	4.2	39
TPhP	0.7	1	0.5
EHDPP	—	1.8×10 <sup>-2</sup>	—
TCP	29	—	—

PNEC<sub>sediment</sub> value was calculated using equation<sup>[5]</sup>:

$$PNEC_{\text{sediment}} = \frac{K_{\text{SPM-water}}}{RHO_{\text{SPM}}} \times PNEC_{\text{water}}$$

$$K_{\text{SPM-water}} = F_{\text{waterSPM}} + F_{\text{solidSPM}} \times \frac{F_{\text{ocSPM}} \times K_{\text{oc}}}{1000} \times RHO_{\text{sediment}}$$

where,  $K_{\text{SPM-water}}$  represents the suspended particulate matter (SPM)-water partitioning coefficient (L/L) and  $RHO$  represents the bulk density (the  $RHO$  for SPM and sediment were 1150 g/L and 2500 g/L, respectively).  $F_{\text{water/solidSPM}}$  is the volume fraction of water/solid matter in suspended particulate solid (0.9/0.1 L/L), while  $F_{\text{ocSPM}}$  is the organic carbon content of solid matter in suspended particulate matter (0.1g/g) and  $K_{\text{oc}}$  is the organic carbon-water partitioning coefficient (L/kg).

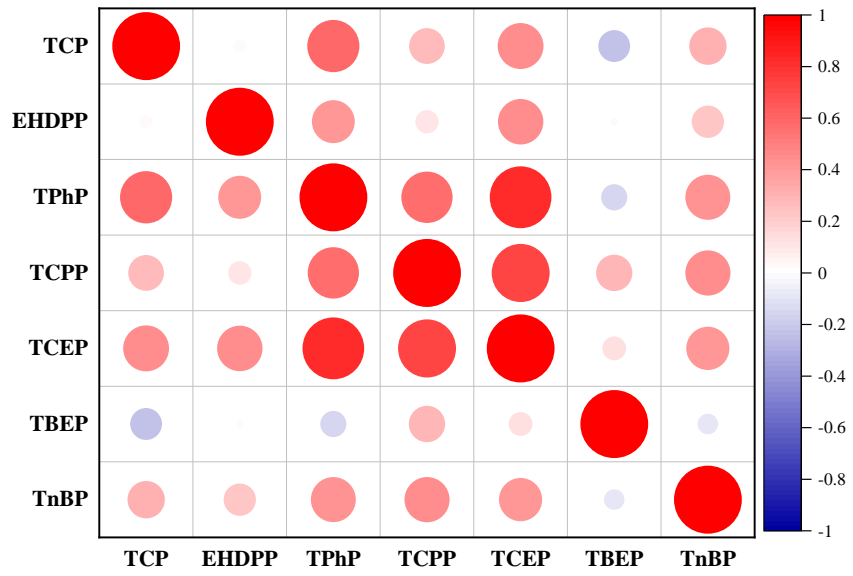
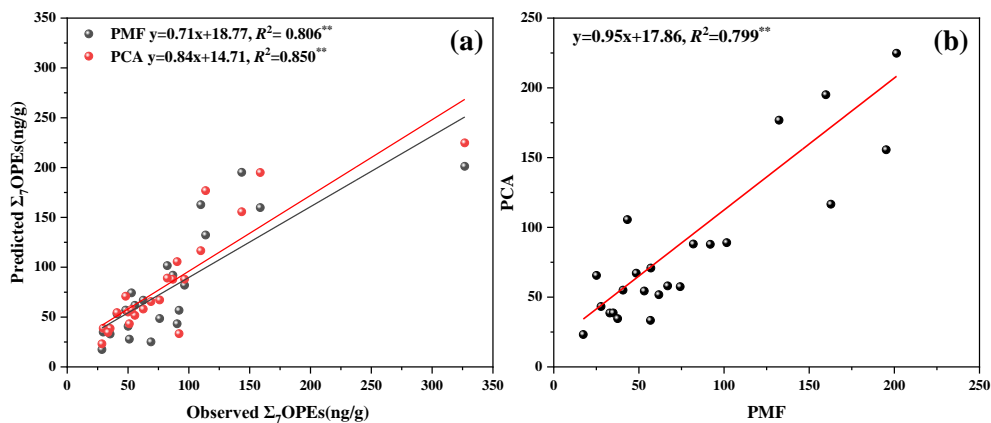


Figure S1. Relevance of OPEs in Taihu Lake



**Figure S2. Linear regression: (a) model fit of observed-versus-predicted  $\Sigma_7$ OPEs of PCA and PMF; (b) linear fit for predicted  $\Sigma_7$ OPEs between PCA-PMF.**

Note: \*\* Correlation is significant at the 0.1 level (2-tailed).

#### References:

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