

Supplementary Materials

# Occurrence Characteristics and Ecological Risk Assessment of Organophosphorus Compounds in a Wastewater Treatment Plant and Upstream Enterprises

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**Table S1.** Solid phase extraction of water samples.

Operation	Solvent	Flow Rate (ml/min)	Volume (ml)	Time (min)
Activation	Methylene chloride	2.0	5	16.87
Activation	Methanol	2.0	5	16.87
Activation	Water	2.0	5	16.87
Extraction	/	2.0	50	25.33
Leaching	Water	1.0	3	19.60
Drying	/	/	/	30.00
Cleaning injection pump	Methanol	2.0	5	1.53
Cleaning injection pump	Methylene chloride	2.0	5	1.53
Elution	Methylene chloride	2.0	5	16.87
Constant volume	/	/	/	0.00
End	/	/	/	145.47

**Table S2.** ECOSAR alculation results (mg/L) .

Organophosphonic	Abbreviated Name	Fish		Daphnid		Green Algae	
		96-hr LC <sub>50</sub>	ChV	48-hr LC <sub>50</sub>	ChV	96-hr EC <sub>50</sub>	ChV
Triphenyl phosphine	TEP	716.89	277.37	542.27	70.97	4041.35	486.44
Tris-b-chloroethyl phosphate	TCEP	3.14	0.01	0.09	/	221.77	45.75
Trimethyl phosphate	TMP	35194.58	18641.81	20316.16	1976.61	468296.28	19264.07
Triphenyl phosphate	TPP	1.00	0.24	1.13	0.23	1.54	0.94
Phosphoric acid tris(2-chloro-1-methylethyl) ester	TCPP	1.52	0.01	0.10	/	23.81	8.70
Dibutyl phosphate	DBP	131.80	45.15	110.70	16.25	532.74	97.20
Triphenyl phosphine oxide	TPPO	92.77	18.54	1.97	0.08	/	/
Triphenyl phosphine sulfide	TPPS	0.65	0.09	0.48	0.10	1.07	0.50
(MethoxyMethyl) diphenylphosphine oxide	MDPO	11581.51	1435.28	8.93	0.54	/	/

N-Dimethylaminomethyl-tert-butyl-isopropylphosphine	NDTPI	10.08	0.43	1.33	0.12	0.90	0.32
Octicizer	-	0.06	0.01	0.08	0.02	0.05	0.06
Dichloro[1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl]phosphine	DCPP	0.22	0.03	0.17	0.04	0.45	0.23
Dimethyl methane phosphonate	DMMP	16573.67	8260.57	10081.45	1038.84	186733.86	9457.22
Diethyl methyl phosphonite	DEMP	1657.77	681.63	1190.00	147.06	11036.67	1079.02

Note: / indicates that it was not queried in ECOSAR

**Table S3.** Concentration dependent toxic classification (mg/L) .

Class	The Acute Toxicity	The Chronic Toxicity
Harmless	$LC_{50} > 100$ or $EC_{50} > 100$	$ChV > 10$
Harmful	$10 < LC_{50} < 100$ or $10 < EC_{50} < 100$	$1 < ChV < 10$
Toxic	$1 < LC_{50} < 10$ or $1 < EC_{50} < 10$	$0.1 < ChV < 1$
Highly toxic	$LC_{50} < 1$ or $EC_{50} < 1$	$ChV < 0.1$

**Table S4.** Prediction of acute toxicity of organophosphorus components.

Water samples	Organophosphonic	Abbreviated Name	Toxicity	LC <sub>50</sub> (mg/L)
Pharmaceutical company	Triphenyl phosphate	TEP	acute toxicity Category 3	67.25
	Methoxy(methyldiphenyl)phosphine oxide	MDPO	acute toxicity Category 3	45.29
	Triphenyl phosphine oxide	TPPO	acute toxicity Category 2	4.98
	Triphenyl phosphine sulfide	TPPS	acute toxicity Category 2	2.46
Pump station I	Triphenyl phosphate	TEP	acute toxicity Category 3	67.25
	Dichloro[1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl]phosphine-	DCPP	/	/
	Tris-b-chloroethyl phosphate	TCEP	acute toxicity Category 3	17.31
	Triphenylphosphine oxide	TPPO	acute toxicity Category 2	4.98
	Triphenylphosphine sulfide	TPPS	acute toxicity Category 3	67.25
Electronic material enterprise	Triethyl phosphate	TEP	acute toxicity Category 3	67.25
Carbon black material enterprise	Triethyl phosphate	TEP	acute toxicity Category 3	67.25
Tyre material enterprise	Triethyl phosphate	TEP	acute toxicity Category 3	67.25
Environmental protection enterprise	Triethyl phosphate	TEP	acute toxicity Category 3	67.25
	Triphenyl phosphate	TPP	acute toxicity Category 1	0.39

	Octicizer	—	acute toxicity Category 1	0.0982
Food company	Triphenyl phosphate	TEP	acute toxicity Category 3	67.25
	Tris-b-chloroethyl phosphate	TCEP	acute toxicity Category 3	17.31
	Trimethyl phosphate	TMP	chronic toxicity	133.63
Pump station II	Dimethyl methane phosphonate	DMMP	/	/
	Diethyl methyl phosphonite	DEMP	chronic toxicity	120.82
	Dibutyl phosphate	DBP	acute toxicity Category 3	46.10
	Triphenyl phosphate	TEP	acute toxicity Category 3	67.25
	Tris-b-chloroethyl phosphate	TCEP	acute toxicity Category 3	17.31
	Phosphoric acid tris(2-chloro-1-methylethyl) ester	TCPP	acute toxicity Category 2	7.24
	N-Dimethylaminomethyl-tert-butyl- isopropylphosphine	NDTPI	/	/
	Dimethyl methane phosphonate	DMMP	chronic toxicity	143.29
	Diethyl methyl phosphonite	DEMP	acute toxicity Category 3	42.81
	Triphenyl phosphate	TEP	acute toxicity Category 3	67.25
Sewage treatment plant	Dichloro[1,7,7-trimethylbicyclo[2.2.1]heptan-2- yl]phosphine	DCPP	/	/
	Tris-b-chloroethyl phosphate	TCEP	acute toxicity Category 3	17.31

**Table S5.** Prediction of bioconcentration factor and developmental toxicity of organophosphorus components.

Water Samples	Organophosphonic	Abbreviated Name	BCF	DevTox
Pharmaceutical company	Triphenyl phosphate	TEP	4.13	developmental toxicants
	Methoxy(methyldiphenyl)phosphine oxide	MDPO	20.06	non-developmental toxicants
	Triphenylphosphine oxide	TPPO	84.99	non-developmental toxicants
	Triphenylphosphine sulfide	TPPS	378.27	non-developmental toxicants
Pump station I	Triphenyl phosphate	TEP	4.13	developmental toxicants
	Dichloro[1,7,7-trimethylbicyclo[2.2.1]heptan-2- yl]phosphine-	DCPP	/	/
	Tris-b-chloroethyl phosphate	TCEP	5.01	non-developmental toxicants
	Triphenylphosphine oxide	TPPO	84.99	non-developmental toxicants

	Triphenylphosphine sulfide	TPPS	4.13	developmental toxicants
Electronic material enterprise	Triethyl phosphate	TEP	4.13	developmental toxicants
Carbon black material enterprise	Triethyl phosphate	TEP	4.13	developmental toxicants
Tyre material enterprise	Triethyl phosphate	TEP	4.13	developmental toxicants
Environmental protection enterprise	Triethyl phosphate	TEP	4.13	developmental toxicants
	Triphenyl phosphate	TPP	50.67	developmental toxicants
	Octicizer	—	48.98	developmental toxicants
Food company	Triphenyl phosphate	TEP	4.13	developmental toxicants
	Tris-b-chloroethyl phosphate	TCEP	5.01	non-developmental toxicants
Pump station II	Trimethyl phosphate	TMP	0.74	developmental toxicants
	Dimethyl methane phosphonate	DMMP	/	/
	Diethyl methyl phosphonite	DEMP	2.79	developmental toxicants
	Dibutyl phosphate	DBP	5.12	developmental toxicants
	Triphenyl phosphate	TEP	4.13	developmental toxicants
	Tris-b-chloroethyl phosphate	TCEP	5.01	non-developmental toxicants
	Phosphoric acid tris(2-chloro-1-methylethyl) ester	TCPP	13.78	developmental toxicants
	N-Dimethylaminomethyl-tert-butyl-isopropylphosphine	NDTPI	/	/
	Dimethyl methane phosphonate	DMMP	1.97	developmental toxicants
Sewage treatment plant	Diethyl methyl phosphonite	DEMP	1.02	developmental toxicants
	Triphenyl phosphate	TEP	4.13	developmental toxicants
	Dichloro[1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl]phosphine	DCPP	/	/
	Tris-b-chloroethyl phosphate	TCEP	5.01	non-developmental toxicants