SUPPORTING INFORMATION

The results of the *umu* test are calculated by Eq (1)-(3):

$$G = \frac{(A_{600,T} - A_{600,B})}{(A_{600,N} - A_{600,B})} \quad (1),$$

$$IR = \frac{(A_{420,T} - A_{420,B})}{(A_{420,N} - A_{420,B})} \times \frac{1}{G} \quad (2),$$

$$U_T = \frac{(A_{420,T} - A_{420,B})}{(A_{600,N} - A_{600,B})} \quad (3),$$

where G is growth factor (larger than 0.5 can be used to calculate IR), and IR is induction ratio. ($G \geq 0.5$). When R is greater than 2, it can be recognized as mutagenicity positive. U_T is the activity of the β-galactosidase. $A_{600,T}$is the absorption of the sample well at 600 nm , $A_{600,B}$ is the absorption (mean value) of the blank at 600 nm , $A_{600,N}$ is the absorption (mean value) of the negative control at 600 nm, $A_{420,T}$ is the extinction of the sample well at 420 nm. $A_{420,B}$ is the extinction (mean value) of the blank at 420 nm, $A_{420,N}$ is the extinction (mean value) of the negative control respectively solvent control at 420 nm.

As the incubation time and reagent concentration of each *umu* test are slightly different, the results expressed by IR value will also be different. In order to improve the comparability of *umu* test results in different batches, the 4-NQO equivalent concentration of water samples was determined according to the dose-response relationship of 4-NQO in each *umu* test (Chang, Y, et al., 2017) (Grimmett, PE and J.W, Munch, 2013).

Appendix Table1

Appendix Table 1 shows toxicological data of DWTP C predicted by ECOSAR and the Toxicity Estimation Software Tool (TEST). In the case of ECOSAR, the results can be classified as very toxic (<1 mg L^{-1}), toxic (1–10 mg L^{-1}), harmful (10–100 mg L^{-1}), and not harmful (>100 mg L^{-1}) based on the Globally Harmonized System of Classification and Labeling of Chemicals (GHS) (UN, 2011). BAC, biological activated carbon.

very toxic toxic Harmful Not harmful

Organic matter	Raw water	Ozone	BAC	Filter	Finished water	ECOSAR							TEST
						Acute toxicity (mg L^{-1})			Chronic toxicity (mg L^{-1})			ECOSAR Class	Mutagenicity
						Fish (96 h LC_{50})	Daphnid (48 h LC_{50})	Algae (96-h EC_{50})	Fish	Daphnid	Algae		
Isopropylidene acetone	√	0	√	√	√	302.89	245.26	127.56	118.49	32.79	31.46	Vinyl/Allyl/ Propargyl Ketones	Negative
Butane	√	√	0	0	0	0.02	0.02	0.16	0	0	0.09	Thiocyanates	Positive
Trimethylphosp	√	0	0	0	0	278754.16	13.18	23108.14		1.12		Phosphine	Negative

hine oxide												Oxide	
Chloroiodomethane	√	√	√	0	√	199.69	111.77	78.47	19.19	10.47	19.91	Neutral Organics	Positive
Chloro-2-methyl-2-propanol	√	√	0	0	0	729.23	376.98	190.52	63.81	28.32	40.49	Neutral Organics	Negative
methylbenzene	√	√	√	√	√	24.76	14.78	13.53	2.57	1.66	3.96	Neutral Organics	Negative
3-hexanone	√	√	√	0	0	397.54	210.4	117.18	35.76	16.87	26.24	Neutral Organics	Negative
2-hexanone	√	√	0	0	√	397.54	210.4	117.18	35.76	16.87	26.24	Neutral Organics	Negative
4-Methyl-2-pentanol	√	√	0	0	0	163.97	90.36	59.48	15.47	8.11	14.57	Neutral Organics	Negative
Methoxypropionitrile	√	√	0	0	√	10420.18	4731.92	1399.32	782.55	247.79	222.8	Neutral Organics	Negative
2-methylhexan-	√	√	√	0	0	62.71	36.28	29.21	6.27	3.73	7.97	Neutral	Negative

2-ol												Organics	
1,4-dimethyl-benzene	√	0	√	0	0	9.2	5.78	6.52	1.01	0.74	2.13	Neutral Organics	Negative
2-Amino-4-methylbenzoic acid	√	0	0	0	0	721.11	219.88	463.11	34.94	11.24	102.75	Anilines (Hindered)	Negative
Cyclooctatetraene	√	0	0	0	0	5.84	3.74	4.57	0.66	0.51	1.56	Neutral Organics	Negative
2-Mercapto-4-phenylthiazole	√	0	0	0	0	0.71	0.23	0.18	0.1	0.02	0.09	Thiols and Mercaptans	Negative
n-butyl butyrate	√	0	0	0	0	6.33	12.04	4.49	0.4	6.48	1.51	Esters	Negative
Octyl phenol	√	√	0	√	0	0.16	0.3	0.02	0.02	0.06	0.07	phenols	Negative
Octacosane	√	0	0	0	0	0	0	0	0	0	0	Neutral Organics	Negative
Undecane	√	0	0	0	0	0.06	0.04	0.14	0.01	0.01	0.08	Neutral Organics	Negative
o-Phthalic	√	√	√	0	0	105.54	60.31	46.12	10.39	5.99	12.25	Neutral	Negative

anhydride												Organics	
Decane	√	√	√	0	0	0.14	0.11	0.28	0.02	0.02	0.14	Neutral Organics	Negative
Heptacosane	0	√	0	0	0	0	0	0	0	0	0	Neutral Organics	Negative
6-tert-Butyl-3-methylphenol	√	0	0	0	0	0.99	1.04	0.09	0.12	0.16	0.32	phenols	Negative
1-Tetradecene	√	0	0	0	0	0	0	0.02	0	0	0.02	Neutral Organics	Negative
n-tetradecane	√	√	0	0	0	0	0	0.02	0	0	0.01	Neutral Organics	Negative
Styrene oxide	√	0	0	0	0	20.16	55.95	67.95	0.01	5.47	39.58	Epoxides, Mono	Positive
Cyclohexane	√	√	0	0	0	0	0	0.02	0	0	0.02	Neutral Organics	Negative
2,4-Di-tert-butylphenol	√	0	0	0	0	0.14	0.28	0.01	0.02	0.05	0.07	Phenols	Negative

n-Dodecane	√	0	0	0	0	0.02	0.02	0.07	0	0.01	0.04	Neutral Organics	Negative
n-Hexadecane	√	0	0	√	0	0	0	0	0	0	0	Neutral Organics	Negative
Triethylene glycol monoethyl ether	√	0	0	0	0	67283.67	29056.1	6979.75	4762.04	1322.85	993.62	Neutral Organics	Negative
Palmitamide	√	0	0	0	0	0.09	0.05	0.04	0.01	0.03	0.14	Amides	Negative
1,3-Dichlorbenzene	√	0	0	0	0	8.52	5.45	6.62	0.96	0.74	2.26	Neutral Organics	Negative
Ethylcyclopentane	√	0	0	0	0	2.99	1.97	2.69	0.35	0.29	0.98	Neutral Organics	Negative
n-Tridecane	√	0	0	0	0	0.01	0.01	0.03	0	0	0.02	Neutral Organics	Negative
acetophenone	√	√	√	0	0	193.85	106.8	70.24	18.29	9.58	17.2	Neutral Organics	Negative
Triethyl	√	√	0	0	0	111.04	260.46	132.55	10.58	246.36	23.55	Esters	Positive

phosphate													
2,6,6-Trimethyl-2-cyclohexene-1,4-dione	√	√	√	√	0	191.03	131.88	75.95	60.12	19.66	23.25	Vinyl/Allyl/ Propargyl Ketones	Negative
Naphthalene	√	0	0	0	0	9.39	5.94	6.91	1.04	0.78	2.3	Neutral Organics	Negative
Tetramethylene sulfone	√	√	0	0	0	10054.44	4644.11	1473.35	770.38	254.97	243.97	Neutral Organics	Negative
Methylcyclopentenolone	√	√	√	√	0	398.32	330.67	169.27	161.21	43.47	40.36	Vinyl/Allyl/ Propargyl Ketones	Negative
Benzothiazole	√	0	0	0	0	78.3	45.16	35.88	7.8	4.6	9.73	Neutral Organics	Positive
Nitrochlorobenzene	√	0	0	0	0	50.49	29.9	26.5	5.19	3.28	7.62	Neutral Organics	Positive
Heneicosane	√	0	0	0	0	0	0	0	0	0	0	Neutral Organics	negative

1-decoxydecane	0	√	0	0	0	0	0	0	0	0	0	Neutral Organics	negative
Chloroacetyl chloride	0	√	0	0	0	84.36	3066.94	1483.41	9.06	207.13	163.02	Acid Halides	negative
2-Nitroanisole	0	√	0	0	0	157.41	88.49	63.24	15.21	8.39	16.2	Neutral Organics	negative
2-Tetradecene	0	√	0	√	0	0.14	0.16	0.3	0	0.03	0.16	Vinyl/Allyl/ Propargyl Aldehydes	negative
2,4-二叔丁基苯酚	0	√	0	√	0	0.14	0.28	0.01	0.02	0.05	0.07	Phenols	negative
2-nitrotoluene	0	√	0	0	0	53.73	31.54	26.93	5.46	3.37	7.59	Neutral Organics	negative
4-nitrochlorobenzene	0	√	0	0	0	50.49	29.9	26.5	5.19	3.28	7.62	Neutral Organics	positive
5-Methyl-1H-	0	√	0	0	0	21.55	96.27	4.82	2.13	1.94	1.05	Benzotriazol	positive

benzotriazole												es	
Styrene	0	√	0	0	0	13.44	8.29	8.69	1.45	1.02	2.74	Neutral Organics	negative
n-Butyl butyrate	0	√	0	0	0	6.33	12.04	4.49	0.4	6.48	1.51	Esters	negative
Ethane,1-ethoxy-1-methoxy-	0	√	0	0	0	1222.92	616.62	281.1	103.91	43.21	56.51	Neutral Organics	negative
sec-Caprylic alcohol	0	√	0	0	0	23.55	14.31	14.09	2.49	1.68	4.29	Neutral Organics	negative
2,5-Dimethyloxolane	0	0	√	0	0	131.85	73.3	50.05	12.57	6.74	12.51	Neutral Organics	negative
Monobromo-dichloro-methane	0	0	√	0	0	301.16	164.96	105.9	28.21	14.56	25.6	Neutral Organics	negative
2-Methyl-1,3-propanediol	0	0	√	0	0	8450.72	3883.55	1206.42	643.63	210.22	197.25	Neutral Organics	negative

Methyl tert-butyl ketone	0	0	√	0	0	500.22	262.04	139.88	44.46	20.42	30.61	Neutral Organics	negative
Chlorodibromomethane	0	0	√	0	√	318.18	175.73	116.74	30.1	15.87	28.74	Neutral Organics	positive
Tribromomethane	0	0	√	0	√	320.85	178.68	122.82	30.65	16.51	20.8	Neutral Organics	negative
Benzaldehyde	0	0	√	0	0	8.89	8.33	4.75	1.45	0.09	1.79	Aldehydes (Mono)	negative
2-Ethyl-1-hexanol	0	0	√	0	0	23.55	14.31	14.09	2.49	1.68	4.29	Neutral Organics	negative
Dimethyl phthalate	0	0	√	0	0	40.82	87.97	39.49	3.3	66.27	9.08	Esters	negative
Diisobutyl phthalate	0	0	√	0	0	28.32	17.31	17.48	3.02	2.07	5.39	Neutral Organics	N/A
Dibutyl phthalate	0	0	√	0	0	1.11	1.75	0.49	0.05	0.56	0.29	Esters	negative
3-	0	0	0	√	√	10420.18	4731.92	1399.32	782.5	247.79	222.8	Neutral	negative

Methoxypropionitrile 3-Methoxypropionitrile									5			Organics	
1-氨基蒽	0	0	0	√	0	2.44	0.86	1.76	0.01	0.01	0.27	Anilines (Unhindered)	positive
DL-3-Methyl-2-butano	0	0	0	√	0	390.56	205.69	112.25	34.93	16.27	24.86	Neutral Organics	negative
4-Hydroxy-4-methyl-2-pentanone	0	0	0	√	0	230.64	105.99	22.31	22.23	10.18	94.5	Ketone Alcohols	negative
N-Hydroxymethyl acetamide	0	0	0	0	√	43974.05	80273.89	1170.56	92.47	2875.06	118.94	Amides	negative
m-Xylene	0	0	0	0	√	9.2	5.78	6.52	1.01	0.74	2.13	Neutral	negative

												Organics	
2,2-dibromoacetonitrile	0	0	0	0	√	1.58	0.77	0.07	1.06	0.06	0.02	Halonitriles	positive
2-BROMO-2-NITROPROPANE	0	0	0	0	√	176	98.85	70.4	16.98	9.35	18	Neutral Organics	positive
trimethyl chlorosilane	0	0	0	0	√	32.97	19.57	17.52	3.4	2.16	5.07	Neutral Organics	negative