Supplementary material

Quaternary Ammonium Compounds in Wastewater During COVID-19 Pandemic: Occurrence, Exposure Evaluation and Risk Assessment

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Appendix S1. Instrumental parameters

The Thermo Vanquish ultrahigh-performance liquid chromatography coupled to an Orbitrap Exploris 480 high resolution mass spectrometer system (UPLC-Orbitrap HRMS, Thermo Fisher Scientific Inc, Waltham, MA) was used for sample analysis. Electrospray ionization was operated in positive mode, and full scan MS^1 and data dependent MS^2 method was performed for data acquisition. A Hypersil GOLD™ VANQUISH™ C18 column (1.9 μm, 2.1 mm i.d. × 100 mm length, ThermoFisher Scientific) was used for chromatographic separation, and column temperature was set at 35°C. The mobile phases were (A) methanol and isopropanol (80:20, v/v), and (B) ultrapure water and isopropanol (80: 20, v/v), both containing 0.1% acetic acid and 10 mM ammonium acetate. The flow rate was set at 0.3 mL/min, and the gradient was 90% B in 0 – 1 min, 90% – 40% B in 1 – 5 min, 40% – 0% B in 11– 14 min, 0% B in 14 – 15 min, 90% B in 15 – 18 min. The injection volume was 5 μL. The ion spray voltage, ion transfer tube temperature, vaporizer temperature, sheath gas and auxiliary gas were 3500V, 350 °C, 250 °C, 35 Arb and 10 Arb, respectively. The scan range was 80 – 800 m/z. The Orbitrap resolution was 120,000 FWHM and 15,000 FWHM for full scan MS^1 and data dependent MS^2 method, respectively. The stepped higher-energy collisional dissociation (HCD) energy was set at 10%, 30% and 60%.

Table S1. Detailed information on chemical name, acronym, CAS, formula, manufacturer, *m/z* and Log Kow of the target QACs.

Chemical name	**Acronym**	**CAS**	**Formula**	**Manufacturer**	***m/z***	**Log *Kow*[a]**
Benzyldimethyloctylammonium chloride	BAC-C8	959-55-7	$C_{17}H_{30}ClN$	Sigma-Aldrich	248.2373	0.96
Benzyldimethyldecylammonium chloride	BAC-C10	965-32-2	$C_{19}H_{34}ClN$	Sigma-Aldrich	276.2686	1.95
Benzyldimethyldodecylammonium chloride	BAC-C12	139-07-1	$C_{21}H_{38}ClN$	J&K Scientific	304.2999	2.93
Benzyldimethyltetradecylammonium chloride	BAC-C14	139-08-2	$C_{23}H_{42}ClN$	Tokyo Chemical Industry	332.3312	3.91
Benzylcetyldimethylammonium chloride	BAC-C16	122-18-9	$C_{25}H_{46}ClN$	Tokyo Chemical Industry	360.3625	4.89
n-Octyltrimethylammonium chloride	ATMAC-C8	10108-86-8	$C_{11}H_{26}ClN$	Tokyo Chemical Industry	172.2060	-0.74
Decyltrimethylammonium chloride	ATMAC-C10	10108-87-9	$C_{13}H_{30}ClN$	Tokyo Chemical Industry	200.2373	0.24
Dodecyltrimethylammonium chloride	ATMAC-C12	112-00-5	$C_{15}H_{34}ClN$	Tokyo Chemical Industry	228.2686	1.22
Trimethylteradecylammonium chloride	ATMAC-C14	4574-04-3	$C_{17}H_{38}ClN$	Tokyo Chemical Industry	256.2999	2.2
Hexadecyltrimethylammonium chloride	ATMAC-C16	112-02-7	$C_{19}H_{42}ClN$	Tokyo Chemical Industry	284.3312	3.18
Trimethylstearylammonium chloride	ATMAC-C18	112-03-8	$C_{21}H_{46}ClN$	Tokyo Chemical Industry	312.3625	4.17
Dimethyldioctylammonium bromide	DADMAC-8:8	3026-69-5	$C_{18}H_{40}BrN$	Tokyo Chemical Industry	270.3155	2.69
Octyl decyldimethyl ammonium chloride	DADMAC-8:10	32426-11-2	$C_{20}H_{44}ClN$	MACKLIN	298.3468	3.68
Didecyldimethylammonium chloride	DADMAC-10:10	7173-51-5	$C_{22}H_{48}ClN$	Tokyo Chemical Industry	326.3781	4.66
Dimethyldimyristylammonium bromide	DADMAC-14:14	68105-02-2	$C_{30}H_{64}BrN$	Tokyo Chemical Industry	438.5033	8.59
Dimethyldipalmitylammonium bromide	DADMAC-16:16	70755-47-4	$C_{34}H_{72}BrN$	Tokyo Chemical Industry	494.5659	10.6
Benzyldimethyltetradecylammonium-d7 chloride	BAC-C14-d7	1219178-72-9	$C_{23}H_{35}D7ClN$	Bellancom Life Sciences Dep.	339.3751	

[a] The octanol-water partition coefficient predicated by EPI Suite.

Table S2. Weather conditions during the sampling period.

Date	Mean temperature (°C)	Precipitation	Date	Mean temperature (°C)	Precipitation
2022/12/15	1.0	sunny	2023/1/10	3.0	sunny
2022/12/18	-1.5	sunny	2023/1/11	7.5	cloudy
2022/12/19	-2.5	sunny	2023/1/12	8.0	snow/rain
2022/12/20	2.5	cloudy	2023/1/13	4.5	snow/rain
2022/12/21	-0.5	snow/rain	2023/1/14	-3.0	cloudy
2022/12/23	-2.5	sunny	2023/1/15	-3.5	cloudy
2022/12/24	-2.0	sunny	2023/1/16	-1.0	sunny
2022/12/25	1.5	cloudy	2023/1/17	3.5	sunny
2022/12/26	-0.5	sunny	2023/1/18	1.0	sunny
2022/12/27	0.5	cloudy	2023/1/19	2.5	sunny
2022/12/28	0.0	sunny	2023/1/20	-1.5	sunny
2022/12/29	0.5	sunny	2023/1/21	4.0	sunny
2022/12/30	1.5	sunny	2023/1/22	3.5	cloudy
2022/12/31	2.5	sunny	2023/1/23	-5.0	snow/rain
2023/1/1	2.0	cloudy	2023/1/24	-10.5	sunny
2023/1/2	1.5	sunny	2023/1/25	-3.5	sunny
2023/1/3	3.0	sunny	2023/1/26	-3.5	cloudy
2023/1/4	4.5	cloudy	2023/1/27	-3.0	sunny
2023/1/5	4.0	sunny	2023/1/28	-0.5	sunny
2023/1/6	3.5	sunny	2023/1/29	3.0	sunny
2023/1/7	7.5	sunny	2023/1/30	2.5	sunny
2023/1/8	6.0	cloudy	2023/1/31	4.5	cloudy
2023/1/9	3.5	sunny			

Table S3. Accurate mass, theoretical mass and MS^2 fragmentations of the target QACs.

Acronym	Accurate mass (m/z)	Theoretical mass (m/z)	Error (mDa)	MS^2 fragmentations
BAC-C8	248.2373	248.2376	-0.30	58.0651, 91.0543
BAC-C10	276.2686	276.2680	0.60	58.0650, 91.0541
BAC-C12	304.2999	304.2998	0.10	58.0651, 91.0542
BAC-C14	332.3312	332.3308	0.40	58.0650, 91.0542
BAC-C16	360.3625	360.3626	-0.10	58.0651, 91.0542
ATMAC-C8	172.2060	172.2059	0.10	57.0698, 60.0807
ATMAC-C10	200.2373	200.2371	0.20	57.0698, 60.0807
ATMAC-C12	228.2686	228.2681	0.50	60.0807, 71.0855
ATMAC-C14	256.2999	256.3001	-0.20	57.0698, 60.0807
ATMAC-C16	284.3312	284.3310	0.20	57.0698, 60.0807
ATMAC-C18	312.3625	312.3621	0.40	57.0698, 60.0807
DADMAC-8:8	270.3155	270.3155	0.00	57.0699, 158.1904
DADMAC-8:10	298.3468	298.3466	0.20	57.0698, 158.1904
DADMAC-10:10	326.3781	326.3781	0.00	57.0698, 186.2216
DADMAC-14:14	438.5033	438.5052	-1.90	57.0698, 306.9835
DADMAC-16:16	494.5659	494.5653	0.60	57.0699, 270.3160
BAC-C14-d7	339.3751	339.3748	0.30	58.0650, 98.0981

Table S4. Instrument stability assessment (During the sequence run, the relative standard deviation of the target QACs signals in the QC sample was within 20%, indicating good instrument stability).

Analytes	RSD (%)	Analytes	RSD (%)
BAC-C8	8.69	ATMAC-C14	10.8
BAC-C10	6.26	ATMAC-C16	8.76
BAC-C12	2.05	ATMAC-C18	4.25
BAC-C14	9.81	DADMAC-8:8	5.62
BAC-C16	18.1	DADMAC-8:10	3.89
ATMAC-C8	3.15	DADMAC-10:10	20.0
ATMAC-C10	13.2	DADMAC-14:14	12.9
ATMAC-C12	2.82	DADMAC-16:16	2.01

Table S5. Recoveries and matrix effects of the 16 target QACs in spiked influent and effluent matrices.

Acronym	Recovery (± SD[a], %)		Matrix effect (± SD, %)	
	Influent	Effluent	Influent	Effluent
BAC-C8	105 ± 5.42	103 ± 4.18	103 ± 7.65	99.6 ± 6.17
BAC-C10	116 ± 6.43	118 ± 4.13	116± 9.05	111 ± 6.57
BAC-C12	107 ± 6.45	97.9 ± 6.37	107 ± 10.0	85.7 ± 5.97
BAC-C14	40.7 ± 2.80	50.7 ± 3.69	45.9 ± 1.62	44.1 ± 1.99
BAC-C16	54.3 ± 6.19	57.6 ± 6.72	61.3 ± 1.57	51.9 ± 2.70
ATMAC-C8	79.7 ± 5.71	79.6 ± 4.89	79.8 ± 5.93	78.1 ± 4.24
ATMAC-C10	75.8 ± 6.87	79.6 ± 6.33	74.8 ± 6.30	77.2 ± 4.93
ATMAC-C12	112 ± 5.22	113 ± 4.21	112 ± 9.67	106 ± 7.26
ATMAC-C14	48.2 ± 4.48	48.1 ± 3.36	48.2 ± 2.72	41.2 ± 2.98
ATMAC-C16	55.3 ± 12.9	57.2 ± 5.62	65.1 ± 5.29	51.4 ± 1.67
ATMAC-C18	135 ± 7.18	96.3 ± 7.75	114 ± 22.8	97.7 ± 4.13
DADMAC-8:8	109 ± 5.25	111 ± 3.57	111 ± 9.66	105 ± 6.52
DADMAC-8:10	68.5 ± 5.17	68.6 ± 4.56	76.2 ± 8.09	69.2 ± 7.81
DADMAC-10:10	57.8 ± 4.84	62.3 ± 5.30	65.2 ± 2.43	57.5 ± 3.39
DADMAC-14:14	86.7 ± 6.12	80.5 ± 4.26	90.7 ± 6.35	79.7 ± 7.35
DADMAC-16:16	84.0 ± 7.15	78.9 ± 3.46	92.1 ± 6.06	77.1 ± 2.90

[a]Standard deviation.

Table S6. Method detection limits (MDLs) and method quantification limits (MQLs) of the 16 target QACs.

Acronym	**MDL (ng/L)**	**MQL (ng/L)**
BAC-C8	0.0581	0.194
BAC-C10	7.39	24.6
BAC-C12	12.2	40.5
BAC-C14	5.21	17.4
BAC-C16	0.0880	0.293
ATMAC-C8	0.0667	0.222
ATMAC-C10	0.359	1.20
ATMAC-C12	2.15	7.17
ATMAC-C14	6.27	20.9
ATMAC-C16	9.51	31.7
ATMAC-C18	21.1	70.5
DADMAC-8:8	1.20	4.00
DADMAC-8:10	17.9	59.8
DADMAC-10:10	0.501	1.67
DADMAC-14:14	0.495	1.65
DADMAC-16:16	0.344	1.15

Table S7. Daily concentration (ng/L) of the target QACs in influent during the sampling period.

Date	BAC					ATMAC						DADMAC				
	C8	**C10**	**C12**	**C14**	**C16**	**C8**	**C10**	**C12**	**C14**	**C16**	**C18**	**8:8**	**10:10**	**14:14**	**16:16**	**8:10**
2022/12/15	9.62	17.4	830	21.9	1.02	0.106	< MDL	127.8	5.44	185	314	8.83	0.74	0.838	3.12	< MDL
2022/12/18	< MDL	< MDL	< MDL	< MDL	< MDL	0.093	< MDL	< MDL	< MDL	< MDL	< MDL	1.33	< MDL	0.845	2.02	< MDL
2022/12/19	< MDL	< MDL	< MDL	< MDL	0.124	< MDL	< MDL	< MDL	< MDL	13.7	52.1	< MDL	< MDL	0.857	5.21	< MDL
2022/12/20	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.80	< MDL
2022/12/21	< MDL	< MDL	< MDL	< MDL	0.105	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.23	< MDL	0.798	5.44	< MDL
2022/12/23	< MDL	< MDL	36.0	6.17	0.087	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.44	6.27	< MDL
2022/12/24	0.608	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.20	< MDL	14.7	44.2	< MDL	< MDL	1.13	4.90	< MDL
2022/12/25	14.2	< MDL	37.2	8.16	< MDL	0.176	< MDL	< MDL	< MDL	< MDL	< MDL	3.06	< MDL	2.17	11.2	< MDL
2022/12/26	5.55	< MDL	127	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.72	< MDL	< MDL	7.70	< MDL
2022/12/27	< MDL	< MDL	< MDL	< MDL	0.308	0.103	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.18	4.63	< MDL
2022/12/28	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.83	< MDL	< MDL	< MDL	1.64	< MDL	< MDL	2.23	< MDL
2022/12/29	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	3.70	0.79	0.795	2.47	< MDL
2022/12/30	6.32	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	38.8	75.2	< MDL	< MDL	0.924	9.66	< MDL
2022/12/31	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	9.53	116	1.24	5.11	54.6
2023/1/1	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.03	< MDL	1.20	14.8	< MDL
2023/1/2	7.71	< MDL	< MDL	< MDL	0.894	< MDL	< MDL	< MDL	< MDL	< MDL	73.4	1.66	1.65	3.17	33.5	< MDL
2023/1/3	< MDL	< MDL	< MDL	< MDL	< MDL	35.8	< MDL	< MDL	< MDL	< MDL	< MDL	336	2183	0.910	13.2	12311
2023/1/4	< MDL	< MDL	88.9	19.5	0.553	< MDL	< MDL	2.04	< MDL	< MDL	28.3	2.79	< MDL	1.16	18.7	< MDL
2023/1/5	16.9	< MDL	40.0	12.1	0.443	0.054	< MDL	1.74	< MDL	< MDL	< MDL	0.82	< MDL	1.42	9.28	< MDL
2023/1/6	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.54	< MDL	1.29	11.4	< MDL
2023/1/7	< MDL	< MDL	945	268	4.97	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	17.0	< MDL
2023/1/8	1.55	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.37	0.430	2.62	19.6	< MDL
2023/1/9	< MDL	< MDL	< MDL	< MDL	0.132	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.93	21.4	< MDL
2023/1/10	< MDL	< MDL	< MDL	< MDL	0.69	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	3.24	11.3	< MDL
2023/1/11	20.1	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.07	< MDL	< MDL	< MDL	< MDL	< MDL	1.78	19.0	< MDL

Date	BAC					ATMAC						DADMAC				
	C8	**C10**	**C12**	**C14**	**C16**	**C8**	**C10**	**C12**	**C14**	**C16**	**C18**	**8:8**	**10:10**	**14:14**	**16:16**	**8:10**
2023/1/12	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.03	4.43	< MDL
2023/1/13	< MDL	< MDL	< MDL	< MDL	0.116	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.33	< MDL	0.996	6.57	< MDL
2023/1/14	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	6.55	< MDL
2023/1/15	24.5	67.9	884	74.8	6.60	< MDL	< MDL	70.3	< MDL	570	1381	14.4	2.71	1.61	10.3	< MDL
2023/1/16	8.83	< MDL	< MDL	< MDL	0.208	< MDL	< MDL	< MDL	< MDL	< MDL	33.8	< MDL	< MDL	2.59	39.0	< MDL
2023/1/17	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	43.4	< MDL	< MDL	0.865	20.6	< MDL
2023/1/18	5.73	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.29	11.2	< MDL
2023/1/19	4.58	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.03	< MDL	< MDL	< MDL	< MDL	< MDL	1.64	11.5	< MDL
2023/1/20	2.53	< MDL	< MDL	< MDL	0.104	< MDL	< MDL	< MDL	< MDL	< MDL	28.1	1.27	0.616	2.69	30.3	< MDL
2023/1/21	5.29	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	7.79	6.02	< MDL	< MDL	1.31	< MDL	1.41	3.36	< MDL
2023/1/22	6.91	29.4	1436	246.9	13.5	< MDL	< MDL	62.2	8.43	916	2216	18.3	15.4	6.71	21.5	65.0
2023/1/23	6.43	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	4.15	< MDL	< MDL	2.92	< MDL
2023/1/24	1.20	< MDL	< MDL	< MDL	0.105	< MDL	< MDL	< MDL	< MDL	11.6	43.0	< MDL	< MDL	1.45	7.70	< MDL
2023/1/25	6.51	23.0	206	9.82	< MDL	< MDL	< MDL	143	6.31	< MDL	< MDL	5.90	0.900	0.770	1.85	< MDL
2023/1/26	7.67	14.6	227	13.3	0.537	< MDL	< MDL	37.5	< MDL	16.8	36.6	4.89	0.881	0.763	2.00	< MDL
2023/1/27	5.19	< MDL	142	12.8	1.30	< MDL	< MDL	12.7	< MDL	16.8	< MDL	3.36	1.41	< MDL	< MDL	< MDL
2023/1/28	7.42	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.18	4.32	< MDL
2023/1/29	3.64	18.4	662	82.6	4.73	< MDL	< MDL	35.7	< MDL	653	1948	8.98	3.24	1.87	5.37	< MDL
2023/1/30	3.53	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.36	< MDL	< MDL	< MDL	1.34	< MDL	< MDL	3.10	< MDL
2023/1/31	6.20	< MDL	107	6.32	< MDL	< MDL	< MDL	9.33	< MDL	14.9	< MDL	1.91	< MDL	0.936	1.82	< MDL

Table S8. Daily concentration (ng/L) of the target QACs in effluent during the sampling period.

Date	BAC					ATMAC						DADMAC				
	C8	C10	C12	C14	C16	C8	C10	C12	C14	C16	C18	8:8	10:10	14:14	16:16	8:10
2022/12/15	< MDL	< MDL	36.2	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	0.89	0.75	< MDL	1.68	< MDL
2022/12/18	< MDL	< MDL	21.6	5.90	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	3.48	2.17	< MDL	1.65	36.6
2022/12/19	< MDL	< MDL	22.8	< MDL	< MDL	< MDL	< MDL	2.07	< MDL	< MDL	< MDL	1.38	0.900	< MDL	2.56	< MDL
2022/12/20	< MDL	< MDL	88.2	17.1	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.70	< MDL	1.84	< MDL
2022/12/21	< MDL	< MDL	119	18.0	< MDL	< MDL	< MDL	1.57	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.96	< MDL
2022/12/22	< MDL	< MDL	147	25.4	< MDL	0.339	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.41	< MDL	< MDL	< MDL
2022/12/23	< MDL	< MDL	54.7	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.65	< MDL
2022/12/24	< MDL	< MDL	145	31.1	0.136	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.45	0.747	1.204	1.69	< MDL
2022/12/25	< MDL	< MDL	21.1	6.43	< MDL	0.101	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.06	< MDL	1.70	< MDL
2022/12/26	< MDL	< MDL	59.7	15.2	0.529	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.75	< MDL	1.85	< MDL
2022/12/27	< MDL	< MDL	72.3	17.3	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.02	< MDL	1.81	< MDL
2022/12/28	< MDL	< MDL	35.8	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.68	< MDL
2022/12/29	< MDL	< MDL	114	32.8	0.602	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.99	16.8	< MDL	1.75	< MDL
2022/12/30	< MDL	< MDL	46.8	7.34	< MDL	0.188	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.34	< MDL	1.84	< MDL
2022/12/31	< MDL	< MDL	56.0	11.8	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.32	0.732	< MDL	< MDL
2023/1/1	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.18	< MDL	1.65	< MDL
2023/1/2	< MDL	< MDL	57.5	10.0	0.356	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	0.967	5.07	< MDL	1.68	< MDL
2023/1/3	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.72	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.99	< MDL
2023/1/4	< MDL	< MDL	67.8	14.8	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.65	< MDL
2023/1/5	< MDL	< MDL	21.8	< MDL	< MDL	< MDL	< MDL	1.62	< MDL	< MDL	< MDL	< MDL	1.13	< MDL	1.68	< MDL
2023/1/6	< MDL	< MDL	36.2	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.09	0.710	1.95	< MDL
2023/1/7	< MDL	< MDL	< MDL	< MDL	0.097	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	0.94	< MDL	1.84	< MDL

Date	BAC					ATMAC						DADMAC				
	C8	C10	C12	C14	C16	C8	C10	C12	C14	C16	C18	8:8	10:10	14:14	16:16	8:10
2023/1/8	< MDL	< MDL	< MDL	< MDL	0.078	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	0.39	0.754	1.66	< MDL
2023/1/9	< MDL	< MDL	49.9	7.78	0.095	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.38	2.17	0.952	1.72	< MDL
2023/1/10	< MDL	< MDL	55.0	14.2	< MDL	0.057	< MDL	1.46	< MDL	< MDL	< MDL	< MDL	1.42	< MDL	2.11	< MDL
2023/1/11	< MDL	< MDL	22.7	7.79	0.173	< MDL	< MDL	7.13	< MDL	< MDL	< MDL	2.38	0.97	0.834	1.74	< MDL
2023/1/12	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.18	5.64	1.68	< MDL
2023/1/13	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.40	< MDL	< MDL	< MDL	< MDL	0.75	< MDL	< MDL	< MDL
2023/1/14	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.41	< MDL	< MDL	< MDL	< MDL	0.43	0.907	1.94	< MDL
2023/1/15	< MDL	< MDL	20.4	10.6	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.01	< MDL	1.97	< MDL
2023/1/16	< MDL	< MDL	35.2	< MDL	< MDL	< MDL	< MDL	2.24	< MDL	< MDL	< MDL	< MDL	0.75	< MDL	1.66	< MDL
2023/1/17	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	0.75	< MDL	1.68	< MDL
2023/1/18	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.16	< MDL	1.97	< MDL
2023/1/19	< MDL	< MDL	39.0	10.8	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.42	< MDL	1.82	< MDL
2023/1/20	< MDL	< MDL	59.3	13.4	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	5.85	< MDL	1.64	< MDL
2023/1/21	< MDL	< MDL	19.5	6.31	< MDL	< MDL	< MDL	4.34	< MDL	< MDL	< MDL	< MDL	1.93	< MDL	N.D.	< MDL
2023/1/22	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.03	0.790	1.86	< MDL
2023/1/23	< MDL	< MDL	26.8	< MDL	0.126	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	0.862	1.65	1.14	1.97	< MDL
2023/1/24	< MDL	< MDL	< MDL	5.98	0.430	< MDL	< MDL	3.61	< MDL	< MDL	< MDL	1.39	2.53	< MDL	1.92	< MDL
2023/1/25	< MDL	< MDL	29.6	< MDL	0.077	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.58	< MDL	1.84	< MDL
2023/1/26	< MDL	< MDL	< MDL	9.10	0.252	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	2.63	0.988	2.08	< MDL
2023/1/27	< MDL	< MDL	20.1	7.99	0.171	< MDL	< MDL	2.35	< MDL	< MDL	< MDL	< MDL	1.08	< MDL	1.72	< MDL
2023/1/28	< MDL	< MDL	< MDL	< MDL	< MDL	0.125	< MDL	2.04	< MDL	< MDL	< MDL	0.993	1.41	< MDL	1.73	< MDL
2023/1/29	< MDL	< MDL	< MDL	< MDL	0.065	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	< MDL	1.77	< MDL
2023/1/30	< MDL	< MDL	61.2	< MDL	< MDL	< MDL	< MDL	4.77	< MDL	< MDL	< MDL	< MDL	0.711	< MDL	1.77	< MDL

Table S9. Daily removal efficiency (%) of the target QACs during the sampling period.

Date	BACs					∑BACs	ATMACs					∑ATMACs	DADMACs					∑DADMACs	∑QACs
	C8	C10	C12	C14	C16		C8	C12	C14	C16	C18		8:8	8:10	10:10	14:14	16:16		
2022/12/15	100	100	95.6	100	100	95.9	100	100	100	100	100	100	89.9	-	-7.1	100	45.8	75.2	97.4
2022/12/18	-[a]	-	-255[b]	-126	-	-216	100	-	-	-	-	100	-168	-308	-768	100	17.5	-229	-223
2022/12/19	-	-	-275	-	100	-269	-	-93.5	-	100	100	96.9	-130	-	-260	100	50.8	30.4	62.9
2022/12/20	-	-	-1350	-554	-	-1111	-	-	-	-	-	-	-	-	-980	-	-2.2	-121	-922
2022/12/21	-	-	-1851	-591	100	-1455	-	-46.7	-	-	-	-46.7	100	-	-	100	63.7	73.5	-712
2022/12/23	-	-	-51.9	100	100	-29.3	-	-	-	-	-	-	-	-	-	100	74.6	79.2	-12.6
2022/12/24	100	-	-2282	-1092	-150	-1786	-	100	-	100	100	100	-133	-	-180	-9.1	65.3	27.0	-134
2022/12/25	100	-	43.3	22.0	-	53.9	50.0	-	-	-	-	50.0	100	-	-340	100	84.8	83.3	60.3
2022/12/26	100	-	52.7	-482	-1150	43.9	-	-	-	-	-	-	100	-	-620	-	76.6	62.7	45.2
2022/12/27	-	-	-1089	-563	100	-897	100	-	-	-	-	100	-	-	-300	100	60.9	53.7	-510
2022/12/28	-	-	-489	-	-	-489	-	100	-	-	-	100	100	-	-	-	22.7	55.3	-196
2022/12/29	-	-	-1772	-1157	-1400	-1586	-	-	-	-	-	-	45.9	-	-2000	100	28.0	-164	-915
2022/12/30	100	-	-670	-180	-	-261	-567	-	-	100	100	99.8	-	-	-420	100	81.4	71.4	59.0
2022/12/31	-	-	-821	-352	-	-680	-	-	-	-	-	-	100	100	98.9	41.7	100.0	98.9	64.2
2023/1/1	-	-	-	-	-	-	-	-	-	-	-	-	100	-	-380	100	88.5	83.2	83.2
2023/1/2	100	-	-846	-283	55.6	-293	-	-	-	-	100	100.0	41.2	-	-200	100	94.9	80.5	42.1
2023/1/3	-	-	-	-	-	-	100	-152	-	-	-	92.7	100	100	100	100	84.8	100	100
2023/1/4	-	-	23.7	24.1	100	24.2	-	100	-	-	100	100.0	100	-	-	100	91.4	93.0	48.0
2023/1/5	100	-	45.5	100	100	68.6	100	5.9	-	-	-	11.1	100	-	-340	100	81.7	76.2	68.4
2023/1/6	-	-	-495	/	/	-495	-	-	-	-	-	-	100	-	-340	46.2	83.3	74.4	-94.3
2023/1/7	-	-	100	100	98.0	100	-	-	-	-	-	-	-	-	-260	-	89.4	84.3	99.8
2023/1/8	100	-	-	-	-150	93.9	-	-	-	-	-	-	100	-	0.0	69.2	91.3	88.4	88.7

2023/1/9	-	-	-721	-199	0.0	-558	-	-	-	-	-	-	-133	-	-780	47.4	92.1	73.9	-94.6
2023/1/10	-	-	-805	-444	100	-678	-233	-40.2	-	-	-	-45.5	-	-	-460	100	81.4	76.3	-200
2023/1/11	100	-	-273	-199	-400	-6.5	-	-238	-	-	-	-238	-300	-	-300	55.6	91.1	72.7	16.9
2023/1/12	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-380	-460	61.4	-50.4	-50.4
2023/1/13	-	-	-	-	100	100	-	-124	-	-	-	-124	100	-	-220	100	68.2	68.3	48.6
2023/1/14	-	-	-	-	-	-	-	-30.8	-	-	-	-30.8	-	-	-60.0	-260	71.2	54.9	43.7
2023/1/15	100	100	97.7	85.8	100	97.1	-	100	-	100	100	100	100	-	63.0	100	80.6	89.7	98.9
2023/1/16	100	-	-479	-	100	-133	-	-106	-	-	100	93.7	-	-	-220	100	95.6	94.0	56.5
2023/1/17	-	-	-	-	-	-	-	-	-	-	100	100	-	-	-180	100	91.7	89.0	96.3
2023/1/18	100	-	-	-241	-	-7.1	-	-	-	-	-	-	-	-	-380	100	82.1	74.9	42.5
2023/1/19	100	-	-541	-314	-	-275	-	100	-	-	-	100	-	-	-460	100	84.3	76.0	-85.1
2023/1/20	100	-	-875	-413	100	-544	-	-	-	-	100	100	100	-	-867	100	94.7	78.8	-7.8
2023/1/21	100	-	-221	-141	-	-84.4	-	44.9	-	-	-	68.8	100	-	-660	100	100	70.1	6.3
2023/1/22	100	100	100	100	100	100	-	100	-	100	100	100	100	100	87.0	88.1	91.2	96.3	99.9
2023/1/23	100	-	-341	-	-150	-115	-	-	-	-	-	-	78.0	-	-580	-340	31.0	24.0	-62.8
2023/1/24	100	-	-	-130	-300	-63.7	-	-236	-	100	100	93.5	-133	-	-900	100	75.3	41.7	77.3
2023/1/25	100	100	85.7	100	-150	87.9	-	100	-	-	-	100	100	-	-77.8	100	0.0	62.2	91.8
2023/1/26	100	100	100	31.6	40.0	96.4	-	100	-	100	100	100	100	-	-189	-25.0	-5.0	33.7	95.8
2023/1/27	100	-	85.8	37.5	84.6	82.4	-	81.1	-	100	-	91.9	100	-	21.4	-	-900	43.7	82.9
2023/1/28	100	-	-	-	-	100	-233	-86.9	-	-	-	-90.9	-66.7	-	-460	100	60.5	35.4	58.2
2023/1/29	100	100	100	100	97.0	100.	-	100	-	100	100	100	100	-	100.0	100	66.7	90.8	99.9
2023/1/30	100	-	-907	-	-	-539	-	-243	-	-	-	-243	100	-	-180	-	41.9	46.2	-338

[a]Not detected in both influent and effluent samples, [b]for those not detected in influent but detected in effluent samples, MDL/2 was used as substituent value in influent.

Table S10. The real-time population size estimated based on NH_4-N concentration in influent.

Date	Influent flow （L/d）	NH_4-N (mg/L)	m_{NH4-N} (mg/d/inh）	Population size
2022/12/15	15541000	25.91	6000	67111
2022/12/18	15439000	34.77	6000	89469
2022/12/19	15641000	31.97	6000	83340
2022/12/20	15649000	34.89	6000	90999
2022/12/21	15645000	36.68	6000	95643
2022/12/22	14437000	26.14	6000	62897
2022/12/23	14736000	27.87	6000	68449
2022/12/24	14939000	27.27	6000	67898
2022/12/25	14688000	35.52	6000	86953
2022/12/26	15038000	34.94	6000	87571
2022/12/27	14633000	29.20	6000	71214
2022/12/28	14786000	31.31	6000	77158
2022/12/29	15141000	28.59	6000	72147
2022/12/30	16492000	29.20	6000	80261
2022/12/31	15646000	24.78	6000	64618
2023/1/1	14237000	23.72	6000	56284
2023/1/2	14085000	24.67	6000	57913
2023/1/3	15341000	42.24	6000	108001
2023/1/4	15441000	25.82	6000	66448
2023/1/5	15038000	29.00	6000	72684
2023/1/6	15190000	27.35	6000	69241
2023/1/7	15594000	27.64	6000	71836
2023/1/8	16945000	28.85	6000	81477
2023/1/9	15645000	31.83	6000	82997
2023/1/10	17001000	29.09	6000	82427

Date	**Influent flow（L/d）**	**NH_4-N (mg/L)**	**m_{NH4-N} (mg/d/inh）**	**Population size**
2023/1/11	15693000	28.39	6000	74254
2023/1/12	15644000	32.03	6000	83513
2023/1/13	15942000	41.21	6000	109495
2023/1/14	13890000	26.17	6000	60584
2023/1/15	14387000	28.25	6000	67739
2023/1/16	14036000	30.33	6000	70952
2023/1/17	14336000	27.90	6000	66662
2023/1/18	13582000	26.63	6000	60281
2023/1/19	13585000	25.61	6000	57985
2023/1/20	14136000	33.10	6000	77984
2023/1/21	13684000	23.00	6000	52455
2023/1/22	11630000	23.29	6000	45144
2023/1/23	11476000	20.60	6000	39401
2023/1/24	12179000	39.98	6000	81153
2023/1/25	12933000	27.58	6000	59449
2023/1/26	12681000	33.79	6000	71415
2023/1/27	13483000	31.74	6000	71325
2023/1/28	14285000	31.42	6000	74806
2023/1/29	12882000	29.66	6000	63680
2023/1/30	13833000	32.17	6000	74168

Table S11. The estimated median, 95th percentile, mean, range and proportion of daily mass load (mg/1000inh/d) of QACs.

Targets	Median	95th percentile	Mean	Range	Proportion (%)	
					In each group	In Σ QACs
Benzylalkyldimethyl ammonium compounds (BACs)						
BAC-C8	0.323	4.02	0.906	0.0 - 5.21	42.5	7.88
BAC-C10	0.000	6.81	0.830	0.0 - 14.4	0.806	0.315
BAC-C12	0.000	201	29.0	0.0 - 370	34.0	17.3
BAC-C14	0.000	45.7	3.96	0.0 - 63.6	4.19	2.21
BAC-C16	0.000	1.30	0.182	0.0 - 3.48	18.5	0.306
Σ BACs	1.08	252	34.8	0.0 - 446	100	28.0
Alkyltrimethyl ammonium compounds (ATMACs)						
ATMAC-C8	0.000	0.0270	0.115	0.0 - 5.08	14.9	0.0970
ATMAC-C10	0.000	0.000	0.000	0.0 - 0.0	0.000	0.0
ATMAC-C12	0.000	25.5	2.59	0.0 - 31.2	30.0	4.02
ATMAC-C14	0.000	1.51	0.142	0.0 - 2.17	1.81	0.578
ATMAC-C16	0.000	129	12.4	0.0 - 236	12.9	4.02
ATMAC-C18	0.000	364	31.7	0.0 - 571	40.4	14.8
Σ ATMACs	0.4	502.1	46.9	0.0 - 825	100	23.4
Dialkyldimethyl ammonium compounds (DADMACs)						
DADMAC-8:8	0.231	4.23	1.60	0.0 - 47.7	17.0	5.25
DADMAC-8:10	0.000	15.7	39.5	0.0 - 1749	3.63	2.52
DADMAC-10:10	0.000	20.8	7.67	0.0 - 310	4.18	2.06
DADMAC-14:14	0.242	0.740	0.279	0.0 - 1.73	9.39	4.60
DADMAC-16:16	1.312	7.06	2.12	0.0 - 8.15	65.8	34.1
Σ DADMACs	2.17	41.4	51.2	0.309 - 2109	100	48.5
Σ QACs	10.7	1121	133	0.309 - 2114		100

Table S12. EC_{50}/LC_{50}, NOEC, AF and PNEC of the target QACs to calculate risk quotient (RQ) of fish.

Acronym	**EC_{50}[a]/LC_{50}[b] (mg/L)**	**NOEC[c] (mg/L)**	**AF[d]**	**PNEC[e]**	**RQ_{95th}[f]**	**RQ_{50th}[g]**
BAC-C8	1987.7	-	1000	1.99E+00	0.00	0.00
BAC-C10	286.5	-	1000	2.87E-01	0.00	0.00
BAC-C12	40.97	-	1000	4.10E-02	0.00	0.00
BAC-C14	5.82	-	1000	5.82E-03	0.01	0.00
BAC-C16	0.82	-	1000	8.21E-04	0.00	0.00
ATMAC-C8	49729.11	-	1000	4.97E+01	0.00	0.00
ATMAC-C10	7404.53	-	1000	7.40E+00	0.00	0.00
ATMAC-C12	0.28	-	1000	2.80E-04	0.02	0.01
ATMAC-C14	157.75	-	1000	1.58E-01	0.00	0.00
ATMAC-C16	22.68	-	1000	2.27E-02	0.00	0.00
ATMAC-C18	-	0.28	100	2.84E-03	0.00	0.00
DADMAC-8:8	-	5.11	100	5.11E-02	0.00	0.00
DADMAC-10:10	-	0.11	100	1.12E-03	0.00	0.00
DADMAC-14:14	0.00	-	1000	5.17E-07	2.28	1.37
DADMAC-16:16	0.00	-	1000	9.87E-09	212.7	177
DADMAC-8:10	-	0.71	100	7.11E-03	0.01	0.00

[a]Median effect concentration, [b]lethal concentration 50%, [c]no observed effect concentration, [d]assessment factor with values of 1000 and 100 applied to EC_{50}/LC_{50} and NOEC data, respectively, [e]the predicted-no-effect concentration at which on effects on exposed organisms occur, [f]risk quotient calculated by the 95th percentile concentration, which represents the worst scenario, [g]risk quotient calculated by the median concentration (the minimum concentration was used when median was < MDL), which represents the normal scenario.

Table S13. EC_{50}/LC_{50}, NOEC, AF and PNEC of the target QACs to calculate risk quotient (RQ) of daphnid.

Acronym	EC_{50}[a]/LC_{50}[b] (mg/L)	NOEC[c] (mg/L)	AF[d]	PNEC[e]	RQ_{95th}[f]	RQ_{50th}[g]
BAC-C8	1025.67	-	1000	1.03E+00	0.00	0.00
BAC-C10	161.89	-	1000	1.62E-01	0.00	0.00
BAC-C12	0.04	-	1000	3.82E-05	3.55	0.74
BAC-C14	3.94	-	1000	3.94E-03	0.01	0.00
BAC-C16	0.61	-	1000	6.09E-04	0.00	0.00
ATMAC-C8	21916.75	-	1000	2.19E+01	0.00	0.00
ATMAC-C10	3573.13	-	1000	3.57E+00	0.00	0.00
ATMAC-C12	0.02	-	1000	1.60E-05	0.29	0.09
ATMAC-C14	0.09	-	1000	9.10E-05	0.00	0.00
ATMAC-C16	14.37	-	1000	1.44E-02	0.00	0.00
ATMAC-C18	-	0.27	100	2.70E-03	0.00	0.00
DADMAC-8:8	-	3.42	100	3.42E-02	0.00	0.00
DADMAC-10:10	-	0.12	100	1.21E-03	0.00	0.00
DADMAC-14:14	0.02	-	1000	2.30E-05	0.05	0.03
DADMAC-16:16	0.00	-	1000	1.23E-08	170.7	141.9
DADMAC-8:10	0.85	-	1000	8.53E-04	0.04	0.00

[a]Median effect concentration, [b]lethal concentration 50%, [c]no observed effect concentration, [d]assessment factor with values of 1000 and 100 applied to EC_{50}/LC_{50} and NOEC data, respectively, [e]the predicted-no-effect concentration at which on effects on exposed organisms occur, [f]risk quotient calculated by the 95^{th} percentile concentration, which represents the worst scenario, [g]risk quotient calculated by the median concentration (the minimum concentration was used when median was < MDL), which represents the normal scenario.

Table S14. EC_{50}/LC_{50}, NOEC, AF and PNEC of the target QACs to calculate risk quotient (RQ) of green algae.

Acronym	**EC_{50}[a]/LC_{50}[b] (mg/L)**	**NOECc (mg/L)**	**AF[d]**	**PNEC[e]**	**RQ_{95th}[f]**	**RQ_{50th}[g]**
BAC-C8	514.41		1000	5.14E-01	0.00	0.00
BAC-C10	118.13		1000	1.18E-01	0.00	0.00
BAC-C12	0.20	-	1000	2.03E-04	0.67	0.14
BAC-C14	0.17	-	1000	1.74E-04	0.17	0.03
BAC-C16	0.16	-	1000	1.61E-04	0.00	0.00
ATMAC-C8	5726.92		1000	5.73E+00	0.00	0.00
ATMAC-C10	1358.45		1000	1.36E+00	0.00	0.00
ATMAC-C12	317.67	-	1000	3.18E-01	0.00	0.00
ATMAC-C14	0.13		1000	1.28E-04	0.00	0.00
ATMAC-C16	0.14		1000	1.37E-04	0.00	0.00
ATMAC-C18		1.11	100	1.11E-02	0.00	0.00
DADMAC-8:8	-	8.61	100	8.61E-02	0.00	0.00
DADMAC-10:10	1.82	-	1000	1.82E-03	0.00	0.00
DADMAC-14:14	0.01	-	1000	5.00E-06	0.24	0.14
DADMAC-16:16	0.00	-	1000	2.41E-07	8.71	7.24
DADMAC-8:10	2.97		1000	2.97E-03	0.01	0.00

[a]Median effect concentration, [b]lethal concentration 50%, [c]no observed effect concentration, [d]assessment factor with values of 1000 and 100 applied to EC_{50}/LC_{50} and NOEC data, respectively, [e]the predicted-no-effect concentration at which on effects on exposed organisms occur, [f]risk quotient calculated by the 95^{th} percentile concentration, which represents the worst scenario, [g]risk quotient calculated by the median concentration (the minimum concentration was used when median was < MDL), which represents the normal scenario.

Table S15. Calculation of EDI for the detected QACs in effluent.

Acronym	PEC_{water}[a]	BCF[b]	BMF[c]	PEC_{fish}[d]	E_D[e]	E_F[f]	F_{IR}[g]	C_f[h]	AT[i]	W_{AB}[j]	EDI[k]
BAC-C12	2.82	61.73	1	1.74	70	365	29.6	0.208	25550	65	0.0165
BAC-C14	0.594	420.24	1	2.50	70	365	29.6	0.208	25550	65	0.0236
BAC-C16	0.00653	2860.88	2	0.374	70	365	29.6	0.208	25550	65	0.00354
ATMAC-C8	0.00572	0.05	1	2.68E-7	70	365	29.6	0.208	25550	65	2.54E-8
ATMAC-C12	0.141	2.17	1	0.00307	70	365	29.6	0.208	25550	65	2.90E-5
DADMAC-8:8	0.0862	38.59	1	0.0332	70	365	29.6	0.208	25550	65	0.000315
DADMAC-8:10	3.66	267.92	1	9.80	70	365	29.6	0.208	25550	65	0.0928
DADMAC-10:10	0.1111	1823.9	2	4.05	70	365	29.6	0.208	25550	65	0.0384
DADMAC-14:14	0.0710	11454.6	3	24.4	70	365	29.6	0.208	25550	65	0.231
DADMAC-16:16	0.175	84.43	1	0.147	70	365	29.6	0.208	25550	65	0.00140

[a]Median concentration divided by a standard dilution factor of 10 (minimum concentration was used when median was < MDL) of QACs in the effluent (ng/L), [b]bioconcentration factor (L/kg), log BCF = 0.85× log *Kow* – 0.70 (when log *Kow* ≤ 6), log BCF = -0.20 × (log *Kow*) ^2 + 2.74 × log *Kow* – 4.72 (when log *Kow* > 6), [c]biomagnification factor, [d] predicted QACs concentrations in fish (μg/kg), [e]exposure duration (years), [f] exposure frequency (days/year), [g]intake rate of fish consumption (g/person/day), [h]wet-to-dry weight conversion factor (reflecting 79% moisture in fish fillets), [i]average exposure time (days), [j]average adult body weight (kg), [k]estimated daily intake (μg/kg/day).

Table S16. The median concentration, DF, PNEC, persistence, BAF, mobility and calculated ToxPi score of the target QACs.

Acronym	**C[a]**	**DF[b] (%)**	**PNEC[c]**	**P[d] (day)**	**BAF[e]**	**M[f]**	**ToxPi Score**
BAC-C8	0.03	0.00	5.14E-01	32.07	1.64	0.73	0.20
BAC-C10	3.70	0.00	1.18E-01	37.25	8.22	0.52	0.36
BAC-C12	28.20	67.39	3.82E-05	42.16	52.18	0.41	0.65
BAC-C14	5.90	50.00	1.74E-04	107.35	192.80	0.33	0.71
BAC-C16	0.04	32.61	1.61E-04	108.05	440.90	0.28	0.57
ATMAC-C8	0.03	10.87	5.73E+00	30.88	0.08	2.34	0.24
ATMAC-C10	0.18	0.00	1.36E+00	31.10	1.05	1.03	0.24
ATMAC-C12	1.07	30.43	1.60E-05	32.90	2.50	0.66	0.50
ATMAC-C14	3.14	0.00	9.10E-05	38.97	16.07	0.49	0.42
ATMAC-C16	4.76	0.00	1.37E-04	42.62	126.80	0.38	0.45
ATMAC-C18	10.57	0.00	2.70E-03	107.70	524.00	0.32	0.57
DADMAC-8:8	0.60	23.91	3.42E-02	41.45	43.22	0.43	0.45
DADMAC-8:10	8.97	2.17	8.53E-04	43.06	277.90	0.35	0.46
DADMAC-10:10	1.10	86.96	1.12E-03	43.25	945.90	0.29	0.57
DADMAC-14:14	0.25	23.91	5.17E-07	108.16	83150.00	0.18	0.65
DADMAC-16:16	1.80	91.30	9.87E-09	108.16	10760.00	0.15	0.74

[a]Median concentration, [b]detection frequency, [c]the lowest predicted-no-effect concentration among the three trophic organisms, for which the reciprocal was taken for processing, [d]persistence, [e]bioaccumulation factor, [f]mobility, potential for compounds to migrate over long distances through water flow, which was calculated as 1/log *Koc*.

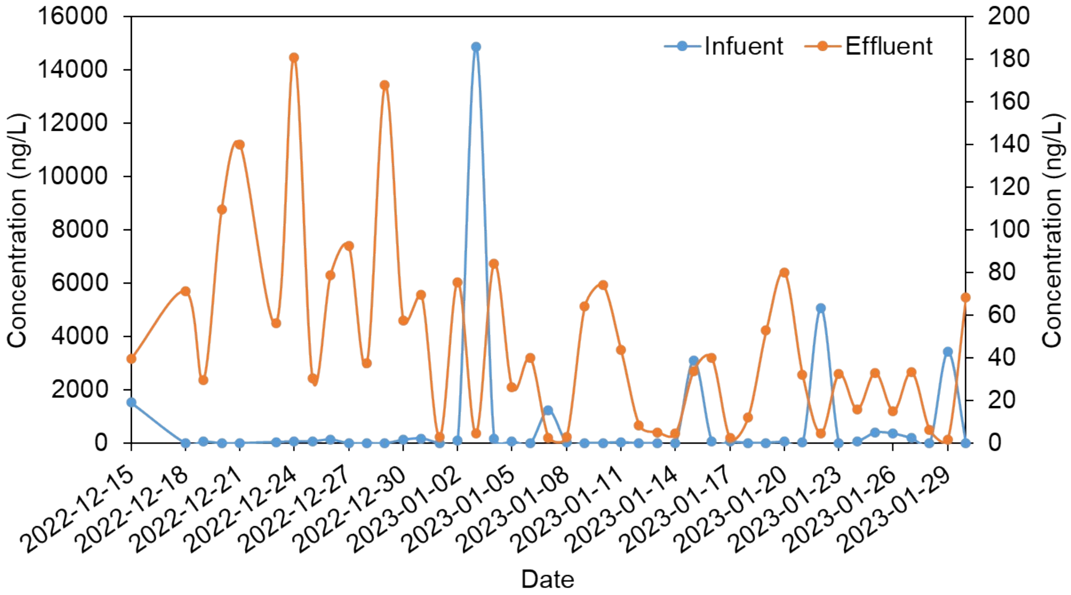


Figure S1. Trends of total QACs concentrations in influent and effluent samples over the sampling period. (The left and right Y-axis represents total QACs concentrations in influent and effluent samples, respectively)

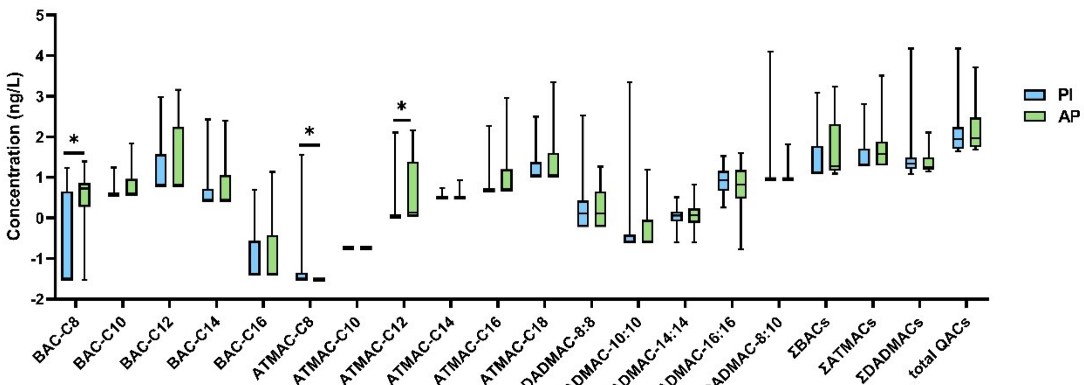


Figure S2. Comparison of QACs concentrations in influent samples during the infection peak period (PI) and abatement period (AP) (*$p < 0.05$).

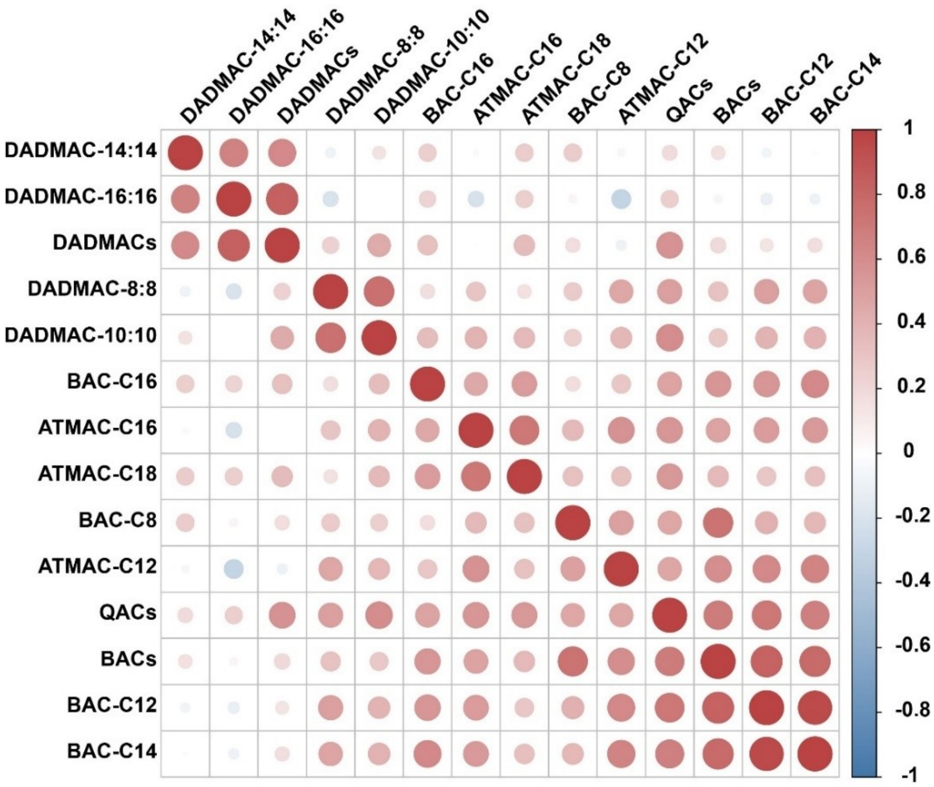


Figure S3. Spearman correlation analysis of the detected QACs with DF > 20% in influent samples.

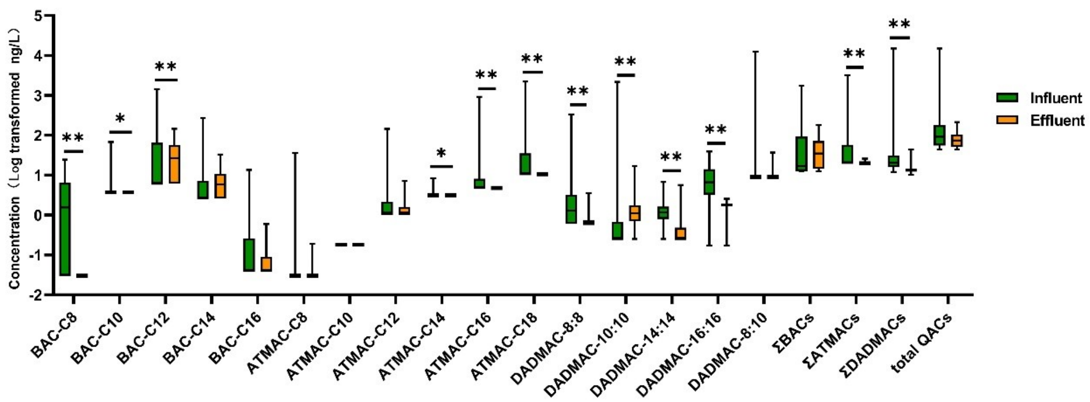


Figure S4. Comparison of target QACs concentrations in influent and effluent samples.

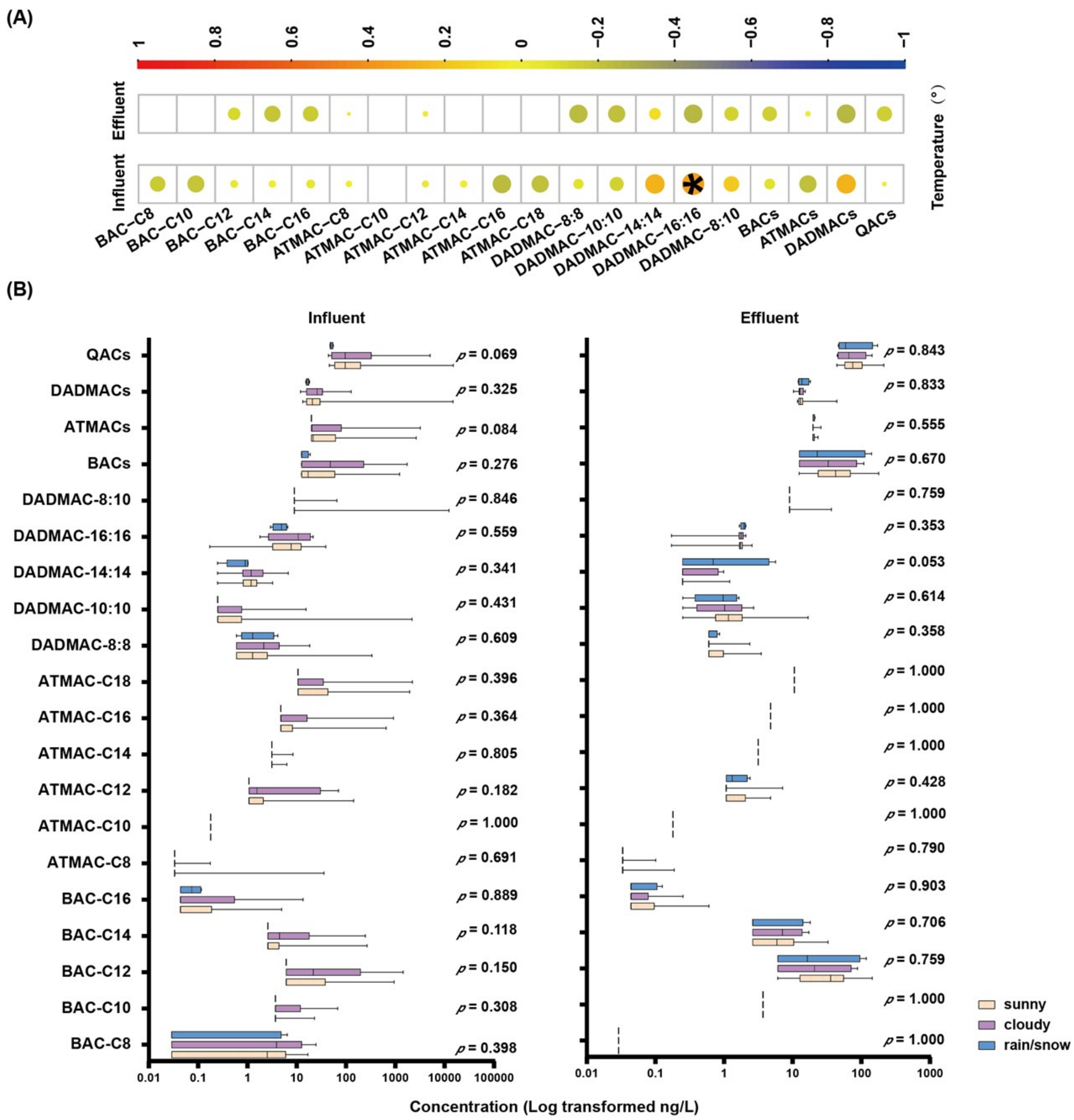
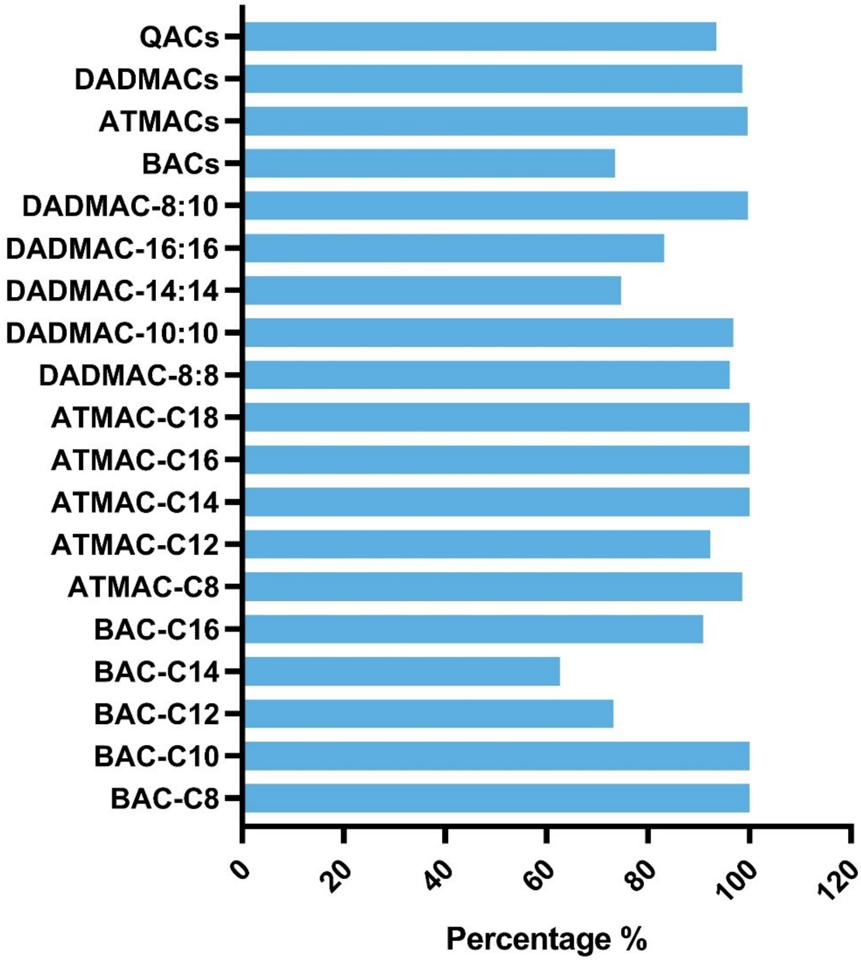


Figure S5. Comparison of QACs concentrations under different weather conditions during the sampling period: (A) spearman correlation analysis between QACs concentrations and temperature (*p < 0.05), (B) Kruskal-Wallis test of QACs concentrations at different weather conditions.



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173 **Figure S6.** Mean removal efficiencies of the target QACs.