Supplementary information for

Direct Generation of DBPs from City Dust during Chlorine-based Disinfection

by

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Summary: SI contains 34 pages, 7 figures, and 8 tables.

MATERIALS AND METHODS

SEC Measurements

This was achieved using a Waters HPLC system (1525 Binary Pump, Model 1500 Column Heater, 2998 Photodiode Array Detector, 2707 Autosampler) equipped with an SEC column (Phenomenex, BioSep 5 μm, SEC-s3000, 290 Å) and SecurityGuard™ Cartridges (Phenomenex, KJ0-4282) with 10 mM sodium acetate (CG grade, Aladdin, Shanghai, China) as the mobile phase[1]. The measurements were carried out at wavelength of 254 nm. The flow rate was set at 1.0 mL/min, and the injection volume for water samples was 100 μL.

Quality Control and Quality Assurance

To avoid contamination, all the glassware used during the tests were ultrasonically cleaned and rinsed with methanol, and then dried at 60 ^{0}C in an oven prior to use. Targeted dust samples were extracted in a single batch, and dust samples without chlorination process were regarded as the control. Since most annotated compounds were novel compounds that no authentic standards were available, peak counts were utilized to semi-quantify their concentrations. Methods detection limits (MDLs) could not be calculated, and an absolute peak area of 10000 counts was used as the MDL.

Chemical Standards for Regulated DBP Calibration

The chemical standards were as follows: a THM mixture certified reference material (100 mg/L of each component in methanol, TanMo Quality Inspection Technology Co., Ltd (China)), a HAA mixture certified reference material (1000 mg/L of each component in methanol, Sigma-Aldrich (USA)).

Measurement of Regulated DBPFP

THMs and HAAs were extracted with methyl-tert-butyl ether (MTBE) (HPLC Grade, J.T. Baker, USA)[2]. For the extraction of THMs, 4 mL methyl tert-butyl ether (MTBE) and 8 g Na_2SO_4 were added to 20 mL water samples. After shaking the water samples for 2 min and standing them for 20 min, the supernatant was drawn and transferred to the gas chromatograph (GC)-vial, and compounds subsequently determined by GC- electron capture detector (ECD). For HAAs, 20 mL water samples were adjusted to pH $\leqslant$ 0.5 with 1 mL concentrated sulfuric acid. Na_2SO_4 was then added and the sample was immediately shaken until all the solid had dissolved. After that, MTBE was added and the sample was shaken vigorously for 2 min. The supernatant containing HAAs were then methylated by adding acidic methanol (containing

10%wt H_2SO_4) followed by water bath heating for 2 h at 50 ^{0}C. Finally, the methylated HAAs were separated by adding $NaSO_4$ (150 g/L), and neutralized with $NaHCO_3$ before determination by GC-ECD.

Quantitative analysis of the DBPs was performed on a gas chromatograph (Clarus 590, PerkinElmer, U.S.) with an electron capture detector (ECD). Conditions for the analyses were as follows: (1) THMs, injector temperature 200 ^{0}C, column temperature 35 ^{0}C (holding 4 min) to 260 ^{0}C (10 ^{0}C/min), detector temperature 290 ^{0}C; (2) HAAs, injector temperature 200 ^{0}C, column temperature 35 ^{0}C (holding 4 min) to 65 ^{0}C (2 ^{0}C/min), detector temperature 290 ^{0}C.

Analysis of Unknown DBPs

For GC-qTOF-MS analysis, the GC oven temperature profile was started at 35 °C and kept for 5 min, then ramped to 290 ^{0}C at 10 ^{0}C/min and kept for 10 min, then the back flush was performed for 0.5 min at 310 ^{0}C. Splitless (50 ml/min) injections of 1 μL sample extract were carried out at 280 ^{0}C and with a splitless time of 0.7 min. Helium 99.999% was used as carrier gas at a constant flow of 1.0 mL/min. Nitrogen was used as collision gas at a flow rate of 1.5 mL/min. Analyses were performed with LE-EI at 70 eV, ion source temperature: 230 ^{0}C, quadrupole temperature: 150 ^{0}C, extended dynamic range: 5GHz. The instrument operated in full scan mode from m/z 45 to 500, with acquisition rate and time of 5 spectra/s and 200 ms/spectrum, respectively. The data obtained from GC-qTOF-MS was processed using MassHunter Qualitative Analysis software, for the deconvolution and non-targeted feature extraction. The extracted data was then statistically analysed using Mass Profiler Professional 13.0 software, and then compared to the mass spectral library NIST-17 for the identification.

Calculation of NOSC and DBE

The nominal oxidation state of carbon in an organic compound can be calculated from the number of electrons transferred in the half reaction, n_{e-}, and the number of carbon atoms (a) in the compound as:

$$\mathrm{NOSC} = -\left(\frac{n_{e-}}{\mathrm{a}}\right) + 4$$

The double bond equvilant can be calculated based on:

$$\mathrm{DBE} = 1 + \frac{\sum n_i(V_i - 2)}{2}$$

Where V_i is the formal valence of an element, and n_i is the number of element in the molecular formula.

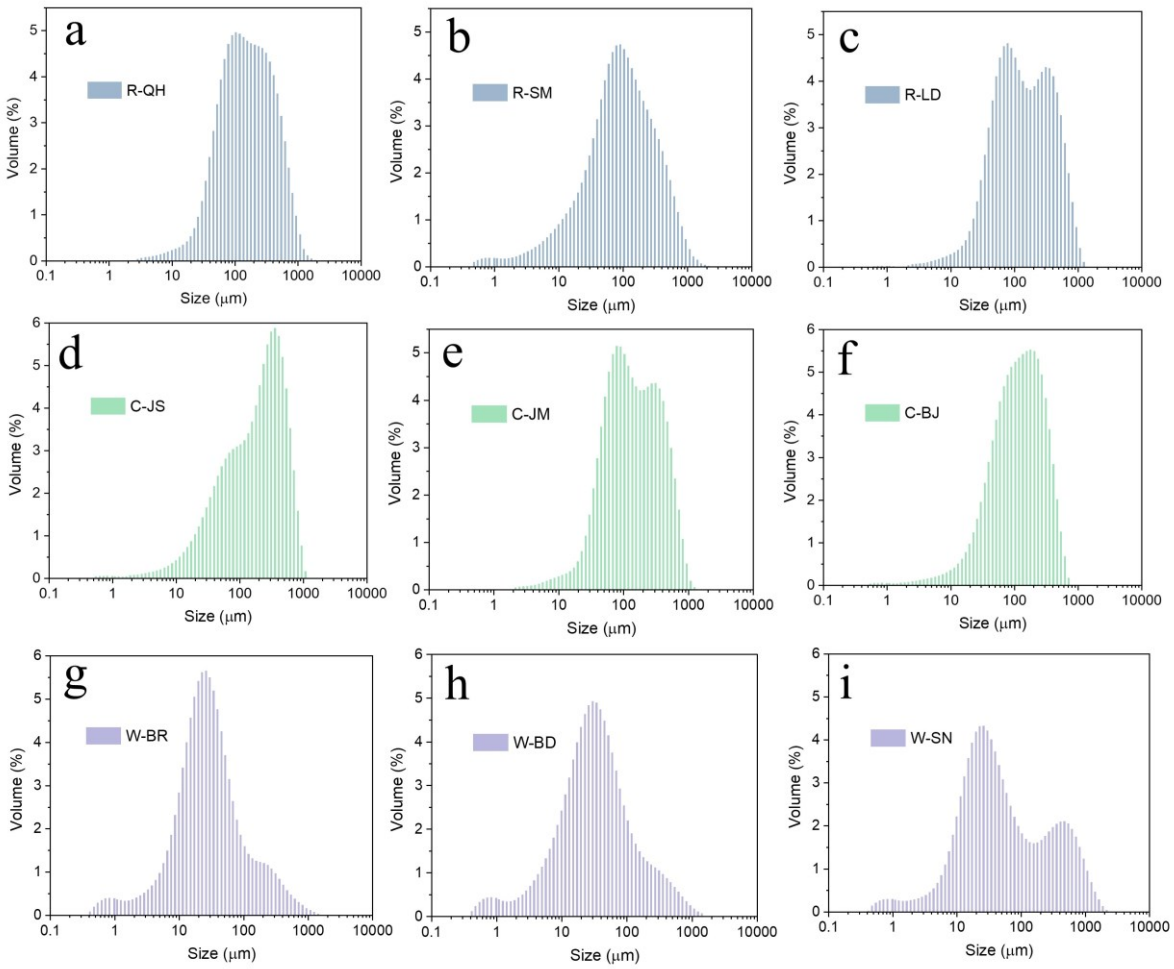


Figure S1. Size distribution of dust collected from public road (a-c), community areas (d-f), and indoor spaces (g-i), respectively.

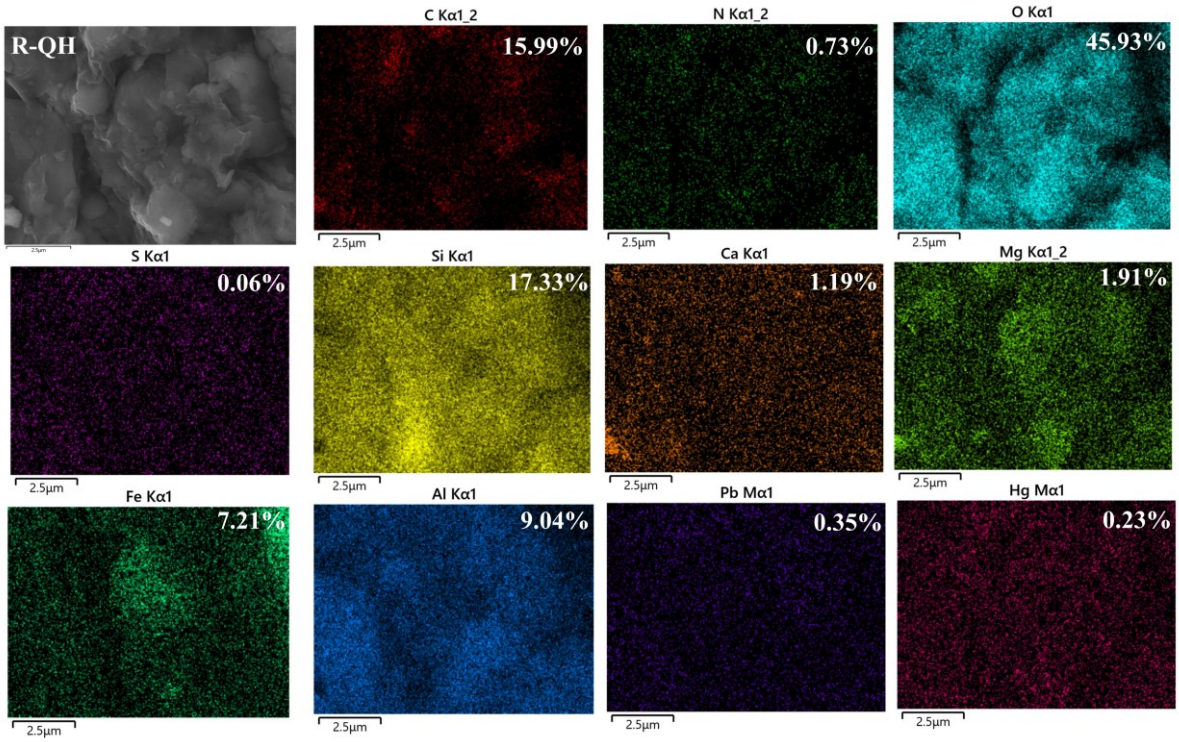


Figure S2. SEM-EDS images of dust collected from R-QH.

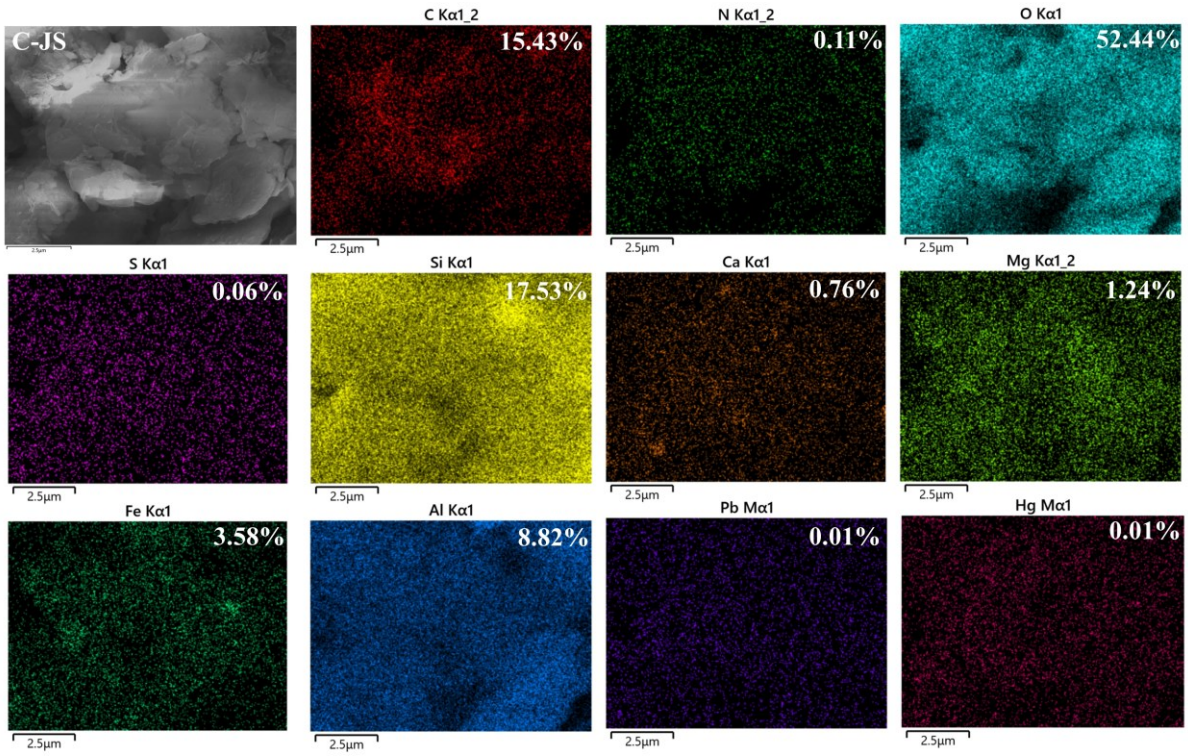


Figure S3. SEM-EDS images of dust collected from C-JS.

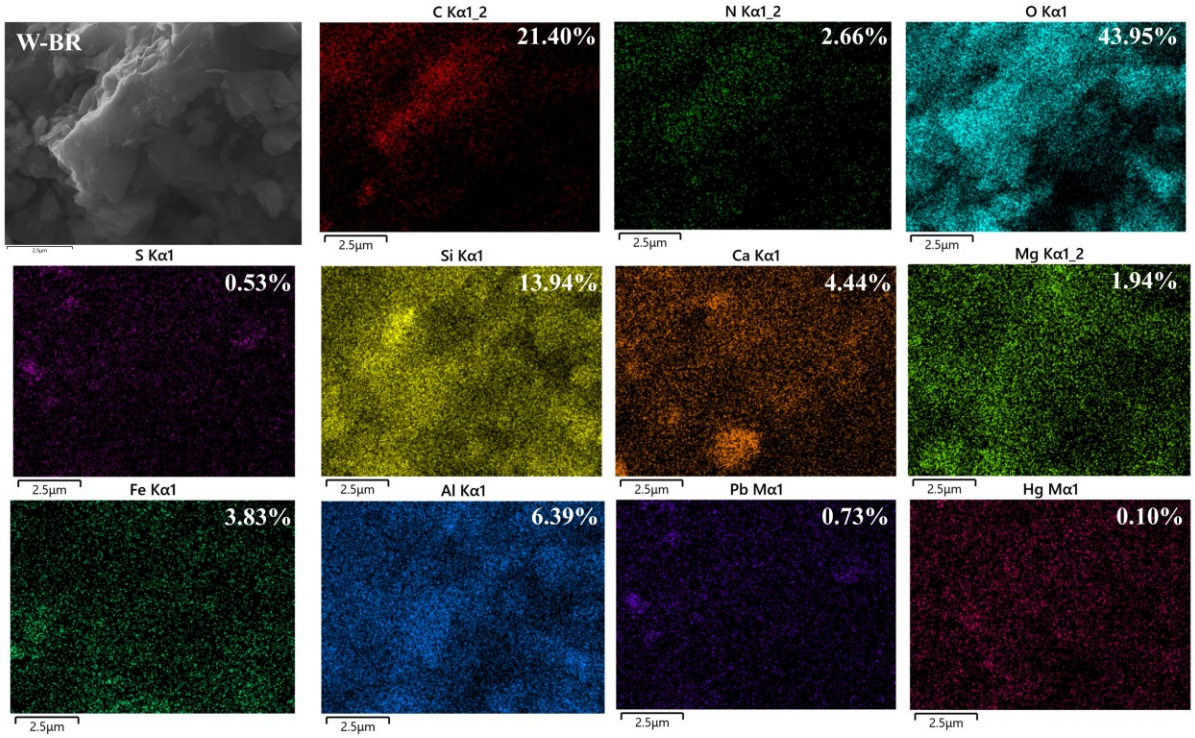
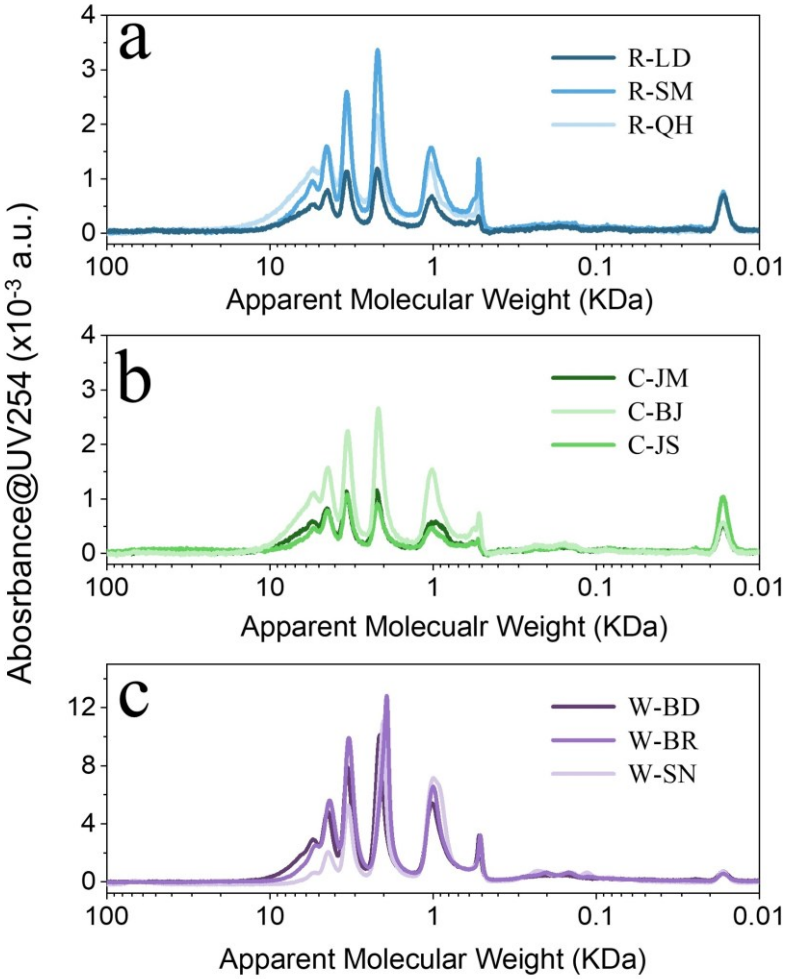


Figure S4. SEM-EDS images of dust collected from W-BR.



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95 **Figure S5**. Apparent molecular weight distribution of dissolved organics on representative
96 dust collected from different areas.

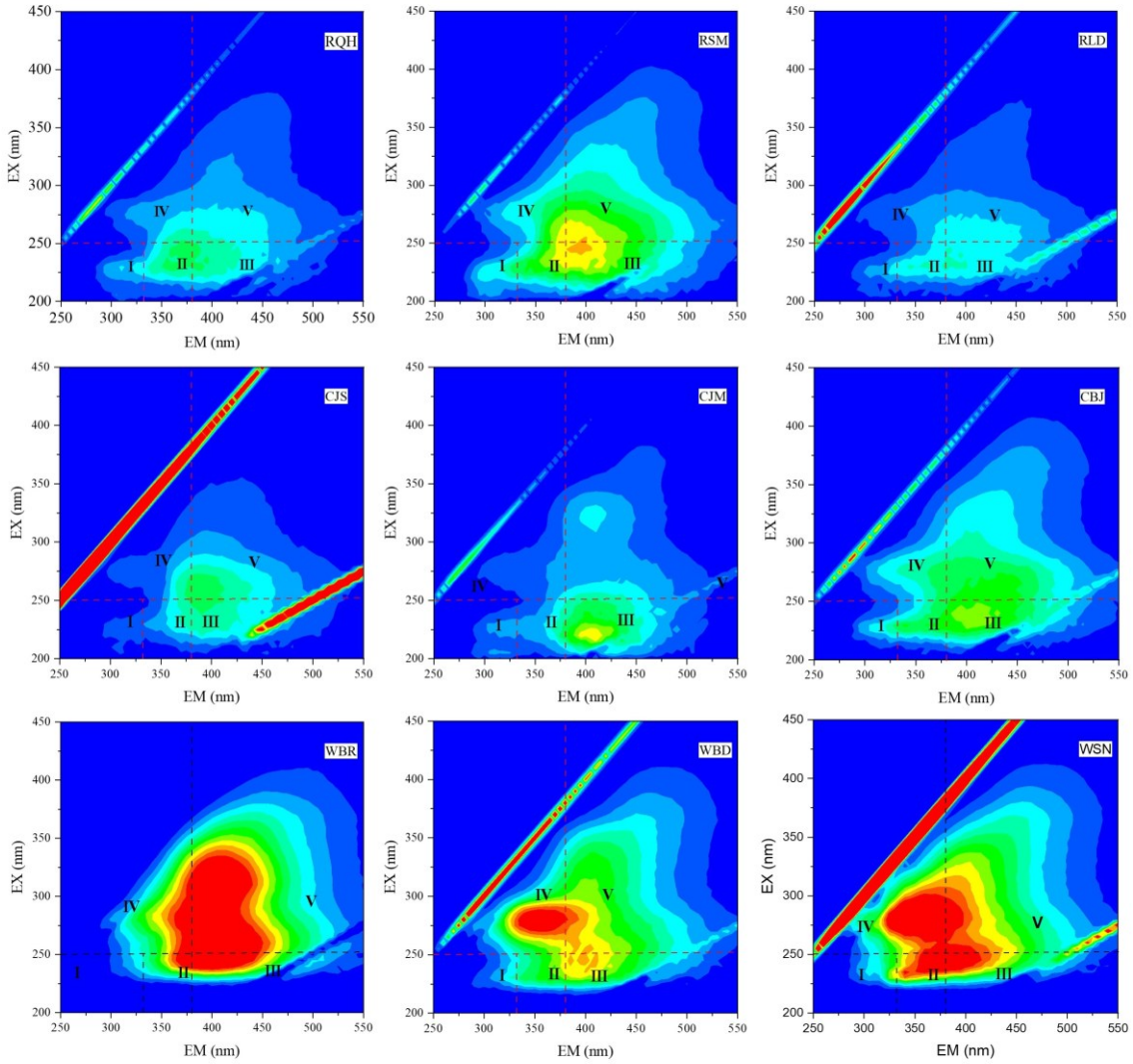


Figure S6. EEM analysis of the organics containing on the representative dust collected from different areas.

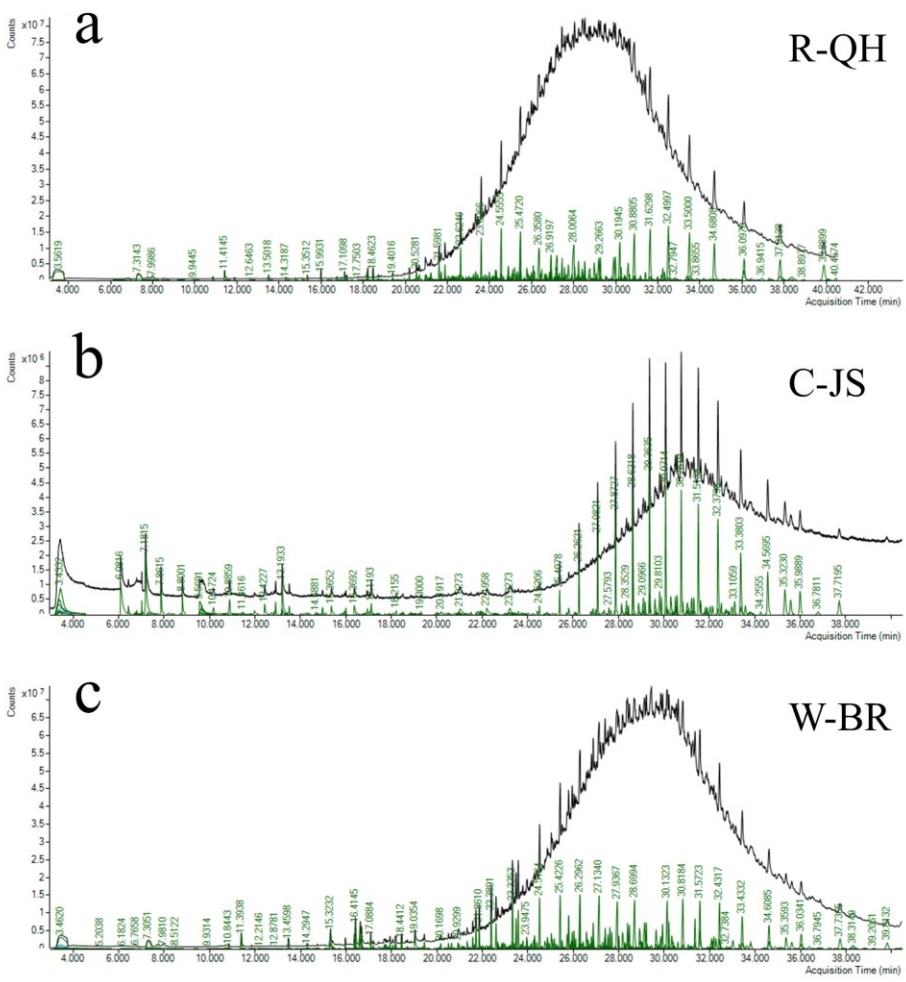


Figure S7. Non-target identification of organics originally from the dust collected from R-QH (a), C-JS (b), and W-BR (c), without the disinfection process using GC-qTOF-MS.

Table S1. Elemental composition of the dust collected from the respective areas (R-QH, C-JS, and W-BR).

Elements	Weight percentage (%)		
	R-QH	C-JS	W-BR
O	45.026	43.544	42.778
Na	1.2324	1.0276	1.3072
Mg	2.3644	3.0035	4.8369
Al	7.1179	7.2091	6.32
Si	25.539	21.947	19.456
P	0.21964	0.24019	0.15197
S	0.23145	0.41218	1.466
Cl	0.23441	0.31448	0.70841
K	2.1418	1.5983	1.7297
Ca	10.693	15.413	16.665
Ti	0.60362	0.71776	0.42933
Cr	0.023428	0.023385	0.030968
Mn	0.094353	0.10731	0.08731
Fe	4.0899	4.1994	3.579
Ni	<0.01	<0.01	0.010263
Cu	0.013483	0.016081	0.015796
Zn	0.077432	0.14278	0.11639
Br	<0.01	<0.01	<0.01
Rb	0.0134	<0.01	<0.01
Sr	0.057759	0.060212	0.028735
Zr	0.033903	0.024006	0.013895
Ba	0.12549	<0.01	0.14893
Ce	0.067353	<0.01	0.1105
Pb	<0.01	<0.01	0.008792

Table S2. Fitting area proportion of peaks at different binding energy for C 1s in respective organics contained on the representative dust collected from different areas.

Samples	C 1s (Approx. binding energy/eV) Peak area (%)			
	284.5 eV C-(C,H)	285.9 eV C-(O,N)	287.6 eV C=O,O-C-O	288.8 eV O=C-OH or O=C-OR
R-QH	46.76	28.92	14.78	9.54
C-JS	46.45	27.81	11.37	14.37
W-BR	51.24	29.92	8.12	10.72

Table S3. Retention time (RT), compound name, formula, CAS number, and match factor of unknown DBPs identified from R-QH dust after the disinfection process.

Component RT	Compound Name	Formula	CAS#	Match Factor
1.6832	2-Propenoyl chloride	C_3H_3ClO	814-68-6	75.63
1.7686	Acetonitrile, bromo-	C_2H_2BrN	590-17-0	60.53
1.8454	Propanoyl chloride	C_3H_5ClO	79-03-8	70.57
1.9148	Chloromethane	CH_3Cl	74-87-3	74.28
2.1441	Chlorotrifluoromethane	$CClF_3$	75-72-9	70.50
2.6172	Dichlorodifluoromethane	CCl_2F_2	75-71-8	78.53
2.6522	Trichloromethane	$CHCl_3$	67-66-3	93.83
2.9358	Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl-	$C_{18}H_{22}BrNO$	3565-72-8	85.34
7.3249	Benzene, chloro-	C_6H_5Cl	108-90-7	95.98
7.4116	Propane, 1,2,3-trichloro-	$C_3H_5Cl_3$	96-18-4	53.72
8.3381	N-(4-Chloro-3,3-dimethyl-2-butylidene)methylamine	$C_7H_{14}ClN$	1000137-59-4	52.62
8.5143	Ethanone, 2-bromo-1,2-diphenyl-	$C_{14}H_{11}BrO$	1484-50-0	76.67
8.5391	Acetonitrile, chlorodifluoro-	C_2ClF_2N	421-05-6	53.45
9.2408	5-Chloro-1,3-dimethyl-1H-pyrazole-4-sulfonic acid, 2-methyl-5-trifluoromethyl-2H-pyrazol-3-yl ester	$C_{10}H_{10}ClF_3N_4O_3S$	1000265-45-4	55.16
9.3835	1-Propene, 1,2,3,3-tetrachloro-	$C_3H_2Cl_4$	20589-85-9	77.51
10.0370	3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	$C_{15}H_{10}Cl_2O_3$	1000331-26-9	85.09
10.1285	4-Chlorobutanoic anhydride	$C_8H_{12}Cl_2O_3$	1000333-91-1	55.79
11.5334	Benzene, 1,2-dichloro-	$C_6H_4Cl_2$	95-50-1	67.27
13.2420	p-Chloroaniline	C_6H_6ClN	106-47-8	90.55
13.3186	Benzene, 1-chloro-4-isocyanato-	C_7H_4ClNO	104-12-1	66.99

13.9238	Maleic monoacid chloride, methyl ester	$C_5H_5ClO_3$	1000152-93-6	52.28
13.9808	Carbon Tetrachloride	CCl_4	56-23-5	81.89
14.6044	p-Chlorophenyl benzylcarbamate	$C_{14}H_{12}ClNO_2$	124068-98-0	53.79
14.6181	L-Proline, 1-(chlorocarbonyl)-, methyl ester	$C_7H_{10}ClNO_3$	85665-59-4	53.21
14.8062	Clopidol	$C_7H_7Cl_2NO$	2971-90-6	67.89
14.8911	1-[3,4-Dichlorophenyl]-3-[4-.alpha.-[diethylamino]-4-hydroxy-m-toluimino-6-methyl]pyrimidin-2-yl-guanidine	$C_{23}H_{27}Cl_2N_7O$	51387-29-2	64.70
15.0902	Piperazine, 1,4-bis[2-(3-chlorophenoxy)ethyl]-	$C_{20}H_{24}Cl_2N_2O_2$	294877-72-8	50.72
15.2978	4-Chloro-2-trifluoromethylbenzo[h]quinoline	$C_{14}H_7ClF_3N$	1700-98-7	59.10
15.9140	2-Bromo dodecane	$C_{12}H_{25}Br$	13187-99-0	61.72
16.0366	Benzene, (1-bromoethyl)-	C_8H_9Br	585-71-7	73.40
16.2802	Benzenamine, 3,4-dichloro-	$C_6H_5Cl_2N$	95-76-1	54.40
16.4576	Benzene, (1-iodoethenyl)-	C_8H_7I	51246-20-9	51.90
16.4878	Decane, 1-iodo-	$C_{10}H_{21}I$	2050-77-3	64.02
17.2465	1,3-Difluoro-2-trichloromethylbenzene	$C_7H_3Cl_3F_2$	93632-85-0	57.12
17.4465	Ethane, iodo-	C_2H_5I	75-03-6	69.29
17.5097	1,3-Benzenediol, 4-bromo-	$C_6H_5BrO_2$	6626-15-9	70.00
17.5838	5-Fluoro-2-trifluoromethylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	$C_{15}H_6Cl_2F_4O_3$	1000331-61-0	65.87
18.8491	Dodecane, 1-iodo-	$C_{12}H_{25}I$	4292-19-7	69.16
18.9001	7-Chloro-2,3-dihydro-3-(4-N,N-dimethylaminobenzylidene)-5-phenyl-1H-1,4-benzodiazepin-2-one	$C_{24}H_{20}ClN_3O$	55056-35-4	59.94

18.9579	Decane, 1-bromo-2-methyl-	$C_{11}H_{23}Br$	127839-47-8	62.12
19.7831	Fenclorim	$C_{10}H_6Cl_2N_2$	3740-92-9	68.67
20.0555	4-Trichloromethyl-1-oxa-2-thiacyclobutane-2,2-dioxide	$C_3H_3Cl_3O_3S$	6989-70-4	55.80
20.6500	(3-Chloropropyl)trimethoxysilane	$C_6H_{15}ClO_3Si$	2530-87-2	51.07
20.7965	4-Iodo-1-methyl-3-nitropyrazole	$C_4H_4IN_3O_2$	75092-34-1	58.69
20.8479	3-Methoxybenzoic acid, 2,4,6-trichlorophenyl ester	$C_{14}H_9Cl_3O_3$	1000325-55-6	58.77
21.0822	3-Chlorobenzamide	C_7H_6ClNO	618-48-4	54.74
21.2511	1,2-Benzenediol, o-(4-methoxybezoyl)-o'-(5-chlorovaleryl)-	$C_{19}H_{19}ClO_5$	1000325-98-7	71.95
21.3068	2,6-Difluoro-3-methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	$C_{15}H_8Cl_2F_2O_3$	1000343-76-0	54.41
21.4489	Benzamide, 2-chloro-N-phenyl-	$C_{13}H_{10}ClNO$	6833-13-2	68.60
21.7459	2-Propanol, 1-chloro-, phosphate (3:1)	$C_9H_{18}Cl_3O_4P$	13674-84-5	87.04
21.7609	2,2'-Oxybis(ethane-2,1-diyl) bis(3-chlorobenzoate)	$C_{18}H_{16}Cl_2O_5$	1000367-01-8	55.09
21.9559	Phenylacetic acid, 2,3-dichlorophenyl ester	$C_{14}H_{10}Cl_2O_2$	1000331-14-2	67.90
23.3962	1,1,7,7-Tetramethyl-4,4-divinyl-1,7-dichlorotrisilethylene	$C_{12}H_{26}Cl_2Si_3$	80153-58-8	65.75
24.3564	Ibomal-permethylated	$C_{12}H_{17}BrN_2O_3$	1000298-81-2	52.20
25.1894	2-Chloro-3-pyridinol	C_5H_4ClNO	6636-78-8	52.23
25.6243	Myclobutanil	$C_{15}H_{17}ClN_4$	88671-89-0	95.49
25.8090	Methanone, (4-chlorophenyl)(4-hydroxyphenyl)-	$C_{13}H_9ClO_2$	42019-78-3	55.35
26.0726	4,4'-Isopropylidene-bis(2-chlorophenol)	$C_{15}H_{14}Cl_2O_2$	79-98-1	57.57

26.0892	Benzene, 2-bromo-3,4-dimethoxy-1-(phenoxymethyl)-	$C_{15}H_{15}BrO_3$	164228-20-0	55.91
28.1982	Terephthalic acid, 3,4-dichlorophenyl ethyl ester	$C_{16}H_{12}Cl_2O_4$	1000323-68-5	53.85
29.9417	2-Fluoro-6-trifluoromethylbenzoic acid, 2,4,5-trichlorophenyl ester	$C_{14}H_5Cl_3F_4O_2$	1000357-30-9	54.30
31.2917	6-Fluoro-2-trifluoromethylbenzoic acid,4-chloro-2-methylphenyl ester	$C_{15}H_9ClF_4O_2$	1000343-74-1	63.07
31.5870	Anthraergostatetraenol p-chlorobenzoate	$C_{35}H_{45}ClO_2$	105818-38-0	52.50
31.6512	2-Piperidinoethyl p-chlorobenzoate	$C_{14}H_{18}ClNO_2$	15483-41-7	56.44
32.0100	Ethane, 1,2-dibromo-1-chloro-	$C_2H_3Br_2Cl$	598-20-9	53.70
32.2784	Pyrazole, 3-(2-bromoethyl)-	$C_5H_7BrN_2$	211738-72-6	55.36
33.1274	Benzamide, N-(4-chloro-3-trifluoromethylphenyl)-2,6-dimethoxy-	$C_{16}H_{13}ClF_3NO_3$	316128-21-9	55.60
33.2747	6-Fluoro-2-trifluoromethylbenzoic acid, 2,3-dichlorophenyl ester	$C_{14}H_6Cl_2F_4O_2$	1000343-74-3	59.72

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Table S4. Retention time (RT), compound name, formula, CAS number, and match factor of unknown DBPs identified from C-JS dust after the disinfection process.

Component RT	Compound Name	Formula	CAS#	Match Factor
1.6575	Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl-	$C_{18}H_{22}BrNO$	3565-72-8	78.83
2.0030	Propane, 1-(t-butylthio)-2-(chloroacetoxy)-	$C_9H_{17}ClO_2S$	1000161-43-7	55.82
2.1335	Acrolein, 2-chloro-	C_3H_3ClO	683-51-2	58.22
2.1811	Ethyne, chloro-	C_2HCl	593-63-5	54.77
2.5008	Propane, 1-chloro-2-nitro-	$C_3H_6ClNO_2$	2425-66-3	59.08
2.5437	Methane, dichloronitro-	$CHCl_2NO_2$	7119-89-3	72.08
2.7464	Chloromethanesulfonyl-dichloromethanesulfonyl chloride	$C_2H_2Cl_4O_4S_2$	66629-57-0	60.13
2.8153	Methane, oxybis[dichloro-	$C_2H_2Cl_4O$	20524-86-1	84.76
6.2665	Tetrachloroethylene	C_2Cl_4	127-18-4	89.54
7.0633	2-Butyne, 1,4-dibromo-	$C_4H_4Br_2$	2219-66-1	54.94
7.3205	Benzene, chloro-	C_6H_5Cl	108-90-7	95.36
7.3413	Acetonitrile, chlorodifluoro-	C_2ClF_2N	421-05-6	60.35
7.3906	Methane, bromofluoro-	CH_2BrF	373-52-4	65.24
7.7658	4-Chloro-3-buten-2-one	C_4H_5ClO	1000432-33-8	52.88
7.9128	2-Chloro-5-iodobenzoic acid	$C_7H_4ClIO_2$	19094-56-5	54.13
8.3266	Carbonochloridothioic acid, S-methyl ester	C_2H_3ClOS	18369-83-0	52.06
8.4935	Bicyclo[4.2.0]octa-1,3,5-triene, 7-bromo-	C_8H_7Br	21120-91-2	56.26

9.3688	1-Propene, 1,2,3,3-tetrachloro-	$C_3H_2Cl_4$	20589-85-9	59.98
10.0454	Propanal, 2-chloro-2-methyl-	C_4H_7ClO	917-93-1	56.43
10.0582	1-Bromo-1-phenylpropane	$C_9H_{11}Br$	2114-36-5	65.82
10.1031	2-Cyclohexene-1,4-dione, 5,6-dichloro-2,3-dimethyl-, 1-oxime, o-benzoyl-	$C_{15}H_{13}Cl_2NO_3$	324051-55-0	74.90
10.4762	2-Chloropropionyl chloride	$C_3H_4Cl_2O$	08-09-23	61.69
10.5189	Acetonitrile, dichlorofluoro-	C_2Cl_2FN	353-82-2	53.23
10.6627	Cyclopropene, 1-chloro-2,3,3-trifluoro-	C_3ClF_3	24921-89-9	67.68
11.1037	2-Chloro-6-fluorophenol, isopropyl ether	$C_9H_{10}ClFO$	1000395-35-5	55.13
11.5144	Furan, 3-bromo-	C_4H_3BrO	22037-28-1	71.33
11.6832	2-Chloroisobutylanilide	$C_{10}H_{12}ClNO$	5434-52-6	51.05
11.7699	Benzeneethanamine, N-(3-chloropropyl)-3,4-dimethoxy-N-methyl-	$C_{14}H_{22}ClNO_2$	36770-74-8	52.91
12.8534	Clindamycin	$C_{18}H_{33}ClN_2O_5S$	18323-44-9	71.96
13.2348	p-Chloroaniline	C_6H_6ClN	106-47-8	73.26
13.2960	4-Chlorobenzoic acid, 4-nitrophenyl ester	$C_{13}H_8ClNO_4$	1000307-76-2	62.04
13.9789	Carbon Tetrachloride	CCl_4	56-23-5	87.14
14.5949	1,2-Benzenediol, o-(2-chloropropionyl)-o'-(4-ethylbenzoyl)-	$C_{18}H_{17}ClO_4$	1000325-96-9	74.32
14.9087	Benzenamine, 2,5-dichloro-	$C_6H_5Cl_2N$	95-82-9	68.72
14.9091	Propanil	$C_9H_9Cl_2NO$	709-98-8	57.13
15.7082	Succinic acid, 2,4,6-trichlorophenyl 2-naphthylmethyl ester	$C_{21}H_{15}Cl_3O_4$	1000390-01-0	77.89

15.8462	Trichloroacetic acid, 6-ethyl-3-octyl ester	$C_{12}H_{21}Cl_3O_2$	1000282-57-4	72.62
15.8788	4-Chlorobenzyl mercaptan	C_7H_7ClS	6258-66-8	66.01
15.9360	Succinic acid, 2-chloro-6-fluorophenyl 2-naphthylmethyl ester	$C_{21}H_{16}ClFO_4$	1000390-00-6	65.76
16.0581	Trichloromethane	$CHCl_3$	67-66-3	82.58
18.0396	Propane, 1,1'-oxybis[2,3-dichloro-	$C_6H_{10}Cl_4O$	7774-68-7	56.11
18.1610	3-Chloro-2-fluorobenzoic acid, 4-nitrophenyl ester	$C_{13}H_7ClFNO_4$	1000357-73-4	65.80
18.4716	Glutaric acid, naphth-2-ylmethyl 2,4-dichlorophenyl ester	$C_{22}H_{18}Cl_2O_4$	1000391-86-1	53.95
19.2547	Benzenecarboimidic acid, N-(3,4-dichlorobenzyloxy)-	$C_{14}H_{11}Cl_2NO_2$	107517-57-7	64.85
19.3487	Tioconazole	$C_{16}H_{13}Cl_3N_2OS$	65899-73-2	51.26
20.1350	d-Proline, N-(2-chloroethoxycarbonyl)-, octadecyl ester	$C_{26}H_{48}ClNO_4$	1000328-23-5	58.94
20.7617	Dodecane, 1-iodo-	$C_{12}H_{25}I$	4292-19-7	72.58
21.0647	1,2-Benzenediol, o-(4-methoxybezoyl)-o'-(5-chlorovaleryl)-	$C_{19}H_{19}ClO_5$	1000325-98-7	72.52
21.7101	Tetradecane, 1-iodo-	$C_{14}H_{29}I$	19218-94-1	68.56
21.7144	N-(2-Bromophenyl)-N'-methylsuccinamide	$C_{11}H_{13}BrN_2O_2$	300726-02-7	54.78
21.7440	2-Propanol, 1-chloro-, phosphate (3:1)	$C_9H_{18}Cl_3O_4P$	13674-84-5	81.71
21.7579	2,2'-Oxybis(ethane-2,1-diyl) bis(3-chlorobenzoate)	$C_{18}H_{16}Cl_2O_5$	1000367-01-8	57.87
22.8326	Benzamide, N-(3-chlorophenyl)-2-fluoro-	$C_{13}H_9ClFNO$	1000307-08-1	52.72

22.8807	Phthalic acid, (2-chlorocyclohexyl)methyl isobutyl ester	$C_{19}H_{25}ClO_4$	1000315-35-1	74.97
22.8923	Cycloheptane, bromo-	$C_7H_{13}Br$	2404-35-5	60.75
23.6666	Succinic acid, 2,2-dichloroethyl tetrahydrofurfuryl ester	$C_{11}H_{16}Cl_2O_5$	1000390-71-6	53.67
24.0103	2-Chloro-1-(2,3-dihydro-1,4-benzodioxin-6-yl)ethanone	$C_{10}H_9ClO_3$	1000411-42-2	53.40
24.0337	Benzene, 1-fluoro-2-iodo-	C_6H_4FI	348-52-7	53.63
24.1922	Phosphonous dichloride, [[chloro(1,1-dimethylethyl)phosphino]methyl]-	$C_5H_{11}Cl_3P_2$	87648-08-6	51.54
24.8710	Ethanone, 2-chloro-1,2-diphenyl-	$C_{14}H_{11}ClO$	447-31-4	70.16
24.9001	Decane, 1-iodo-	$C_{10}H_21I$	2050-77-3	69.75
26.0400	4-(2-Chloroethyl)naphthalen-1-ol	$C_{12}H_{11}ClO$	40847-82-3	57.26
26.1824	4-Hydroxy-N-[2-(4-(bromoethenyl)-2-thiazolyl)ethyl] butanamide	$C_{11}H_{15}BrN_2O_2S$	1000302-00-8	52.66
26.2673	Tetracosane, 1-iodo-	$C_{24}H_{49}I$	1000406-32-0	74.87
26.4937	2-Fluoro-6-trifluoromethylbenzoic acid, 4-chlorophenyl ester	$C_{14}H_7ClF_4O_2$	1000357-69-7	65.72
26.8706	Phthalic acid, 4-chloro-2-methoxybenzyl octyl ester	$C_{24}H_{29}ClO_5$	1000382-84-2	57.50
26.8838	Chamigran-7-en-9-ol, 2,10-dibromo-3-chloro-	$C_{15}H_{23}Br_2ClO$	1000139-03-8	51.85
26.8949	3,4-Dibromo-1-pentene	$C_5H_8Br_2$	91198-48-0	51.04
26.9347	6-Fluoro-2-trifluoromethylbenzoic acid,4-chloro-2-methylphenyl ester	$C_{15}H_9ClF_4O_2$	1000343-74-1	60.39

27.0018	(1R,2R,4S)-2-(6-Chloropyridin-3-yl)-7-methyl-7-azabicyclo[2.2.1]heptane	$C_{12}H_{15}ClN_2$	232615-84-8	52.28
27.7753	Carbonic acid, ethyl 2,5-dichlorophenyl ester	$C_9H_8Cl_2O_3$	1000325-56-8	56.22
27.8519	6-Fluoro-2-trifluoromethylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	$C_{15}H_6Cl_2F_4O_3$	1000343-74-4	66.83
28.5427	1,3-Dioxolane, 2-(bromomethyl)-2-(2-methylphenyl)-	$C_{11}H_{13}BrO_2$	24169-43-5	63.11
29.0098	4-(4-Iodo-benzyloxy)-3,5-dimethoxy-benzaldehyde	$C_{16}H_{15}IO_4$	1000274-94-0	52.34
29.1459	Isophthalic acid, propyl 2,4,6-trichlorophenyl ester	$C_{17}H_{13}Cl_3O_4$	1000344-56-6	63.22
29.5635	Cyclopropanecarboxylic acid, 3-(2,2-dichloroethenyl)-2,2-dimethyl-, (3-phenoxyphenyl)methyl ester, trans-	$C_{21}H_{20}Cl_2O_3$	61949-77-7	67.51
29.9877	Benzamide, N-[(4-chlorophenyl)methyl]-2-fluoro-N-(2-furanylmethyl)-	$C_{19}H_{15}ClFNO_2$	1000350-60-3	50.67
30.1917	Acetic acid, dichloro-, methyl ester	$C_3H_4Cl_2O_2$	116-54-1	51.32
30.2068	Sebacic acid, di(4-iodobenzyl) ester	$C_{24}H_{28}I_2O_4$	1000380-63-2	63.34
30.4647	2-Thiophenecarboxylic acid, 4-chlorophenyl ester	$C_{11}H_7ClO_2S$	1000308-06-2	58.84
30.4868	Benzamide, 2-fluoro-N-(2-fluorobenzoyl)-N-(5-chloro-2-methoxyphenyl)-	$C_{21}H_{14}ClF_2NO_3$	1000340-08-7	50.05
30.6647	(1,3,3,3-Tetrachloro-2-fluoro-1-propenyl)pentafluorobenzene	$C_9Cl_4F_6$	127722-98-9	51.03
30.6803	Dichloroacetic acid, 1-adamantylmethyl ester	$C_{13}H_{18}Cl_2O_2$	1000282-97-7	64.35
30.9977	1-Propene, 1,2,3-trichloro-, (Z)-	$C_3H_3Cl_3$	13116-57-9	53.68

31.1703	Phosphoric acid, 2-chloroethenyl dimethyl ester	$C_4H_8ClO_4P$	17027-41-7	51.31
32.3895	Chlorotrifluoromethane	$CClF_3$	75-72-9	57.81
33.8299	2-(1-Bromo-2-methoxy-2-(4-methoxyphenyl)ethyl)-3-phenyl-quinazolin-4(3H)-one	$C_{24}H_{21}BrN_2O_3$	77143-52-3	52.91
34.4099	Ethane, 1,2-dibromo-	$C_2H_4Br_2$	106-93-4	60.59
36.0024	Eicosane, 1-iodo-	$C_{20}H_{41}I$	1000406-31-8	55.35

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Table S5. Retention time (RT), compound name, formula, CAS number, and match factor of unknown DBPs identified from W-BR dust after the disinfection process.

Component RT	Compound Name	Formula	CAS#	Match Factor
1.8192	Carbonic acid, 2-chloroethyl 2-methoxyethyl ester	$C_6H_{11}ClO_4$	1000331-45-9	53.19
2.0326	Acetonitrile, chlorodifluoro-	C_2ClF_2N	421-05-6	65.70
2.4409	2-Propenoyl chloride	C_3H_3ClO	814-68-6	64.59
2.5140	Methanesulfonyl chloride	CH_3ClO_2S	124-63-0	77.88
2.6314	Trichloroacetamidoxime	$C_2H_3Cl_3N_2O$	2533-67-7	55.97
2.6314	1,2-Benzenediol, O-dichloroacetyl-O'-(3-methylbut-2-enoyl)-	$C_{13}H_{12}Cl_2O_4$	1000330-46-9	67.28
2.6372	2,2,2-Trifluoroethyl trichloromethanesulfonate	$C_3H_2Cl_3F_3O_3S$	23199-56-6	54.35
2.6494	1,3-Dioxolane, 2-(3-bromo-3-buten-1-yl)-	$C_7H_{11}BrO_2$	333961-98-1	50.33
2.8184	Succinic acid, monochloride 2-methylpent-3-yl ester	$C_{10}H_{17}ClO_3$	1000349-40-1	55.70
2.8303	Methane, oxybis[dichloro-	$C_2H_2Cl_4O$	20524-86-1	68.00
2.8306	Carbon Tetrachloride	CCl_4	56-23-5	56.46
2.9872	Ethylamine, 2-((p-bromo-.alpha.-methyl-.alpha.-phenylbenzyl)oxy)-N,N-dimethyl-	$C_{18}H_{22}BrNO$	3565-72-8	82.92
3.7075	Methane, bromodichloro-	$CHBrCl_2$	75-27-4	74.70
7.2862	Methane, bromofluoro-	CH_2BrF	373-52-4	70.06
7.3501	Benzene, chloro-	C_6H_5Cl	108-90-7	95.93

8.2669	Ethane, 1-chloro-2-isocyanato-	C_3H_4ClNO	1943-83-5	60.67
8.2898	1,2-Benzenediol, o-(6-chlorohexanoyl)-	$C_{12}H_{15}ClO_3$	1000325-91-6	51.07
10.0228	3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	$C_{15}H_{10}Cl_2O_3$	1000331-26-9	84.12
10.1062	Acetaldehyde, chloro-	C_2H_3ClO	107-20-0	52.09
10.5493	4-Chlorobutyric acid, 3,4-dimethylphenyl ester	$C_{12}H_{15}ClO_2$	1000357-38-7	76.53
10.6274	1-Buten-3-yne, 1-chloro-, (E)-	C_4H_3Cl	20374-91-8	50.56
10.6903	Cyclohexene, 3-bromo-	C_6H_9Br	1521-51-3	59.71
11.3597	3-Chloro-1-(chloromethyl)-1,2,4-triazole	$C_3H_3Cl_2N_3$	1000444-92-4	61.40
11.6617	Ethane, 1,2-dibromo-	$C_2H_4Br_2$	106-93-4	68.26
11.7901	Sebacic acid, di(2-chlorophenethyl) ester	$C_{26}H_{32}Cl_2O_4$	1000416-23-5	57.09
12.0891	Oxazole, 2-(dichloromethyl)-4,5-dihydro-4,4-dimethyl-	$C_6H_9Cl_2NO$	65029-00-7	55.03
12.1969	Propane, 2-chloro-2-nitro-	$C_3H_6ClNO_2$	594-71-8	64.06
12.4318	2-Propanol, 1,3-dibromo-	$C_3H_6Br_2O$	96-21-9	53.15
12.4697	Succinic acid, 2-chloro-6-fluorophenyl 4-methoxybenzyl ester	$C_{18}H_{16}ClFO_5$	1000389-69-2	64.19
12.4866	Succinic acid, 3-chlorophenyl 3-phenylprop-2-en-1-yl ester	$C_{19}H_{17}ClO_4$	1000391-04-7	50.97
12.8658	Trichloromethane	$CHCl_3$	67-66-3	82.30
13.2171	p-Chloroaniline	C_6H_6ClN	106-47-8	74.43

13.3221	Benzamide, 4-chloro-, o-dichloroacetyloxime	$C_9H_7Cl_3N_2O_2$	1000262-86-8	67.90
13.3325	Benzeneacetonitrile, .alpha.-bromo-	C_8H_6BrN	5798-79-8	53.24
13.5355	Nicotinic acid, 3,4-dichlorophenyl ester	$C_{12}H_7Cl_2NO_2$	1000307-95-1	52.87
13.9765	Phenol, 2,4-dichloro-	$C_6H_4Cl_2O$	120-83-2	70.30
14.0728	Ethane, 2,2-dichloro-1,1,1-trifluoro-	$C_2HCl_2F_3$	306-83-2	53.87
14.2193	[1,4']Bipiperidinyl-4'-carboxamide, 1'-(4-chlorobenzenesulfonyl)-	$C_{17}H_{24}ClN_3O_3S$	1000303-77-0	61.06
14.4430	2,4,4-Trimethyl-1-pentanol, chlorodifluoroacetate	$C_{10}H_{17}ClF_2O_2$	1000447-27-2	70.52
14.9303	Thiophene, 2,5-dichloro-	$C_4H_2Cl_2S$	3172-52-9	55.93
15.1825	Phenyltrimethylammonium chloride	$C_9H_{14}ClN$	138-24-9	63.71
15.6986	Succinic acid, 2,4,6-trichlorophenyl 2-naphthylmethyl ester	$C_{21}H_{15}Cl_3O_4$	1000390-01-0	68.87
15.9564	ethane, 2,2'-[oxybis(methylenesulfonyl)]bis[1-chloro-	$C_6H_{12}Cl_2O_5S_2$	1000402-13-7	53.84
16.5130	1-Chloroethynyl-4-ethynylbenzene	$C_{10}H_5Cl$	1000283-76-6	51.75
16.5657	Phenol, 2,4,5-trichloro-	$C_6H_3Cl_3O$	95-95-4	72.56
16.5720	Benzamide, 2-fluoro-N-(2-fluorobenzoyl)-N-(5-chloro-2-methoxyphenyl)-	$C_{21}H_{14}ClF_2NO_3$	1000340-08-7	64.76
16.6368	1,3-Benzenediol, o-(2-chlorobenzoyl)-o'-(2-methoxybenzoyl)-	$C_{21}H_{15}ClO_5$	1000330-77-8	55.01

16.8628	Silane, diethyl(2-bromo-4-fluorophenoxy)tridecyloxy-	$C_{23}H_{40}BrFO_2Si$	1000363-18-4	68.04
16.9827	Chloroxylenol	C_8H_9ClO	88-04-0	50.57
17.4571	1H-Purine, 2,6-dichloro-	$C_5H_2Cl_2N_4$	5451-40-1	63.91
17.6112	Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-	$C_2Cl_2F_4$	76-14-2	53.53
18.1788	o-Cresol, 3,4,6-trichloro-	$C_7H_5Cl_3O$	643-14-1	63.62
18.1789	Acetamide, 2,2-dichloro-N-butyl-N-(hept-2-yl)-	$C_{13}H_{25}Cl_2NO$	1000437-56-9	51.79
18.3824	6-Bromohexanoic acid, 4-methoxyphenyl ester	$C_{13}H_{17}BrO_3$	1000307-61-6	56.20
18.9064	2,6-Difluoro-3-methylbenzoic acid, 2,3-dichlorophenyl ester	$C_{14}H_8Cl_2F_2O_2$	1000343-75-9	50.65
19.0471	Propane, 1,2-dibromo-	$C_3H_6Br_2$	78-75-1	62.37
19.2251	Erythro-2,3-dibromopentane	$C_5H_{10}Br_2$	22415-74-3	53.18
19.4808	Phthalic acid, 4-bromophenyl ethyl ester	$C_{16}H_{13}BrO_4$	1000309-80-8	73.16
19.7613	3,5-Dimethyl-2,4,6-trichlorophenol	$C_8H_7Cl_3O$	6972-47-0	81.23
20.3378	Carbinoxamine	$C_{16}H_{19}ClN_2O$	486-16-8	53.61
20.4655	Thiazolidine-2,4-dione, 5-(4-chlorobenzylidene)-3-(2,6-dimethylmorpholin-4-ylmethyl)-	$C_{17}H_{19}ClN_2O_3S$	1000276-76-6	56.16
20.6977	4-Fluorobenzoic acid, 2,4,6-trichlorophenyl ester	$C_{13}H_6Cl_3FO_2$	1000325-53-1	70.43
21.2323	Dodecane, 1-iodo-	$C_{12}H_{25}I$	4292-19-7	56.78

21.3601	Tri(2-chloroethyl) phosphate	$C_6H_{12}Cl_3O_4P$	115-96-8	95.62
21.3980	p-Toluic acid, 3-chloroprop-2-enyl ester	$C_{11}H_{11}ClO_2$	1000292-51-0	68.68
21.7436	2-Propanol, 1-chloro-, phosphate (3:1)	$C_9H_{18}Cl_3O_4P$	13674-84-5	96.26
22.6624	.beta.-Chloro-para-fluoropropiophenone	C_9H_8ClFO	347-93-3	56.13
22.8913	Dotriacontane, 1-iodo-	$C_{32}H_{65}I$	1000406-32-4	81.88
23.2159	1,3-Dimethyl-5-pylazolyl-2,4-dichlorobenzoate	$C_{12}H_{10}Cl_2N_2O_2$	1000425-21-6	72.95
24.3056	l-Leucine, N-(2-chloroethoxycarbonyl)-N-methyl-, octadecyl ester	$C_{28}H_{54}ClNO_4$	1000328-52-8	51.84
25.2303	Glutaric acid, naphth-2-ylmethyl 2-bromo-4-fluorophenyl ester	$C_{22}H_{18}BrFO_4$	1000391-84-2	57.61
25.8106	Benzene, (1,2-dibromoethyl)-	$C_8H_8Br_2$	93-52-7	66.51
26.7400	Tris(1,3-dichloroisopropyl)phosphate	$C_9H_{15}Cl_6O_4P$	13674-87-8	51.83
26.9283	4-Fluoro-2-trifluoromethylbenzamide, N-(3-chlorophenyl)-	$C_{14}H_8ClF_4NO$	1000358-09-1	52.24
27.4978	Acetic acid, chlorodifluoro-, ethyl ester	$C_4H_5ClF_2O_2$	383-62-0	50.63
27.5740	4,4'-Isopropylidene-bis(2-chlorophenol)	$C_{15}H_{14}Cl_2O_2$	79-98-1	59.98
28.9388	2,3,4,5-Tetrafluorobenzyl alcohol, bromomethyldimethylsilyl ether	$C_{10}H_{11}BrF_4OSi$	1000376-06-0	50.96
29.0003	10,10-Dichloro-9-oxa-10-sila-9,10-dihydrophenanthrene	$C_{12}H_8Cl_2OSi$	20470-98-8	50.81
29.1636	Ethane, iodo-	C_2H_5I	75-03-6	61.03

31.3333	Isophthalic acid, di(2-bromo-4-fluorophenyl) ester	$C_{20}H_{10}Br_2F_2O_4$	1000344-40-4	59.99
32.3861	Triacontane, 1-iodo-	$C_{30}H_{61}I$	1000406-32-3	72.66
32.8111	3-Biphenyl-4-yl-N-[2-(4-chloro-phenoxy)-ethyl]-acrylamide	$C_{23}H_{20}ClNO_2$	1000295-37-2	51.43
32.8307	Dimethomorph	$C_{21}H_{22}ClNO_4$	110488-70-5	56.18
33.9390	Isophthalic acid, 2,6-dichlorophenyl ethyl ester	$C_{16}H_{12}Cl_2O_4$	1000344-61-8	52.74
35.3224	2-Propanone, 1,1,3,3-tetrachloro-	$C_3H_2Cl_4O$	632-21-3	50.78
36.0132	Tetracosane, 1-iodo-	$C_{24}H_{49}I$	1000406-32-0	64.17
37.7466	Succinic acid, 2,2-dichloroethyl tetrahydrofurfuryl ester	$C_{11}H_{16}Cl_2O_5$	1000390-71-6	63.24

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Table S6. Retention time (RT), compound name, formula, CAS number, and match factor of original organics identified from R-QH dust.

Component RT	Compound Name	Formula	CAS#	Match Factor
7.3143	Benzene, chloro-	C_6H_5Cl	108-90-7	96.85
7.3152	Pyridine, 3-chloro-	C_5H_4ClN	626-60-8	74.82
11.5285	(4-Fluorophenyl)carbamic acid, 2-chloro-4-fluorophenyl ester	$C_{13}H_8ClF_2NO_2$	1000305-16-6	61.66
16.9601	Decane, 1-iodo-	$C_{10}H_{21}I$	2050-77-3	81.03
19.9563	2-Piperidinone, N-[4-bromo-n-butyl]-	$C_9H_{16}BrNO$	195194-80-0	63.13
20.9969	Octadecane, 1-chloro-	$C_{18}H_{37}Cl$	3386-33-2	60.77
21.2130	Tetradecane, 1-chloro-	$C_{14}H_{29}Cl$	2425-54-9	57.22
22.2489	Hexadecane, 1-iodo-	$C_{16}H_{33}I$	544-77-4	79.75
22.5881	2,4,6-Trimethyliodobenzene	$C_9H_{11}I$	4028-63-1	55.65
23.3277	Octadecane, 1-iodo-	$C_{18}H_{37}I$	629-93-6	54.04
24.2780	1-(3-bromophenyl)-2-(piperazin-1-yl)propan-1-one	$C_{13}H_{17}BrN_2O$	1000455-10-5	50.34
24.5647	2,4-Diamino-6-[p-chlorophenyl]pteridine	$C_{12}H_9ClN_6$	30146-32-8	59.99
25.4385	1,2-Benzenediol, o-(2-bromopropionyl)-o'-(4-ethylbenzoyl)-	$C_{18}H_{17}BrO_4$	1000325-97-0	54.84
26.2663	Isophthalic acid, butyl 4-chloro-3-methylphenyl ester	$C_{19}H_{19}ClO_4$	1000344-59-1	50.18
27.2829	Bromophos	$C_8H_8BrCl_2O_3PS$	2104-96-3	57.80
27.4940	6-Chloro-2-ethyl-4-phenylquinoline	$C_{17}H_{14}ClN$	22609-10-5	64.11

27.8431	5-(4-Iodo-phenylamino)-thiazolidine-2,4-dione	$C_9H_7IN_2O_2S$	1000278-36-9	55.66
28.5396	Bumetrizole	$C_{17}H_{18}ClN_3O$	05-11-96	78.65
28.8557	Phthalic acid, 2-(4-bromophenoxy)ethyl hexyl ester	$C_{22}H_{25}BrO_5$	1000382-89-5	52.74
28.8721	Phosphorochloridic acid, diisopropyl ester	$C_6H_{14}ClO_3P$	2574-25-6	59.62
29.2720	Pyridine, 4-(biphenyl-4-yloxy)-3-chloro-2,5,6-trifluoro-	$C_{17}H_9ClF_3NO$	1000302-84-4	55.63
29.8077	3,5-Diiodosalicylaldehyde	$C_7H_4I_2O_2$	2631-77-8	50.03
29.9017	(4-Amino-furazan-3-yl)-[4-(2-chloro-4-nitro-phenyl)-piperazin-1-yl]-methanone oxime	$C_{13}H_{14}ClN_7O_4$	1000294-85-9	50.68
30.1527	Butane, 1,4-diiodo-	$C_4H_8I_2$	628-21-7	54.29
30.4827	4-Hydroxy-2',3',5',6'-tetrachlorobiphenyl, trimethylsilyl ether	$C_{15}H_{14}Cl_4OSi$	1000447-78-9	52.40
30.8199	2-[(3-Iodo-benzylidene)-amino]-4,5,6,7-tetrahydro-benzo[b]thiophene-3-carbonitrile	$C_{16}H_{13}IN_2S$	330682-81-0	55.43
30.8960	5-(p-Aminophenyl)-4-(m-iodophenyl)-2-thiazolamine	$C_{15}H_{12}IN_3S$	94064-19-4	63.83
31.1828	3-(4-Dimethylaminobenzylideneamino)-7-chloro-10-methyl-phenothiazine	$C_{22}H_{20}ClN_3S$	57824-42-7	55.58

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Table S7. Retention time (RT), compound name, formula, CAS number, and match factor of original organics identified from C-JS dust.

Component RT	Compound Name	Formula	CAS#	Match Factor
7.0157	Methanesulfonyl chloride	CH_3ClO_2S	124-63-0	79.76
7.2959	Methane, bromofluoro-	CH_2BrF	373-52-4	70.04
14.9555	5-Chloro-1,3-dimethyl-1H-pyrazole-4-sulfonic acid, 2-methyl-5-trifluoromethyl-2H-pyrazol-3-yl ester	$C_{10}H_{10}ClF_3N_4O_3S$	1000265-45-4	51.51
16.9446	9-(3-Chlorobenzyl)-9-hydroxy-3,6,10,10-tetramethyl-9,10-dihydrophenanthrene	$C_{25}H_{25}ClO$	142728-03-8	55.47
19.0926	trans-(2-Chlorovinyl)dimethylethoxysilane	$C_6H_{13}ClOSi$	1000139-71-5	70.47
23.5899	Dodecane, 1-iodo-	$C_{12}H_{25}I$	4292-19-7	82.73
27.5793	Docosane, 1-iodo-	$C_{22}H_{45}I$	1000406-31-9	72.28
29.0966	Tetracosane, 1-iodo-	$C_{24}H_{49}I$	1000406-32-0	79.66
30.5065	Hexacosane, 1-iodo-	$C_{26}H_{53}I$	1000406-32-1	72.47
31.2170	Chlorotrifluoromethane	$CClF_3$	75-72-9	56.90
32.0454	Tetradecane, 1-iodo-	$C_{14}H_{29}I$	19218-94-1	69.76

Table S8. Retention time (RT), compound name, formula, CAS number, and match factor of original organics identified from W-BR dust.

Component RT	Compound Name	Formula	CAS#	Match Factor
7.3051	Benzene, chloro-	C_6H_5Cl	108-90-7	95.93
7.3248	.beta.-Chloroethylurea	$C_3H_7ClN_2O$	6296-42-0	51.09
11.5143	(4-Fluorophenyl)carbamic acid, 2-chloro-4-fluorophenyl ester	$C_{13}H_8ClF_2NO_2$	1000305-16-6	63.85
14.2317	Benzyltributylammonium chloride	$C_{19}H_{34}ClN$	23616-79-7	65.49
20.5810	2,4,4-Trimethyl-1-pentanol, chlorodifluoroacetate	$C_{10}H_{17}ClF_2O_2$	1000447-27-2	70.01
21.3298	Tri(2-chloroethyl) phosphate	$C_6H_{12}Cl_3O_4P$	115-96-8	93.25
21.7194	2-Propanol, 1-chloro-, phosphate (3:1)	$C_9H_{18}Cl_3O_4P$	13674-84-5	93.11
22.7608	Silane, (iodomethyl)trimethyl-	$C_4H_{11}ISi$	4206-67-1	63.18
23.3132	4-Chlorobutanoic anhydride	$C_8H_{12}Cl_2O_3$	1000333-91-1	61.48
23.3478	Phthalic acid, 2,2-dichloroethyll octyl ester	$C_{18}H_{24}Cl_2O_4$	1000356-92-9	52.71
23.8310	1,4-Dibromoheptane	$C_7H_{14}Br_2$	42474-23-7	58.59
24.2202	4-Bromobutyric acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester	$C_9H_9BrF_8O_2$	1000354-68-2	51.62
24.5460	2,4-Diamino-6-[p-chlorophenyl]pteridine	$C_{12}H_9ClN_6$	30146-32-8	64.37
24.5998	Benzene, 1-iodo-3-(trifluoromethyl)-	$C_7H_4F_3I$	401-81-0	52.28
25.1611	Propionamide, N-(4-chlorophenyl)-3-(4-methylpiperazin-1-yl)-	$C_{14}H_{20}ClN_3O$	1000271-68-3	58.00
27.4433	6-Chloro-2-ethyl-4-phenylquinoline	$C_{17}H_{14}ClN$	22609-10-5	55.02

27.8524	2,4(1H,3H)-Pyrimidinedione, 6-iodo-5-methyl-	$C_5H_5IN_2O_2$	31458-38-5	50.52
28.4922	Bumetrizole	$C_{17}H_{18}ClN_3O$	05-11-96	78.28
28.5561	Benzenamine, 2-iodo-	C_6H_6IN	615-43-0	51.22
29.3626	Acetic acid, 2-(5-trifluoromethyl-1-methyl-3-pyrazolyloxy)-, 2,4-dichlorophenyl ester	$C_{13}H_9Cl_2F_3N_2O_3$	1000268-22-1	60.57
29.6426	Propane, 1,3-diiodo-	$C_3H_6I_2$	627-31-6	57.05
30.8380	5-(p-Aminophenyl)-4-(m-iodophenyl)-2-thiazolamine	$C_{15}H_{12}IN_3S$	94064-19-4	50.87
31.3503	3,4,4,4-Tetrafluoro-3-trifluoromethyl-1-iodobutene	$C_5H_2F_7I$	243139-61-9	50.48
31.9831	Silane, (3-chlorophenyloxy)dimethylheptadecyloxy-	$C_{25}H_{45}ClO_2Si$	1000346-88-7	62.05
32.0465	2-[(3-Iodo-benzylidene)-amino]-4,5,6,7-tetrahydro-benzo[b]thiophene-3-carbonitrile	$C_{16}H_{13}IN_2S$	330682-81-0	66.13
32.4697	6-Fluoro-2-trifluoromethylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	$C_{15}H_6Cl_2F_4O_3$	1000343-74-4	59.49
36.7249	1,3-Benzenediol, o-chloroacetyl-o'-cyclohexanecarbonyl-	$C_{15}H_{17}ClO_4$	1000330-67-0	53.68
38.2878	Cyclopropane, 1-butyl-2-iodo-	$C_7H_{13}I$	55682-97-8	53.13

References

(1) Zhang, L.; Xu, L.; Graham, N.; Yu, W. Z., Unraveling Membrane Fouling Induced by Chlorinated Water Versus Surface Water: Biofouling Properties and Microbiological Investigation. *Engineering-Prc* **2022,** *15*, 154-164.

(2) Liu, M. J.; Graham, N.; Xu, L.; Zhang, K.; Yu, W. Z., Bubbleless aerated-biological activated carbon as a superior process for drinking water treatment in rural areas. *Water Res.* **2023,** *240*.