

ORIGINAL RESEARCH ARTICLE

Comparative analysis of chlorination byproduct formation in galvanized iron and high-density polyethylene pipes using low-cost filtration techniques

Supplementary File

Supplementary Note: Equations used to quantify disinfection byproducts

TTHMs + THAAs = Prominent chlorine DBPs (I)

After running the standard calibration, the internal standard peak area was used to construct a linear calibration curve. A linear calibration curve is calculated using the following equation:

$$C_{\text{extract}} = \frac{\text{Measured peak area}}{\text{Peak area of internal standard}} \times (m + b) \quad \text{(II)}$$

where:

- (i) m is the slope of the calibration curve, indicating gas chromatography sensitivity to changes in disinfection byproduct (DBP) concentration.
- (ii) b is the intercept that accounts for the baseline offset.

To determine the concentration of DBPs in the original water sample, the following equation was used:

$$C_{\text{water}} = \frac{C_{\text{extract}} \times V_{\text{extract}}}{V_{\text{water}}} \quad \text{(III)}$$

where:

- (i) C_{water} is the concentration of DBPs in the water sample ($\mu\text{g/L}$)
- (ii) C_{extract} is the concentration in the extract ($\mu\text{g/L}$)
- (iii) V_{extract} is the volume of extraction solvent (mL)
- (iv) V_{water} is the volume of water sample (mL or L)

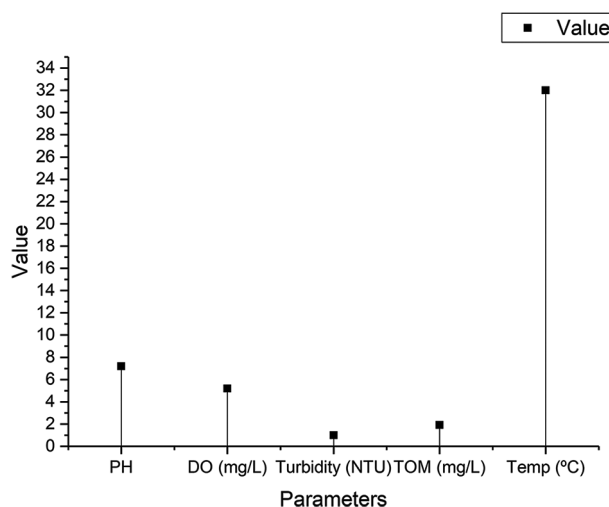


Figure S1. Physicochemical parameters of water samples collected from Zone 1

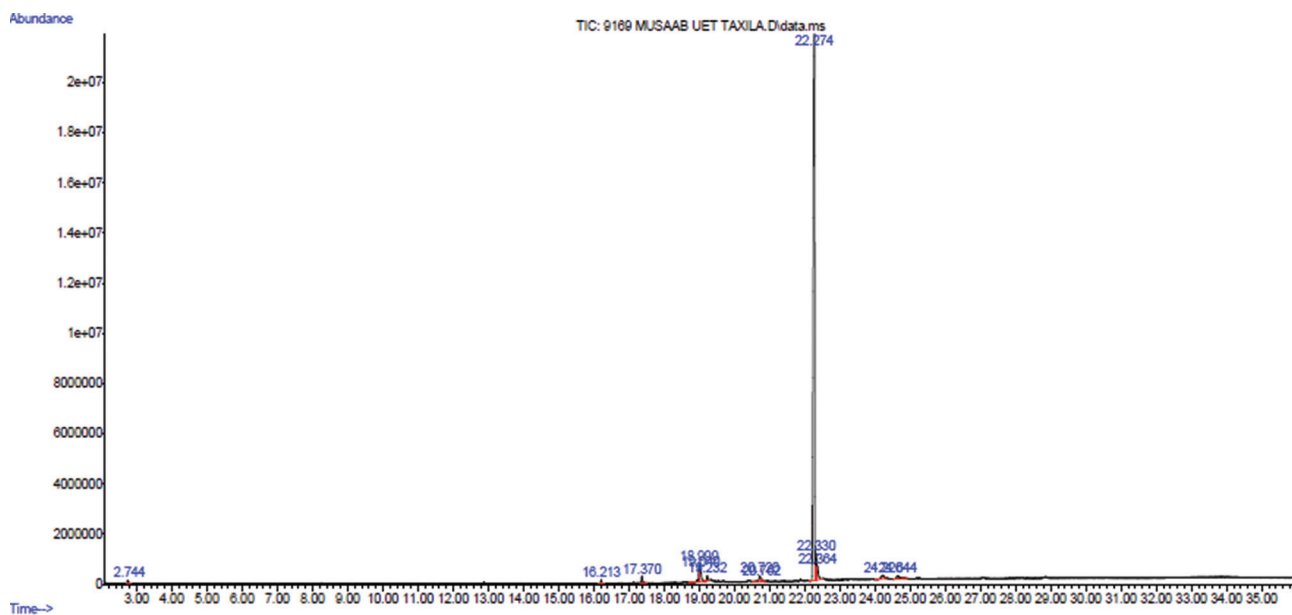


Figure S2. Chromatogram of the water sample treated with a 0.2 mg/L chlorine dosage

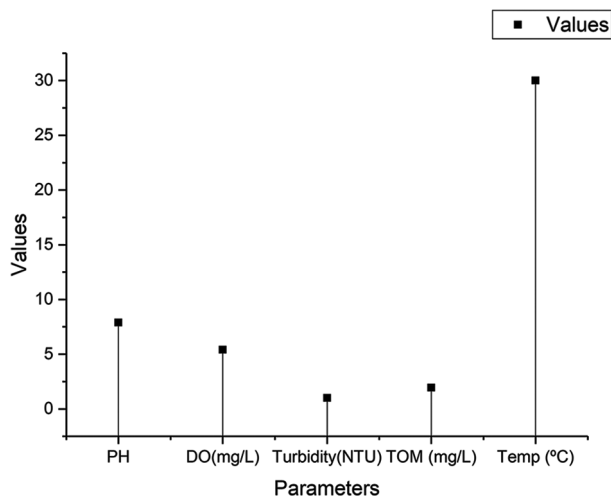


Figure S3. Physicochemical parameters of water samples collected from Zone 2 at a chlorine dosage of 1.8 mg/L

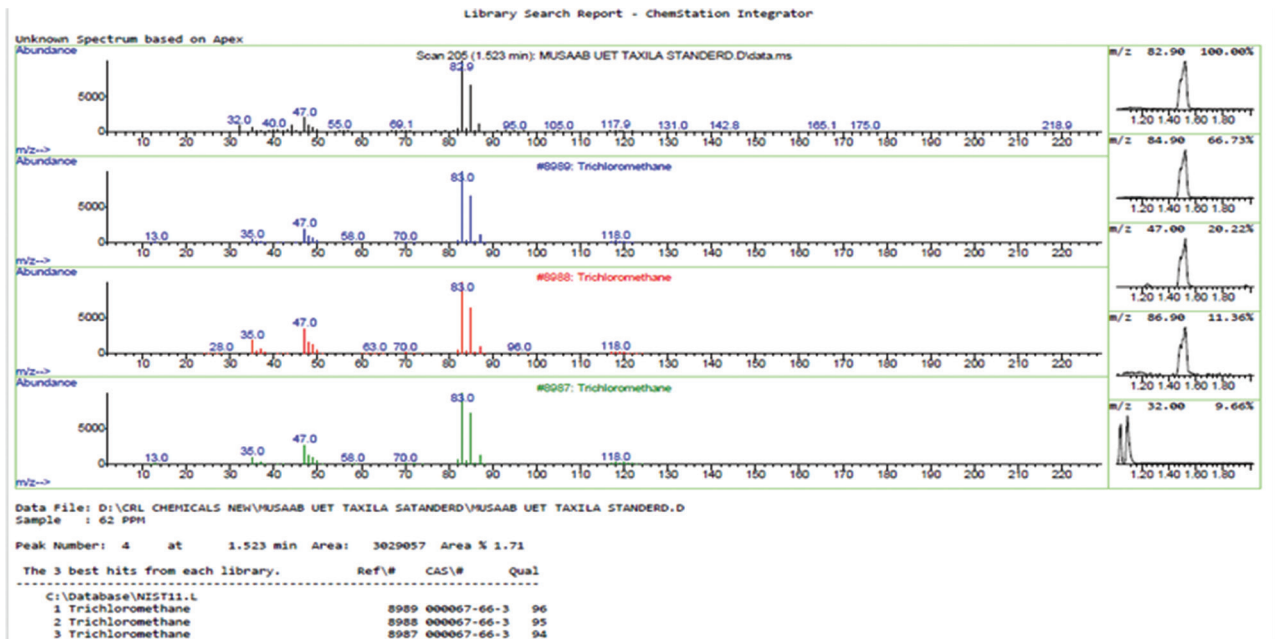


Figure S4. Mass spectrum of trichloromethane detected in the galvanized iron pipe water samples at a chlorine dosage of 1.8 mg/L

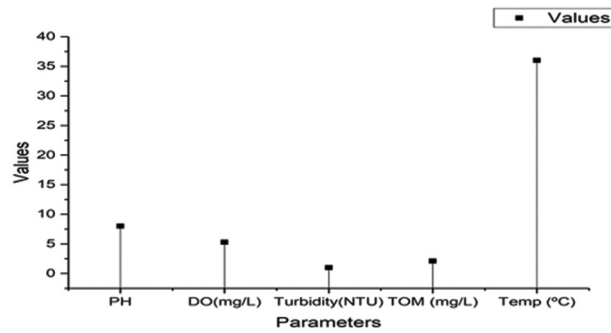


Figure S5. Physicochemical parameters of water samples collected from Zone 3 at a chlorine dosage of 2.4 mg/L

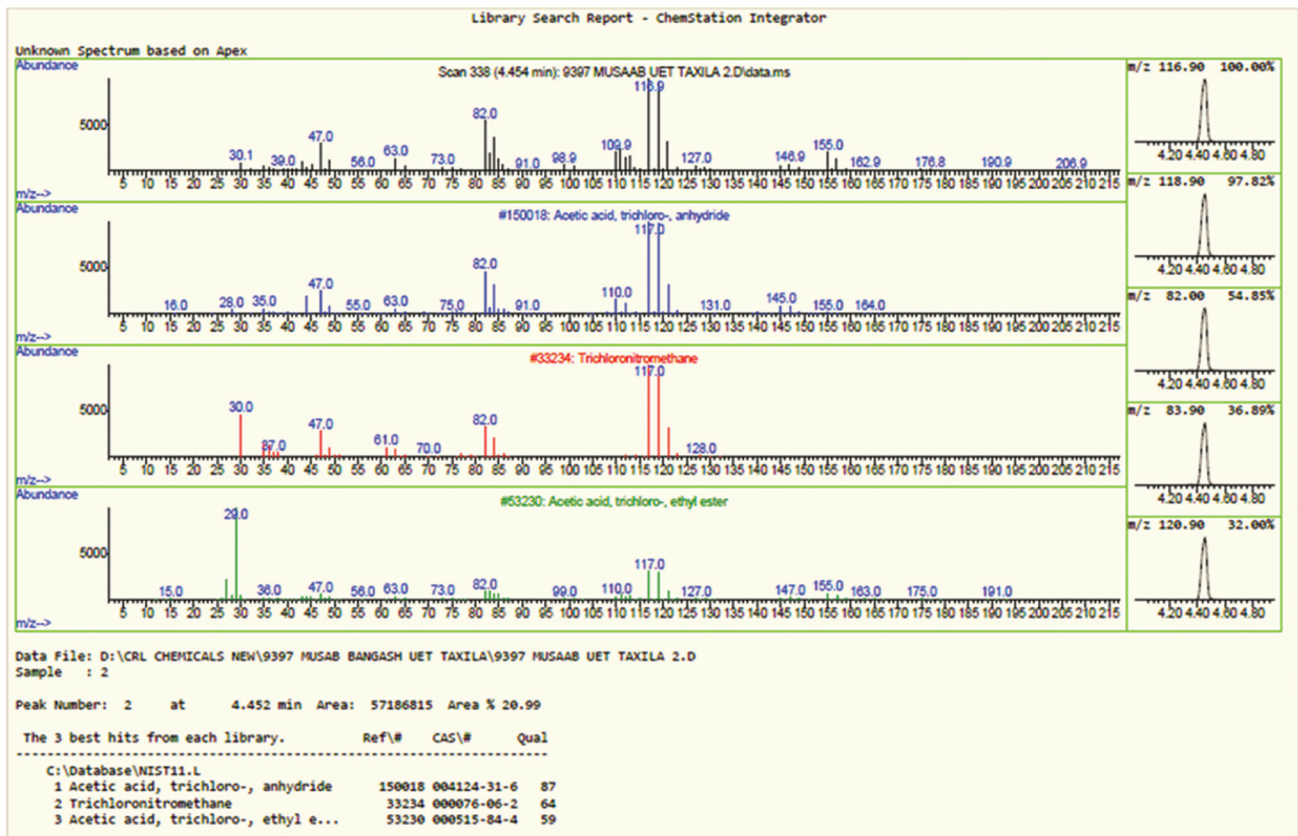


Figure S6. Mass spectra of chlorination disinfection byproducts detected in the galvanized iron pipe water samples at a chlorine dosage of 2.4 mg/L

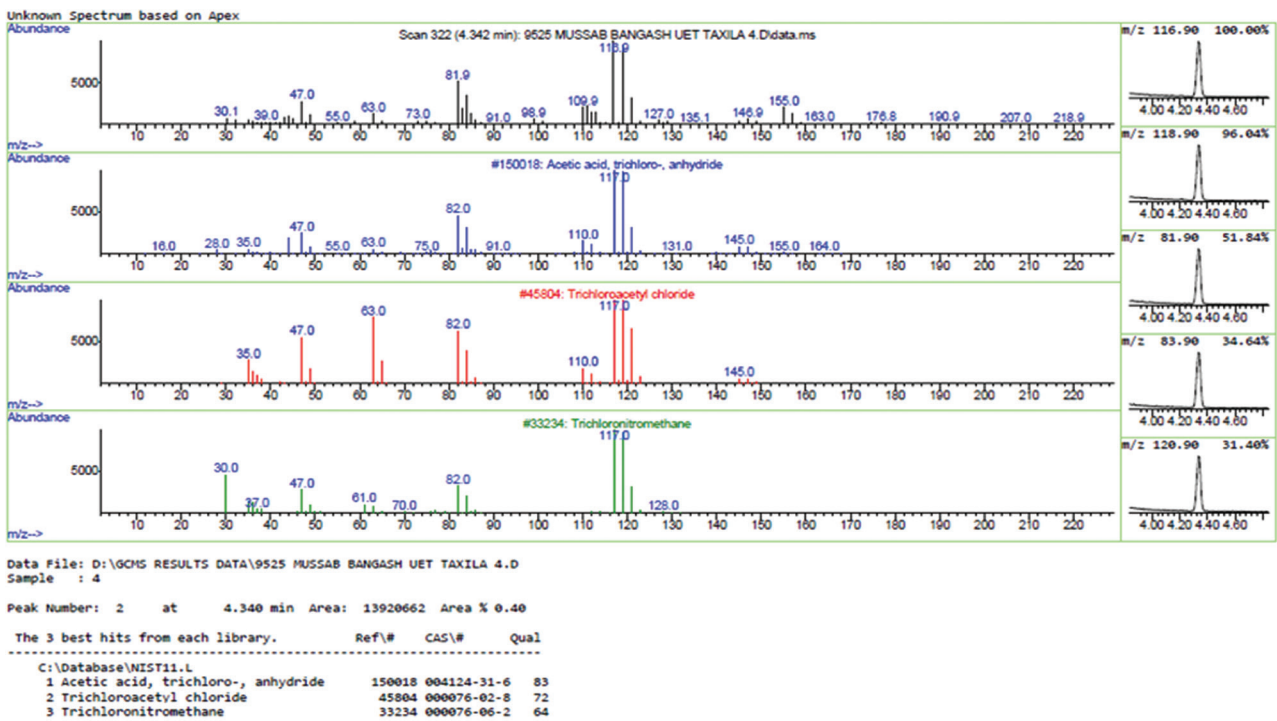


Figure S7. Mass spectra of chlorination disinfection byproducts detected in the high-density polyethylene pipe water samples at a chlorine dosage of 2.4 mg/L

Table S1. Analytical conditions for the gas chromatography-mass spectrometry analysis of disinfection byproducts

No.	Nomenclature	Details
1	Run time	36 min
2	Post-run time	0 min
3	Oven temperature	70°C
4	Hold time	3 min
5	Post-run	50°C
6	Temperature rate	10°C/min
7	Equilibrium time	2 min
8	Maximum temperature	300°C
9	Slow fan	Disabled
10	Mode	Split
11	Heater	250°C
12	Pressure	8.805 psi
13	Jet cleaning	No cleaning
14	Solvent delay	2 min
15	Scanning	Normal
16	Total flow	24 mL/min
17	Septum purge	3 mL/min
18	Gas saver	Off
19	Split ratio	20:1
20	Split flow	20mL/min
21	Thermal annex (initial)	280°C
22	Post-run	0°C
23	Column 1 flow	On
24	Initial (post-run)	1mL/min
25	Column	DB-1
26	Length	25 m×0.250 mm×0.25 μm
27	Gas used	Helium
28	Scanning low mass	30
29	Scanning high mass	650
30	Threshold	150

Table S2. Retention times of compounds detected (excluding prominent disinfection byproducts) in the galvanized iron pipe water samples at a chlorine dosage of 0.2 mg/L

No.	IUPAC name	Retention time
1	1-butanol, 3-methyl-, acetate	2.74 min
2	Phthalic acid, isobutyl octyl ester	16.21 min
3	n-Hexadecanoic acid	17.37 min
4	Oleic acid	18.99 min
5	9-Octadecenoic acid, (E)-	19.04 min
6	Octadecanoic acid	19.232 min
7	Cis-13-eicosenoic acid	20.720 min
8	Cis-11-eicosenoic acid	20.726 min
9	Diisooctyl phthalate	22.274 min
10	Erucic acid	22.330 min
11	Erucic acid	22.364 min
12	1, 2-bis (trimethylsilyl) benzene	24.22 min
13	Erucic acid	24.644 min

Abbreviation: IUPAC: International Union of Pure and Applied Chemistry.

Table S3. Retention times of compounds detected (including prominent disinfection byproducts) in the galvanized iron pipe water samples at 1.8 mg/L chlorine dosage

No.	IUPAC name	Retention time
1	Benzeneethanamine, N-methyl-	1.04 min
2	Acetic acid, hydroxy-	1.100 min
3	7, 11-Hexadecadienal	1.195 min
4	Trichloromethane	1.52 min
5	Hexadecanoic acid, methyl ester	19.03 min
6	n-Hexadecanoic acid	19.380 min
7	9, 12-Octadecadienoic acid (Z, Z)-	20.584 min
8	8-Octadecenoic acid, methyl ester	20.667 min
9	9,12-Octadecadienoic acid (Z, Z)-	20.930 min
10	9-Octadecenoic acid, (E)-	21.01 min
11	Octadecanoic acid	21.243 min

Abbreviation: IUPAC: International Union of Pure and Applied Chemistry.

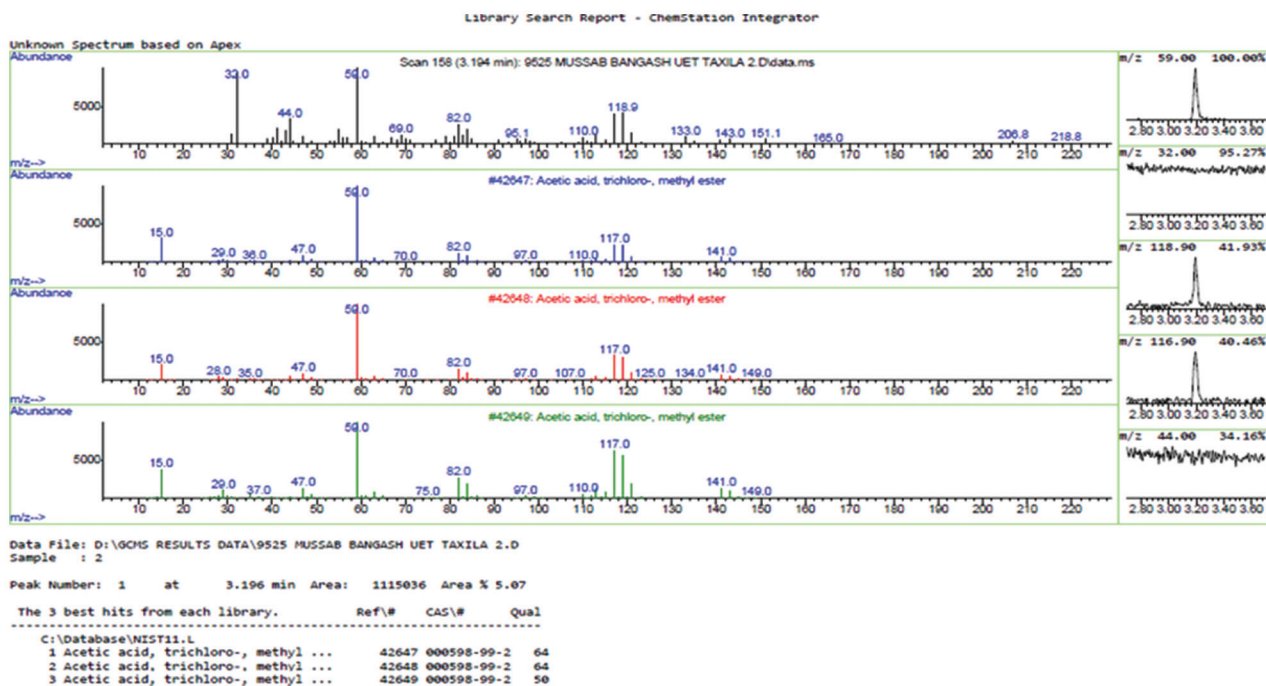


Figure S8. Mass spectra of chlorination disinfection byproducts detected in the galvanized iron pipe water samples after treatment with the first filtration media

Table S4. Retention times of compounds detected (including prominent disinfection byproducts) in the galvanized iron pipe water samples at 2.4 mg/L chlorine dosage

No.	IUPAC name	Retention time
1	Acetic acid, trichloro-, methyl...	3.329 min
2	Acetic acid, trichloro-, anhydride, trichloromethane	4.452 min
3	1,3-dioxolane, 2-methyl-2-phenyl-	10.170 min
4	Phenol, 2,4-bis (1,1-dimethylethyl)-	12.515 min
5	7,9-Di-tert-butyl-1-oxaspiro (4,5...	16.774 min
6	n-Hexadecanoic acid	17.424 min
7	Hexadecanoic acid, ethyl ester	17.738 min
8	9,12-Octadecadienoic acid (Z, Z)-	18.972 min
9	Oleic acid	20.930 min
10	9-Octadecenoic acid, (E)-	19.046 min
11	Octadecanoic acid	19.281 min
12	Octadecanoic acid, ethyl ester	19.569 min
13	Bis (2-ethylhexyl) phthalate	22.279 min

Abbreviation: IUPAC: International Union of Pure and Applied Chemistry.

Table S5. Retention times of detected compounds (including prominent disinfection byproducts) in the high-density polyethylene pipe water samples at 2.4 mg/L chlorine dosage

No.	IUPAC name	Retention time
1	Acetic acid, trichloro-, methyl...	3.370 mins
2	Acetic acid, trichloro-, anhydride, Trichloronitromethane	4.340 min
3	Acetic acid, trichloro-, anhydride	6.120 min
4	Phthalic anhydride	9.181 min
5	Hexadecanoic acid, methyl ester	16.935 min
6	n-Hexadecanoic acid	17.288 min
7	9-Octadecenoic acid, methyl ester	18.565 min
8	Methyl stearate	18.829 min
9	Bis (2-ethylhexyl) phthalate	22.127 min

Abbreviation: IUPAC: International Union of Pure and Applied Chemistry.

Table S6. Retention times of detected compounds at 2.4 mg/L chlorine dosage in the galvanized iron pipe water samples after treatment with sand media (first filtration setup)

No.	IUPAC name	Retention time
1	Acetic acid, trichloro-, methyl...	3.196 min
2	Fumaric acid, propyl trans-hex-3...	8.182 min
3	Phenol, 3,5-bis (1,1-dimethylethyl)-	13.364 min
4	7,9-Di-tert-butyl-1-oxaspiro (4,5...	16.622 min
5	4-Methyl-5-phenyl-imidazol-2 (3H)...	18.941 min
6	Phenethylamine, N-hexyl-	19.460 min
7	Tricyclo[4.3.1.1 (3,8)]undecane-1...	22.132 min
8	Tetrasiloxane, decamethyl-	23.463 min
9	1,2-Benzisothiazol-3-amine tert-butyl dimethylsilyl	23.805 min
10	1,2-Benzisothiazol-3-amine tert-butyl dimethylsilyl	23.965 min
11	1,2-Benzisothiazol-3-amine tert-butyl dimethylsilyl	24.155 min
12	1,2-Benzisothiazol-3-amine tert-butyl dimethylsilyl	27.256 min

Abbreviation: IUPAC: International Union of Pure and Applied Chemistry.

Table S7. Retention times of detected compounds at 2.4 mg/L chlorine dosage in the galvanized iron pipe water samples after treatment with granular activated carbon media (second filtration setup)

No.	IUPAC name	Retention time
1	Cyclotrisiloxane, hexamethyl-	2.337 min
2	Oxime-, methoxy-phenyl-	3.201 min
3	Phenol, 3,5-bis (1,1-dimethylethyl)-	3.201 min
4	Cyclotetrasiloxane, octamethyl-	5.19 min
5	1,2-Benzenedicarboxylic acid, bi...	17.050 min
6	9,12-Octadecadienoic acid (Z, Z)-...	18.620 min
7	7-Octadecenoic acid, methyl ester	18.685 min
8	Methyl stearate	18.946 min
9	Cyclohexane, 1,3,5-triphenyl-	21.455 min
10	13-Docosenoic acid, methyl ester...	22.066 min
11	Erucic acid	22.339 min
12	Silane, dimethyl (dimethyl (2,6-di...	22.947 min
13	1,4-Benzenedicarboxylic acid, bi...	23.944 min

Abbreviation: IUPAC: International Union of Pure and Applied Chemistry.