

「Promising Solution_Application Note」

Analysis of Chlorine Disinfection Byproducts in Drinking Water by ChroZen GC/MS in Reference to EPA 551.1

• GC/MS Application



Abstract

Water is a vital resource for a human being that is used not only for drinking water but the industrial purpose in various fields. Chemical disinfectants, such as chlorine, ozone, and chlorine dioxide are commonly used for the disinfection of water in most water purification plants. When these react with naturally occurring organic matter in water, the disinfection byproducts (DBPs) like trihalomethanes (THMs), haloacetic acids (HAAs) and haloacetonitriles (HANs) are produced, which cause adverse health effects on humans.

For these reasons, DBPs are strictly regulated in drinking water and certain places like swimming pools while ensuring data reliability.

In this study, the analysis of chlorine disinfection byproducts was determined by gas chromatograph-mass spectrometer referring to EPA 551.1.

Applying our promising solution, it was able to reduce the consumption of solvents and samples, and increase productivity and reproducibility with automated workflow rather than using liquid-liquid extraction (LLE).

Instruments and Software

• ChroZen GC/MS System

Item	Description	Part No.
Oven	ChroZen GC Mainframe Assembly for Mass Spectrometer	6701012500
Inlet	Capillary Inlet Assembly for ChroZen GC	6701012550
Detector	ChroZen MS for ChroZen GC incl. built-in turbomolecular pump - Single Quadropole - EI source (UEIS: Ultimated Efficiency Ion Source) - Turbo pump(240 L/sec) - Include fore pump and spares kit - Higher Sensitivity (S/N for OFN 2500:1)	6901012110
Autosampler	ChroZen PAL LSI system for liquid injection	6501011590
	Mounting Kit for ChroZen GC	PAL3-Kit-YI6700
CDS	YL-Clarity software for single instrument of YL GC	5301011020
	MS module of YL-Clarity	5301011180
	Autosampler control of YL-Clarity	5301011040
	Library(NIST/EPA/NIH 2020 edition)-350,643 spectra	9781119750291
Column	DB-5MS (30m, 0.2 mm, 0.33 μ m)	-
ACC	Start-up kit (Installation kit)	1601011110
	Big Universal Trap, 1/8" fttgs, Helium	RMSH-2
	Sample Rack for 15 vials of 10/20mL, pack of 3 pcs Vials are not included	PAL3-Kit-VT15
	YL PAL System Vial 20CV, 20ml Clear Glass with Label, designed for the YL PAL Autosampler. 75.5x22.5mm, 1st Class Hydrolytic Glass with flat finish for better sealing, fits ND18 Screw Caps, Pk of 100 Pcs	Vial-20-ND18-CG-100
	YL PAL System Screw Cap 10CV and 20CV, designed for the YL PAL Autosampler. ND18 Magnetic, Silver, Silicone white/PTFE blue Septa 1.5mm, Pk of 100 pcs	Cap-ND18-St-SP15-100

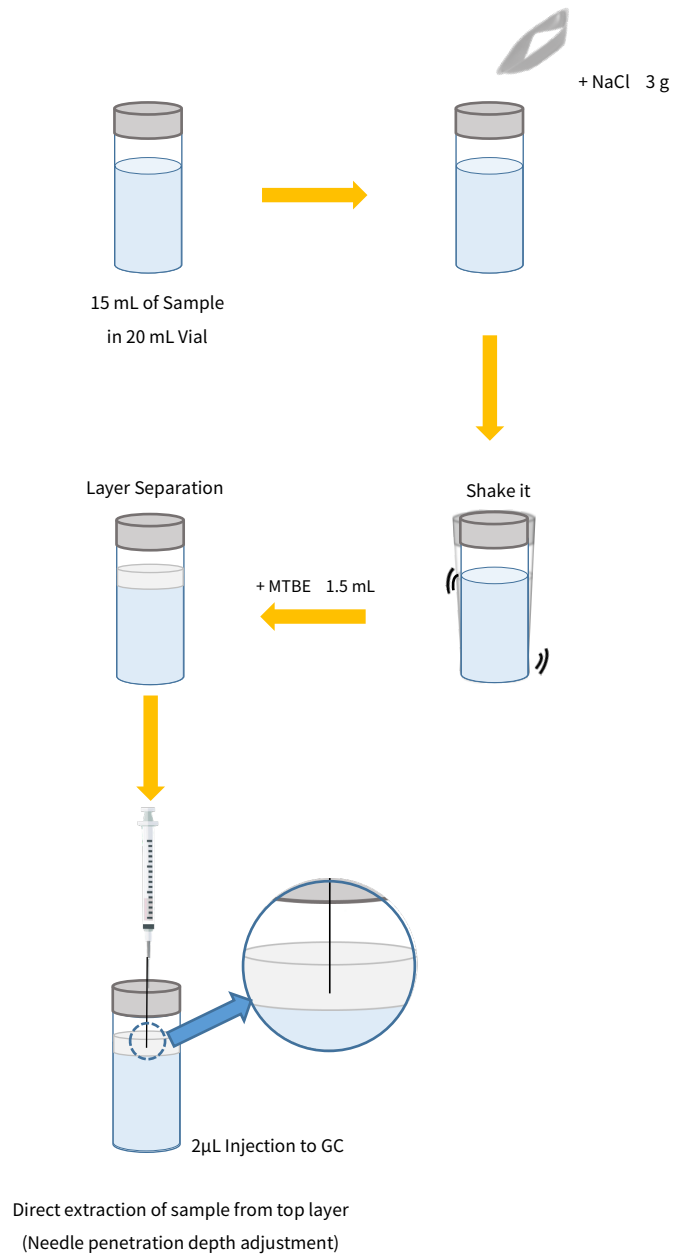
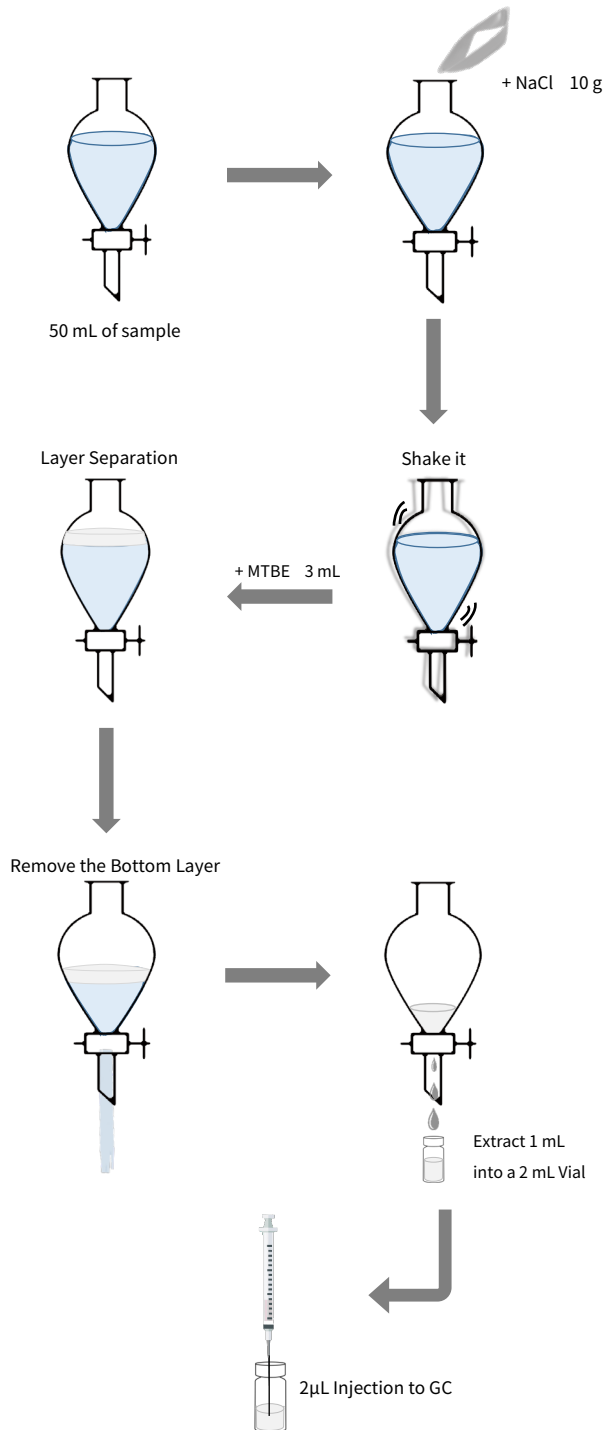
[Reagent]

- Methyl-t-butyl ether (MTBE)
- Sodium Chloride (NaCl) : ACS Reagent Grade

Comparison of Water Samples Preparation

Traditional LLE

Promising Solution



	Liquid-Liquid Extraction	YCM Promising Solution
Consumption of Sample, Reagent, Standard	██████████	██████████
Productivity	██████████	██████████



Fig 1. ChroZen GC/MS with PAL

Methods of Analysis

Table 2. GC/MS conditions

GC conditions	MS conditions
Column: DB-5 (30 m x 0.2 mm i.d. x 0.33 μ m)	Ion source 200°C, Transfer Line 280°C
Inlet: 1 mL/min, split ratio: 1/5, 200°C	
Oven temperature program: 35°C, 6min, 30°C/min to 250°C, 1min	
	Detection: SIM mode

Table 3. GC/MS chromatographic conditions

	Compound	Molecular Weight	Selected ions, m/z
1	Trichloroacetonitrile	147.55	82, 108, 110
2	Chloralhydrate	165.40	82, 84, 111
3	Dichloroacetonitrile	112.05	74, 82, 84
4	Dibromoacetonitrile	201.05	118, 120, 199
5	1,2-dibromo-3-chloropropane	236.58	75, 155, 157

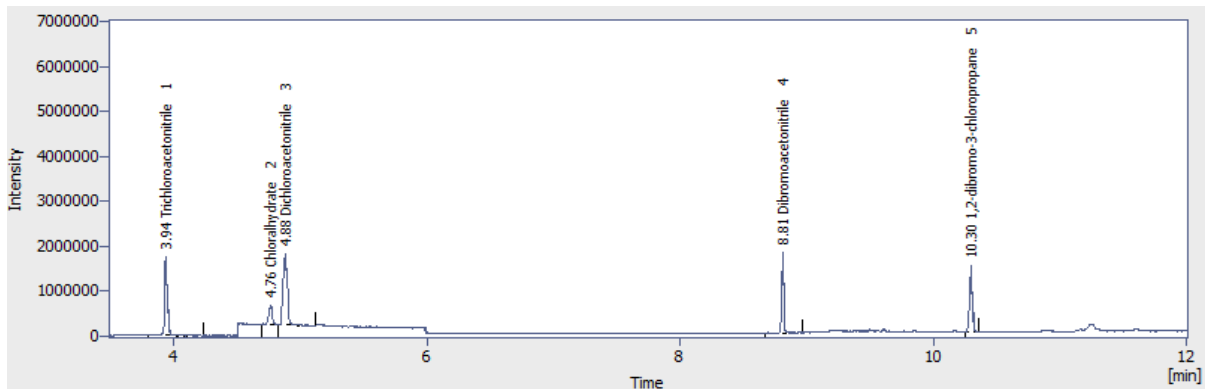


Fig 2. Chromatogram of 10 μ g/L STD

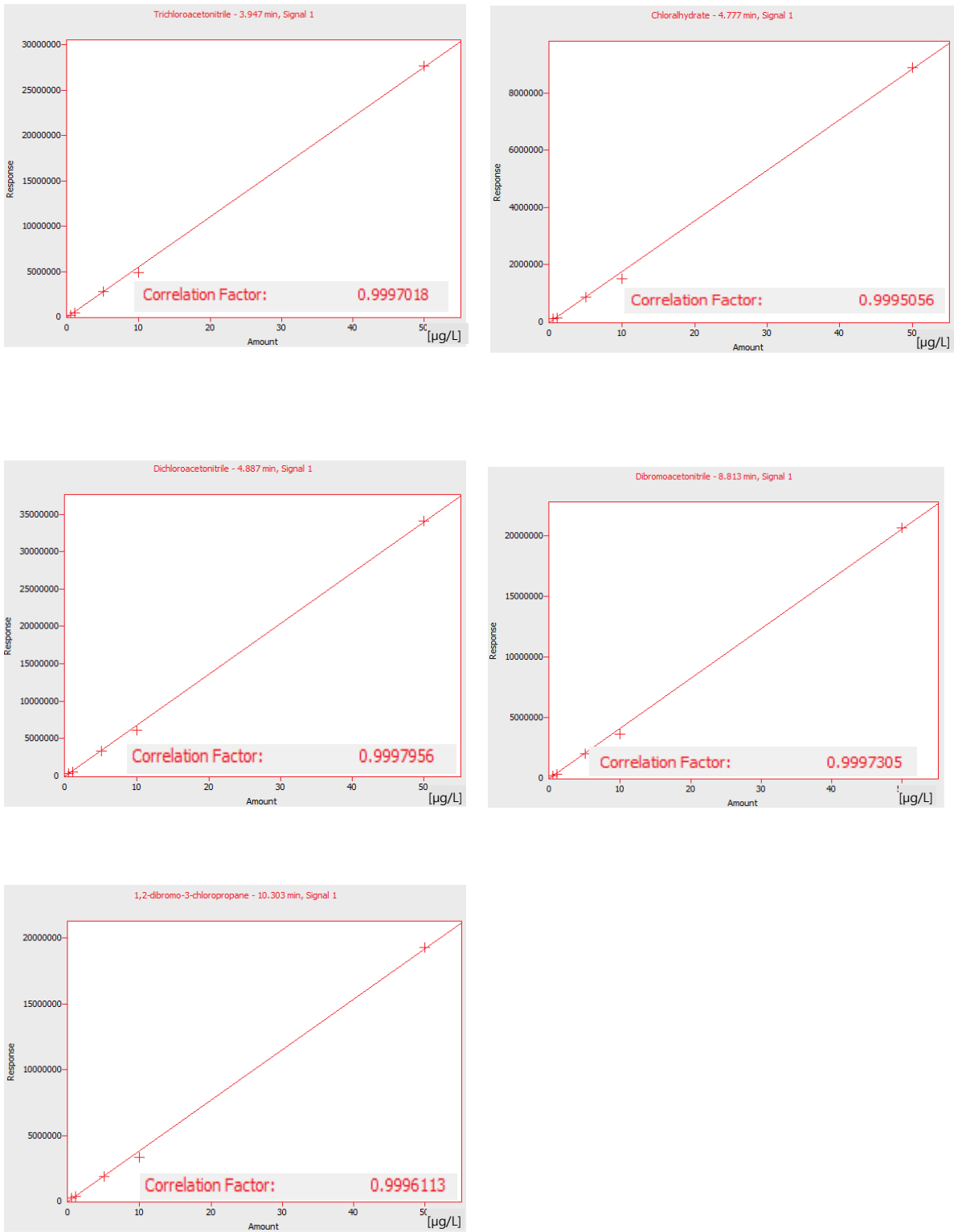


Fig 3. Calibration (0.5, 1, 5, 10, 50 µg/L)

Result

Table 4. Accuracy and Precison of Chlorine Disinfection By-products Analysis

Analyte	Sample name	Response	Calc. Conc ($\mu\text{g/L}$)	Accuracy (%)	Precision (%)
Trichloro-acetonitrile	QC-1	4842236.303	9.716	95.46	2.53
	QC-2	4738809.909	9.509		
	QC-3	4593895.463	9.218		
	QC-4	4853324.453	9.739		
Chloralhydrate	QC-1	1476660.553	9.512	95.34	2.76
	QC-2	1440173.387	9.277		
	QC-3	1536824.562	9.900		
	QC-4	1466366.978	9.446		
Dichloro-acetonitrile	QC-1	6144995.989	9.831	97.26	0.78
	QC-2	6052216.642	9.682		
	QC-3	6082033.713	9.730		
	QC-4	6039081.886	9.661		
Dibromo-acetonitrile	QC-1	3693745.643	9.895	94.98	3.12
	QC-2	3536894.462	9.474		
	QC-3	3426484.642	9.179		
	QC-4	3525737.178	9.445		
1,2-dibromo-3-chloropropane	QC-1	3275444.877	9.522	94.93	0.41
	QC-2	3250809.757	9.451		
	QC-3	3249920.379	9.448		
	QC-4	3271913.578	9.512		

Table 5. MDL(Method Detection Limit) & LOQ(Limit of Quantitation) of Chlorine Disinfection Byproducts

Analyte	QC Name	Data Conc.($\mu\text{g/L}$)	STDEV	MDL ($\mu\text{g/L}$)	LOQ ($\mu\text{g/L}$)
Trichloro-acetonitrile	MDL-1	4.978	0.0439	0.14	0.44
	MDL-2	4.942			
	MDL-3	5.033			
	MDL-4	4.917			
	MDL-5	4.966			
	MDL-6	4.900			
	MDL-7	4.940			
Chloralhydrate	MDL-1	4.960	0.0234	0.07	0.23
	MDL-2	4.981			
	MDL-3	4.966			
	MDL-4	4.948			
	MDL-5	4.976			
	MDL-6	4.971			
	MDL-7	4.912			
Dichloro-acetonitrile	MDL-1	4.899	0.0255	0.08	0.25
	MDL-2	4.967			
	MDL-3	4.955			
	MDL-4	4.947			
	MDL-5	4.946			
	MDL-6	4.916			
	MDL-7	4.965			
Dibromo-acetonitrile	MDL-1	4.936	0.0488	0.15	0.49
	MDL-2	4.861			
	MDL-3	4.980			
	MDL-4	4.847			
	MDL-5	4.951			
	MDL-6	4.932			
	MDL-7	4.943			
1,2-dibromo-3-chloropropane	MDL-1	4.929	0.0431	0.14	0.43
	MDL-2	4.877			
	MDL-3	4.896			

	MDL-4	4.933			
	MDL-5	4.991			
	MDL-6	4.978			
	MDL-7	4.972			

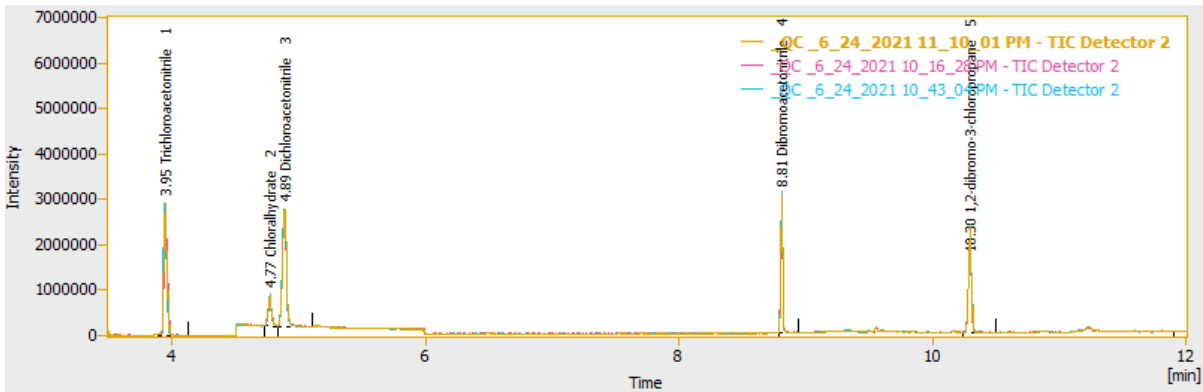
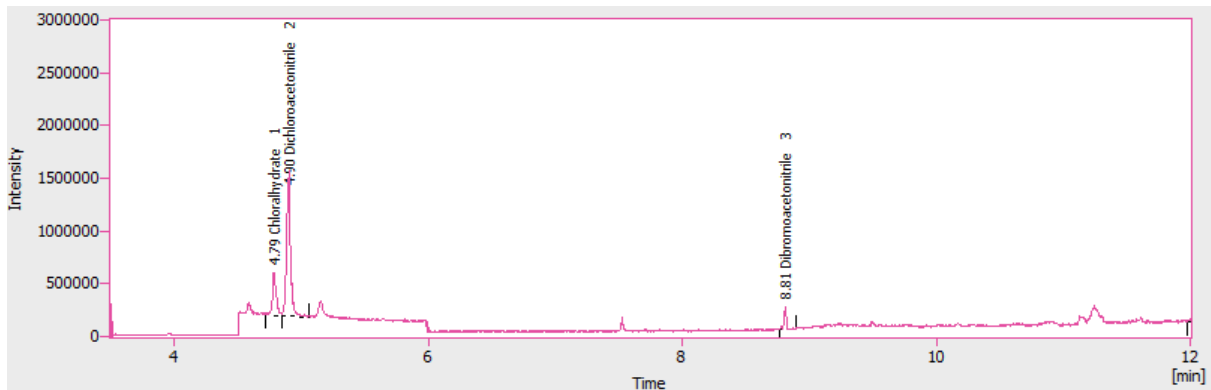


Fig 4. Overlaid-Chromatogram of 10 µg/L STD in 3 Consecutive Injections

Table 6. Analysis of Sample A & B

Sample name	Analyte	Calc. Conc (µg/L)
A	Trichloroacetonitrile	N.D.
	Chloralhydrate	4.898
	Dichloroacetonitrile	4.794
	Dibromoacetonitrile	0.657
	1,2-dibromo-3-chloropropane	N.D.
B	Trichloroacetonitrile	N.D.
	Chloralhydrate	11.518
	Dichloroacetonitrile	3.948
	Dibromoacetonitrile	0.671
	1,2-dibromo-3-chloropropane	N.D.

Sample A



Sample B

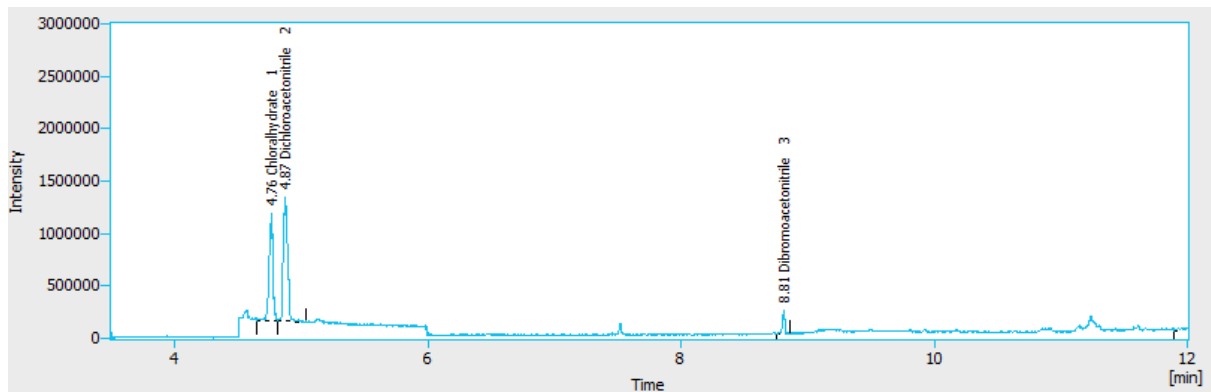


Fig 5. Chromatogram of Sample A & B

Conclusion

Analysis of chlorine disinfection byproducts was conducted by ChroZen GC/MS coupling with PAL system in reference to EPA 551.1. The linearity, accuracy and precision of all analytes were evaluated to verify the validity of analysis results. The accuracy was greater than 94 % and the precision resulted within 4%, of which analytes recoveries meet between 75% and 125% for accuracy and within 25% for precision. [Table 4]

The method detection limit (MDL) and the limit of quantitation (LOQ) were calculated according to the standard method. The LOQ was calculated 0.00044 mg/L for trichloroacetonitrile, 0.00023 mg/L for Chloralhydrate, 0.00025 mg/L for Dichloroacetonitrile, 0.00049 mg/L for Dibromoacetonitrile, and 0.00043 mg/L for 1,2-dibromo-3-chloropropane.

Sample A and B were collected from tap water in 2 different places. Trichloroacetonitrile and 1,2-dibromo-3-chloropropane were not detected in both samples and Chloralhydrate was detected in 4.9 µg/L and 11.5 µg/L each. [Fig 5][Table 6]

As a result, ChroZen GC/MS with PAL system

ensures that the data reliability of chlorine disinfection byproducts analysis and the indicated promising solution for sample preparation works successfully.

Reference

- Standard method for drinking water_ES 05551. 1b [Analysis of Chlorine disinfection byproducts by GC/MS]
- EPA 551.1 Determination of chlorination disinfection byproducts, chlorinated solvent, and halogenated pesticides/herbicides in drinking water by liquid-liquid extraction and gas chromatography with electron-capture detection.



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