

Mass Spectrometry & Spectroscopy

Volatile organic compounds analysis in drinking water with Headspace GC/MSD using hydrogen carrier gas and hydroInert source

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Recent concerns with the price and availability of helium have led laboratories to look for alternative carrier gases for their gas chromatography mass spectrometry (GC/MS) methods. For GC/MS, hydrogen is the best alternative to helium, and offers potential advantages in terms of chromatographic speed and resolution. However, hydrogen is not an inert gas, and may cause chemical reactions in the mass spectrometer electron ionisation (EI) source. This can lead to disturbed ion ratios in the mass spectrum, spectral infidelity, peak tailing, and nonlinear calibration for some analytes. Therefore, a new EI source for GC/MS and GC/MS/MS was developed and optimised for use with hydrogen carrier gas. The new source, named HydroInert, was used in the system evaluated here to test volatile organic compounds (VOCs) in drinking water. In addition to the new source, the chromatographic conditions were optimised to provide separation of 80 volatile compounds in 7 minutes. Standards and samples were analysed in both scan and SIM data acquisition modes. For the scan data, spectra were deconvoluted with MassHunter Unknowns Analysis software and searched against NIST 20 to assess the spectral fidelity. In both modes, quantitative calibration was performed for the 80 compounds over the range of 0.05 to 25 µg/L. As demonstrated in this note, the system gives excellent results for the analysis of VOCs in drinking water.

Introduction

One of the analyses commonly used to ensure that the quality of drinking water is the measurement of volatile organic compounds (VOCs). These compounds can appear in drinking water by contamination from numerous sources, including industrial and commercial operations. Another common source is when VOCs are formed by the addition of chlorine (used to disinfect the water) and react with natural organic matter in the source water.

Regulations governing the allowable concentration of VOCs in drinking water vary by country and region but are typically in the low µg/L (ppb) range. Due to the large number of potential contaminants, and the need to measure them at such low levels, GC/MS systems are commonly used. GC/MS offers both the sensitivity and selectivity required to identify and quantify VOCs. Purge and trap [1] and static headspace [2, 3] are two commonly used automated sampling techniques that extract the VOC analytes from water samples and inject them into the GC/MS. This method uses a system configured to perform static headspace/GC/MS analysis of VOCs in drinking water, optimised for using hydrogen as the carrier gas.

Both scan and SIM modes of data acquisition were evaluated. Scan is useful for confirming the identity of found targets, and for identifying nontarget compounds. It can also be used retrospectively to search for compounds that may become of interest in the future. SIM has a substantial advantage in the signal-to-noise ratio and is preferred where quantitation to low levels is required.

Experimental

The Agilent 5977C Inert Plus MSD was coupled to the Agilent 8890 GC equipped with a multimode inlet (MMI) and an Agilent 8697 headspace sampler. A HydroInert source (G7078-60930 for the fully assembled source with 9 mm lens) was used in the MSD, and autotuned using the etune tuning algorithm. The analytical method used an Agilent Ultra Inert straight-through 1.0 mm GC inlet liner and a DB 624 UI column, 20 m × 0.18 mm, 1 µm. The Headspace Sampler was connected to the GC carrier gas inlet line between the GC control pneumatics and the GC injection port. A pulsed split injection was used with the split ratio set to 21:1.

Eight calibration levels ranging from 0.05 to 25 µg/L were prepared in water by spiking 5 µL of a corresponding stock solution (which also included the ISTD) into 10.0 mL of water in a 20 mL headspace vial. Five grams of anhydrous sodium sulphate were weighed into each vial before the addition of water and spiking solution. After capping, each vial was vortexed vigorously for 20 seconds, before placement in the headspace sampler. The spiking stock solutions were prepared in methanol using an Agilent 73-compound standard (DWM-525-1), an Agilent six-compound gas standard (DWM-544-1), and an Agilent three-compound ISTD mix (STM-320N-1), containing fluorobenzene (internal standard), 1,2-dichlorobenzene-d4 (surrogate), and BFB (surrogate). The ISTD/surrogate mix was added to each calibration stock solution at a level to give 5 µg/mL of each compound in the water. Agilent MassHunter Workstation software was used for data acquisition and processing.

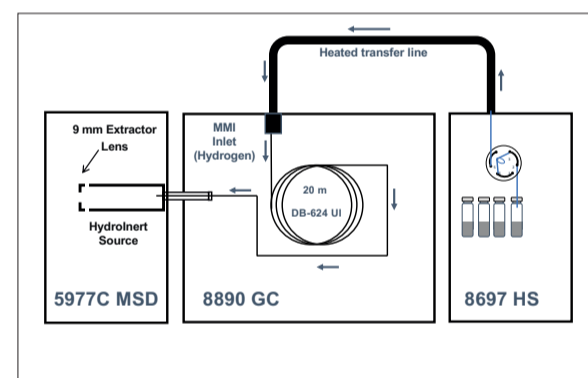


Figure 1. System configuration.

Figure 1 shows the system configuration used here. The operating parameters are listed in Table 1.

Table 1. Gas chromatograph, mass spectrometer, and headspace sampler parameters for VOCs analysis.

Agilent 8890 GC Parameters		Agilent 8697 Headspace Sampler	
Parameters	Setpoints	8697 Loop Size	1 mL
Inlet Temperature	200 °C	Vial Pressurization Gas	Nitrogen
Liner	Agilent Ultra Inert inlet liner, splitless, straight, 1 mm id (p/n 5190-4047)	HS Loop Temperature	75 °C
Carrier Gas	Hydrogen	HS Oven Temperature	75 °C
Column Flow	0.95 mL/min constant flow	HS Transfer Line Temperature	115 °C
Injection Mode	Pulsed split	Vial Equilibration	12.00 min
Split Ratio	21:1	Injection Duration	0.30 min
Pulse Pressure	26 psig until 0.3 min	GC Cycle Time	15.00 min
Septum Purge Flow	3 mL/min	Vial Size	20 mL
Column	Agilent DB-624 Ultra Inert, 20 m × 0.18 mm, 1 µm (p/n 121-1324-UI)	Vial Shaking	Level 9, 250 shakes/min with acceleration of 980 cm/s ²
Oven Program	35 °C (0.25 min), ramp 25 °C/min to 240 °C (0.2 min) Run time 8.65 min	Fill Mode	Default
Agilent 5977C MSD		Fill Flow	50
MS Source	HydroInert Extractor with 9 mm Extractor Lens	Fill Pressure	10 psi
MS Tune	Etune	Pressure Equilibration Time	0.1 min
MSD Transfer Line Temperature	250 °C	Postinjection Purge	100 mL/min for 2 min
MS Source Temperature	250 °C		
MS Quad Temperature	200 °C		
Scan Range	35 to 260 Da		
Scan Speed	A/D samples 4, TID on		
EM Gain Factor (Scan mode)	5		
SIM Method Dwell Time	10 to 60 ms, varied by time segment to maintain minimum cycle time of 6.7 Hz		
EM Gain Factor (SIM Mode)	2		

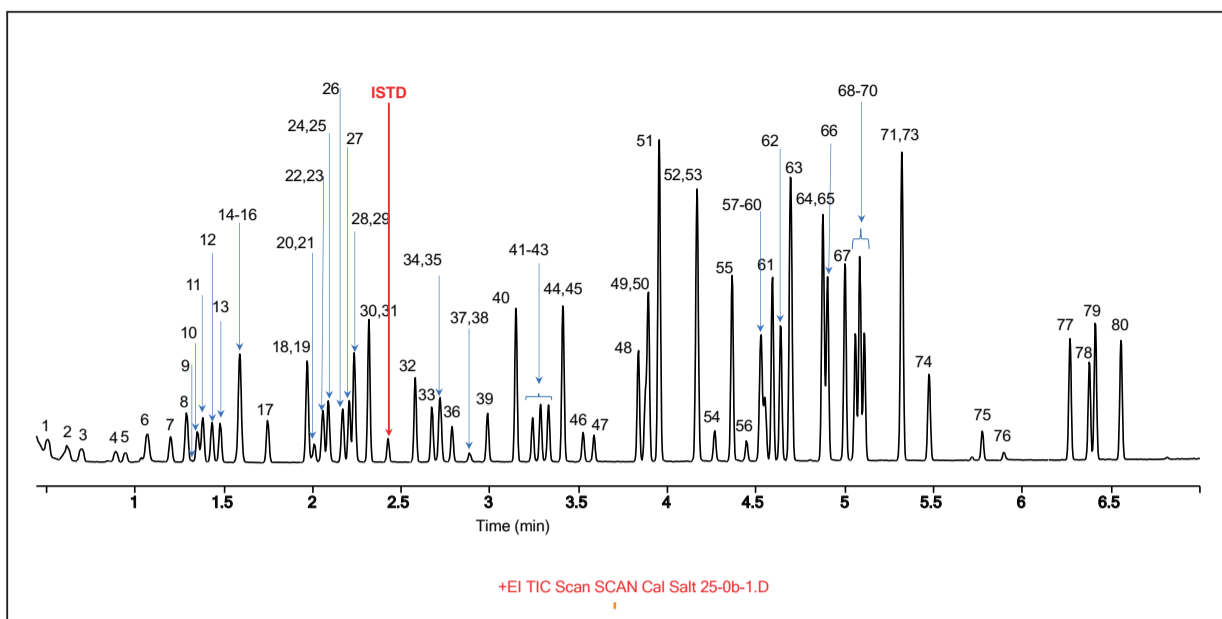


Figure 2. Total ion chromatogram (TIC) from the scan analysis of the 25 µg/L standard. The numbers identifying the peaks correspond to the first column in Table 2.

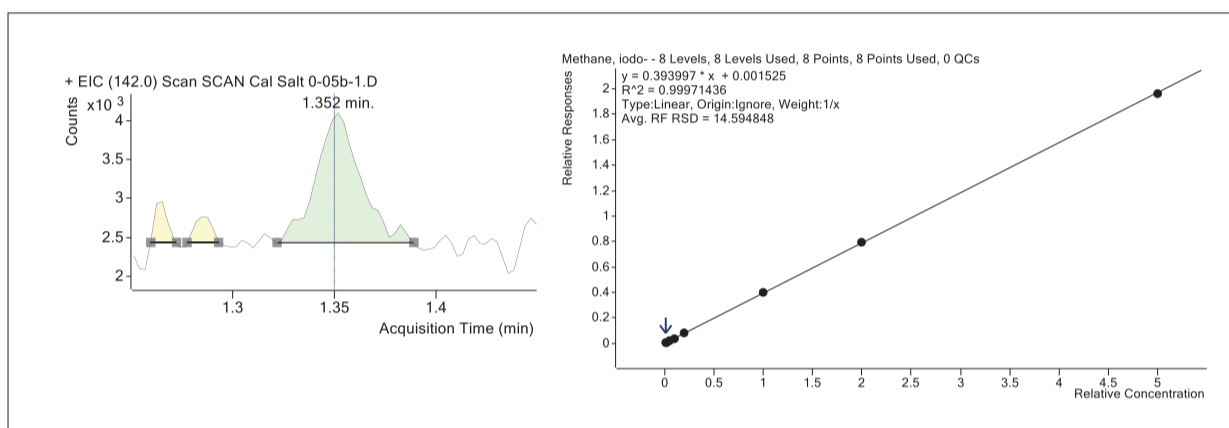


Figure 3. (A) quantifier EIC for iodomethane 0.05 µg/L calibration standard. (B) calibration curve for iodomethane from 0.05 µg/L to 25 µg/L.

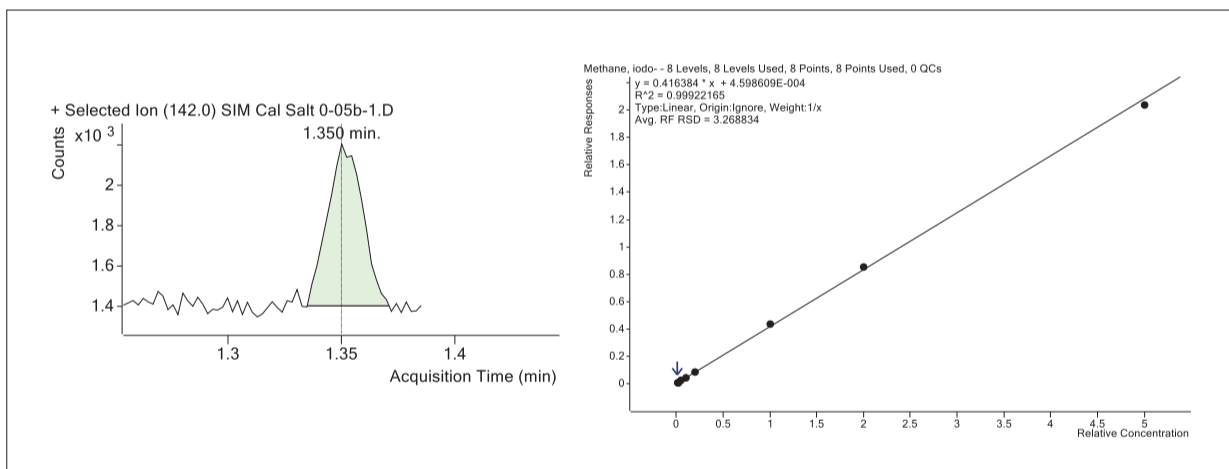


Figure 4. SIM results for iodomethane. (A) quantifier EIC for iodomethane 0.05 µg/L calibration standard. (B) calibration curve for iodomethane from 0.05 µg/L to 25 µg/L.

Initial calibration (ICAL) with scan data

The chromatographic parameters used in the method resulted in good separation of the 80 VOC compounds in less than 7 minutes, as shown in Figure 2. While there are overlapping peaks, their response was measured selectively with the quantifier ions chosen. Most compounds had sufficient response to be measured at or below 0.1 µg/L, and exhibit very good linearity. The average calibration range was 0.16 to 25 µg/L with an average R2 of 0.9978. If necessary, the relative standard error (RSE) value was used to guide removal of the lowest, and in one case highest, calibration points, to achieve an RSE value of <20% (except for acetone). The average Response Factor RSD was <20 for 76 analytes. As expected, polar compounds with higher solubility in water were the worst performers. Acetone is an example, where it also had a contamination issue as observed in the blank, resulting in poor calibration results. A typical example is shown in Figure 3, with the lowest calibrator and calibration curve for iodomethane.

Spectral fidelity

The 25 µg/L VOC standard was analysed with the software, where spectra of the compounds were deconvoluted and searched against the NIST20 library. As seen in Table 2, the library match scores (LMS) are excellent, with an average of 94. There were only six compounds with LMS scores below 90, and these were due to low response and/or interference from overlapping peaks not completely removed by deconvolution. Nitrobenzene (compound 76 in Table 2) gave a very good LMS value of 94. Nitrobenzene reacts readily with hydrogen in a conventional MS source to produce aniline [4], resulting in low LMS values typically in the 60s. The HydroInert source greatly reduces in-source reactions with hydrogen, resulting in the high LMS value for nitrobenzene.

Initial calibration with SIM data

The results of the SIM mode calibration are listed in Table 3. As expected, for most compounds, SIM provided excellent calibration linearity and measurement at or below 0.05 µg/L.

The average calibration range was 0.07 to 24 µg/L, with an average R2 of 0.9990. If necessary, the relative standard error (RSE) value was used to guide removal of the lowest and highest calibration points, to achieve an RSE value of <20% and for choosing between a linear or quadratic fit. For some compounds, a linear fit would meet the <20% RSE criteria, but come close to the limit. However, use of a quadratic fit would significantly improve the RSE. For example, tert-butylbenzene had an RSE of 18.3 with a linear fit, but changing to quadratic lowered the RSE to 8.1. Similar improvements were seen with some of the other substituted benzenes as well. As observed with the scan data calibration, the average response factor RSD was <20 for 76 analytes.

Figure 4 shows a typical example with the lowest calibrator and calibration curve for iodomethane. The improved signal-to-noise ratio provided by SIM, relative to that shown in Figure 3, is clear.

Method detection limits

An MDL study was performed after completion of the initial calibration. Eight trials were performed at the lowest level of calibration, 0.05 µg/L. The calculated MDLs were obtained by applying the formula shown in Equation 1. For compounds with higher reporting limits, eight trials were performed at the concentration of 0.1 µg/L. Table 3 lists the calculated MDLs for 80 VOCs. Six compounds had insufficient response, even at the 0.1 µg/L level, so the lowest calibration level used is listed instead in bold and square brackets. As noted in the scan results, acetone also had a contamination issue as observed in the blank, resulting in poor calibration results. The average MDL for the 80 compounds was 0.026 µg/L.

Equation 1: Formula for MDL calculations.

$$MDL = s \cdot t(n - 1, 1 - \alpha = 99) = s \cdot 2.998$$

Where: $t(n - 1, 1 - \alpha) = t$ value for the 99% confidence level with $n - 1$ degrees of freedom

$n =$ number of trials (8)

$s =$ standard deviation of the eight trials

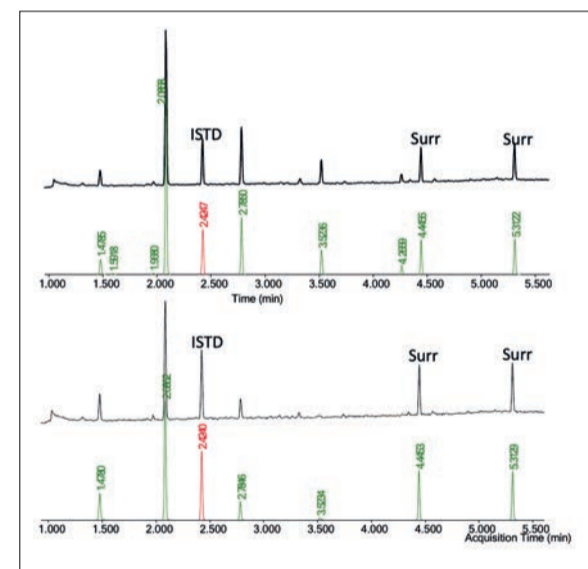


Figure 5. TIC (black) and deconvolution component (green) chromatograms of tap water samples. ISTD is shown in red. Top: Sample from Eastern Pennsylvania. Bottom: Sample from Southeastern Pennsylvania.

VOCs found in drinking water

Samples of municipal tap water from sources in the state of Pennsylvania were analysed using both the scan and SIM methods. Several VOCs were identified by searching their deconvoluted spectra against the NIST20 library. The chromatograms from two of the samples are shown in Figure 5. The concentration of VOCs was determined using quantitative analysis, with both the scan and SIM calibrations. The results are presented in Table 4.

Trichloromethane, bromodichloromethane, dibromochloromethane, and tribromomethane (collectively known as the trihalomethanes) are very common in municipal water treated with chlorine for disinfection purposes.

Table 2. Peak identifications, calibration results, and deconvoluted library match scores against NIST20 for the scan analysis.

Peak No.	Compound	RT (min)	Tgt m/z	Q1	Avg. RF RSD	CF Limit Low (µg/L)	CF Limit High (µg/L)	CF R ²	CF	CF Weight	Rel. Std. Error	LMS NIST20
	Fluorobenzene [ISTD]	2.425	96	77								97
1	Dichlorodifluoromethane	0.508	85	87	12.5	0.1	25	0.9989	Linear	1/x	17.3	92
2	Chloromethane	0.615	50	52	14.4	0.25	25	0.9977	Linear	1/x	16.2	97
3	Chloroethane	0.698	62	64	18.4	0.05	25	0.9995	Linear	1/x	9	91
4	Bromomethane	0.891	94	96	21.7	1	25	0.9995	Linear	1/x	4.2	96
5	Ethyl Chloride	0.945	64	66	13.6	0.25	25	0.9995	Linear	1/x	6.5	92
6	Trichloromonofluoromethane	1.067	101	103	9.6	0.05	25	0.9994	Linear	1/x	9.6	96
7	Ethyl ether	1.198	74	59	12.8	0.25	25	0.9992	Linear	1/x	11.4	97
8	1,1-Dichloroethane	1.288	61	96	6.7	0.05	25	0.9993	Linear	1/x	7.3	98
9	Acetone	1.317	58	43	112.5	1	25	0.9770	Linear	1/x	22.9	87
10	Iodomethane	1.350	142	127	14.6	0.05	25	0.9997	Linear	1/x	7.4	99
11	Carbon disulfide	1.379	76		16.4	0.05	25	0.9997	Linear	1/x	5.7	95
12	Allyl chloride	1.432	76	41	13.9	0.1	25	0.9982	Linear	1/x	17.2	97
13	Methylene chloride	1.478	84	49	5.0	0.1	25	0.9996	Linear	1/x	5.1	97
14	Acrylonitrile	1.572	52	53	16.1	0.5	25	0.9940	Linear	1/x	16.3	90
15	trans-1,2-Dichloroethylene	1.586	61	96	15.9	0.05	25	0.9991	Linear	1/x	17.5	99
16	Methyl tert-butyl ether	1.592	73	57	8.3	0.05	25	0.9991	Linear	1/x	9.6	98
17	1,1-Dichloroethane	1.745	63	65	9.4	0.05	25	0.9998	Linear	1/x	5.2	97
18	cis-1,2-Dichloroethylene	1.966	61	96	7.9	0.05	25	0.9998	Linear	1/x	6.1	95
19	2,2-Dichloropropane	1.969	77	79	3.1	0.5	25	0.9994	Linear	1/x	3.7	80
20	Propanenitrile	1.993	54	52	14.5	0.5	25	0.9943	Linear	1/x	16.4	67
21	2-Propanoic acid, methyl ester	2.008	55	85	12.2	0.1	25	0.9991	Linear	1/x	8.5	97
22	Methylacrylonitrile	2.052	67	52	4.6	0.5	25	0.9994	Linear	1/x	4.4	95
23	Bromochloromethane	2.059	130	128	15.4	0.1	25	0.9946	Linear	1/x	14.2	97
24	Trichloromethane	2.086	83	85	7.0	0.1	25	0.9989	Linear	1/x	11.5	98
25	Tetrahydrofuran	2.090	72	71	19.1	0.25	25	0.9959	Linear	1/x	10.3	96
26	1,1,1-Trichloroethane	2.168	97	99	14.9	0.05	25	0.9995	Linear	1/x	9.6	98
27	1-Chlorobutane	2.205	56	41	5.1	0.1	25	0.9997	Linear	1/x	6.6	97
28	1,1-Dichloropropene	2.231	75	110	18.5	0.05	25	0.9980	Linear	1/x	13.8	96
29	Carbon Tetrachloride	2.235	117	119	8.7	0.1	25	0.9983	Linear	1/x	9.4	96
30	Benzene	2.315	78	77	10.4	0.05	25	0.9991	Linear	1/x	11.4	94
31	1,2-Dichloroethane	2.316	62	64	15.5	0.05	25	0.9989	Linear	1/x	9.8	98
32	Trichloroethylene	2.577	130	132	18.7	0.1	25	0.9981	Linear	1/x	12.4	99
33	1,2-Dichloropropane	2.671	63	62	10.8	0.1	25	0.9997	Linear	1/x	9	98
34	Methyl methacrylate	2.713	100	69	8.4	0.1	25	0.9991	Linear	1/x	10.5	98
35	Dibromomethane	2.722	174	172	13.6	0.1	25	0.9989	Linear	1/x	18	98
36	Bromodichloromethane	2.785	83	85	14.5	0.1	25	0.9997	Linear	1/x	4.1	98
37	2-Nitropropane	2.883	43	41	19.4	0.5	25	0.9973	Linear	1/x	16.2	93
38	Chloromethyl cyanide	2.887	75	77	51.4	1	25	0.9947	Linear	1/x	9.7	63
39	cis-1,3-Dichloropropene	2.985	75	110	12.9	0.1	25	0.9956	Linear	1/x	12.4	98
40	Toluene	3.145	91	92	2.9	0.05	25	0.9995	Linear	1/x	4.3	99
41	trans-1,3-Dichloropropene	3.239	75	110	7.1	0.05	25	0.9963	Linear	1/x	9.3	98
42	Ethyl methacrylate	3.283	69	41	9.6	0.05	25	0.9989	Linear	1/x	10.5	98
43	1,1,2-Trichloroethane	3.328	97	99	11.0	0.1	25	0.9994	Linear	1/x	7.8	98
44	Tetrachloroethylene	3.410	164	166	10.0	0.1	25	0.9991	Linear	1/x	11.3	91
45	1,3-Dichloropropane	3.412	76	78	17.9	0.05	25	0.9991	Linear	1/x	10.7	90
46	Dibromochloromethane	3.524	129	127	6.0	0.1	25	0.9998	Linear	1/x	5.2	98
47	1,2-Dibromoethane	3.585	109	107	6.9	0.25	25	0.9989	Linear	1/x	9.1	99
48	Chlorobenzene	3.835	112	114	8.7	0.05	25	0.9951	Linear	1/x	12.8	99
49	1,1,1,2-Tetrachloroethane	3.875	133	131	10.4	0.1	25	0.9968	Linear	1/x	14.4	96
50	Ethylbenzene	3.892	91	106	5.6	0.05	25	0.9992	Linear	1/x	4.3	98
51	m-Xylene	3.953	91	106	7.7	0.05	25	0.9991	Linear	1/x	4.6	99
52	o-Xylene	4.164	91	106	6.7	0.05	25	0.9995	Linear	1/x	10.8	89
53	Styrene	4.169	104	103	13.0	0.05	25	0.9972	Linear	1/x	8.8	96
54	Tribromomethane	4.266	173	171	14.1	0.1	25	0.9993	Linear	1/x	11.2	99
55	Isopropylbenzene	4.364	105	120	15.9	0.05	25	0.9978	Linear	1/x	6.9	98
56	p-Bromofluorobenzene [SURR]	4.446	174	176								97
57	1,1,2,2-Tetrachloroethane	4.521	83	85	9.4	0.1	25	0.9981	Linear	1/x	12.4	97
58	Bromobenzene	4.530	158	156	11.4	0.1	25	0.9963	Linear	1/x	15.9	97
59	1,2,3-Trichloropropane	4.548	110	112	8.5	0.25	25	0.9960	Linear	1/x	14.7	84
60	trans-1,4-Dichloro-2-butene	4.555	89	88	9.9	0.25	25	0.9985	Linear	1/x	10.7	65
61	Propylbenzene	4.592	91	120	8.6	0.05	25	0.9989	Linear	1/x	8.1	98
62	2-Chlorotoluene	4.638	91	126	7.9	0.05	25	0.9993	Linear	1/x	7.3	98
63	Mesitylene	4.692	105	120	11.6	0.05	25	0.9972	Linear	1/x	8	91
64	tert-Butylbenzene	4.876	134	91	17.4	0.25	25	0.9954	Linear	1/x	15.5	97
65	Pentachloroethane	4.881	167	165	13.3	0.1	25	0.9967	Linear	1/x	17.2	86
66	1,2,4-Trimethylbenzene	4.903	105	120	11.8	0.05	25	0.9975	Linear	1/x	8.4	98
67	1-Methylpropyl benzene	5.001	105	134	19.0	0.05	25	0.9955	Linear	1/x	11.9	98
68	1,3-Dichlorobenzene	5.060	146	148	10.8	0.05	25	0.9979	Linear	1/x	13.3	99
69	p-Cymene (4-Isopropyltoluene)	5.086	119	134	9.9	0.05	25	0.9994	Linear	1/x	6.9	97
70	1,4-Dichlorobenzene	5.110	146	148	9.7	0.05	25	0.9979	Linear	1/x	17.2	99
71	1,2-Dichlorobenzene-D4 [SURR]	5.313	152	150								78
72	n-Butylbenzene	5.322	91	92	9.5	0.1	25	0.9956	Linear	1/x	12.9	96
73	1,2-Dichlorobenzene	5.325	146	148	12.0	0.05	25	0.9993	Quadratic	1/x	12.6	92
74	Hexachloroethane	5.476	166	164	13.7	0.1	25	0.9979	Linear	1/x	14.4	97
75	1,2-Dibromo-3-chloropropane	5.775	155	75	5.1	0.25	25	0.9982	Linear	1/x	8.2	98
76	Nitrobenzene	5.896	77	51	15.6	1	25	0.9981	Linear	1/x	5.5	94
77	1,2,4-Trichlorobenzene	6.270	180	182	13.5	0.05	10	0.9990	Linear	1/x	15.1	99
78	1,1,2,3,4,4-Hexachlorobuta-1,3-diene	6.380	225	223	8.6	0.05	25	0.9997	Linear	1/x	9.6	91
79	Naphthalene	6.413	128	127	7.1	0.05	25	0.9986	Linear	1/x	11.4	99
80	1,2,3-Trichlorobenzene	6.558	180	182	13.4	0.05	25	0.9942	Linear	1/x	12.5	99

* Library match score lower due to low response of compound.

** Library match score lower due to overlapping spectra not completely removed by deconvolution.

They are the products of reaction between chlorine and naturally occurring humic and fulvic acids, often present in source water. All trihalomethanes were confirmed in both samples with precisely matching retention times, qualifier ion ratios, and, except for tribromomethane, with good LMS search results. As expected, LMS values decrease with decreasing concentration of the analyte. The cis-1,2-dichloroethylene and tetrachloroethylene are commonly found at trace levels in ground water from areas with a history of industrial activity. Methyl tert-butyl ether (MTBE) was an additive to gasoline several years ago, used in response to federal mandates requiring specified levels of organic oxygen in gasoline. Its use was later banned when it began showing up in ground water as the result of leaking underground storage tanks at gasoline stations

Figure 6 shows the benefits of using both the scan and SIM methods on tap water samples. Spectral matching provides added confidence in the identification of compounds in the water samples.

Figure 6 also shows the extracted SIM quantifier ions and deconvoluted spectra for four of the seven VOCs found in the Eastern PA water sample. Dibromochloromethane [A] is confidently identified with an RT that precisely matches that in the calibration table, an acceptable ratio of the qualifier to quantifier responses (not shown), and a very high library match score. As the concentration of an analyte decreases, the signal-to-noise ratio in the both the spectra and quantifier chromatograms also decrease. In Figure 6, the spectral information is useful down to about 0.1 µg/L. The SIM data, which identifies using precise RT matching and the ratio of the qualifier to quantifier response can be used to lower levels.

Table 3. Calibration results, and method detection limits (MDL) using SIM acquisition.

Peak No.	Compound Name	RT (min)	Tgt m/z	Q1	Avg. RF RSD	CF Limit Low (µg/L)	CF Limit High (µg/L)	CF R ²	CF	CF Weight	Rel. Std. Error	Conc. for MDL	MDL (µg/L)
	Fluorobenzene [ISTD]	2.425	96	77									
1	Dichlorodifluoromethane	0.508	85	87	15.3	0.05	25	0.9994	Linear	1/x	11.6	0.10	0.011
2	Chloromethane	0.615	50	52	7.3	0.1	25	0.9997	Linear	1/x	8.4	0.10	0.022
3	Chloroethane	0.698	62	64	4.1	0.05	25	0.9998	Linear	1/x	4.7	0.05	0.008
4	Bromomethane	0.891	94	96	4.1	0.05	25	0.9999	Linear	1/x	4.4	0.10	0.029
5	Ethyl Chloride	0.945	64	66	4.5	0.05	25	0.9998	Linear	1/x	4.7	0.05	0.010
6	Trichloromonofluoromethane	1.067	101	103	4.1	0.05	25	0.9997	Linear	1/x	4.3	0.05	0.008
7	Ethyl ether	1.198	74	59	6.4	0.05	25	0.9994	Linear	1/x	11	0.05	0.017
8	1,1-Dichloroethane	1.288	61	96	5.9	0.05	25	0.9996	Linear	1/x	5.3	0.05	0.006
9	Acetone	1.317	58	43	102.2	1	10	0.9994	Linear	1/x	3.5	[cont]	
10	Iodomethane	1.350	142	127	3.3	0.05	25	0.9992	Linear	1/x	4.8	0.05	0.006
11	Carbon disulfide	1.379	76		12.6	0.1	25	0.9994	Linear	1/x	4.6	0.05	0.003
12	Allyl chloride	1.432	76	41	4.9	0.05	25	0.9997	Linear	1/x	6.4	0.05	0.014
13	Methylene chloride	1.478	84	49	12.2	0.1	25	0.9999	Linear	1/x	5.2	0.05	0.007
14	Acrylonitrile	1.572	52	53	8.3	0.1	25	0.9999	Linear	1/x	5.4	[0.25]	
15	trans-1,2-Dichloroethylene	1.586	61	96	7.1	0.05	25	0.9997	Linear	1/x	5	0.05	0.007
16	Methyl tert-butyl ether	1.592	73	57	4.2	0.05	25	0.9995	Linear	1/x	7.5	0.05	0.003
17	1,1-Dichloroethane	1.745	63	65	3.7	0.05	25	0.9998	Linear	1/x	4.6	0.05	0.003
18	cis-1,2-Dichloroethylene	1.966	61	96	10.1	0.05	25	0.9996	Linear	1/x	7.3	0.05	0.007
19	2,2-Dichloropropane	1											

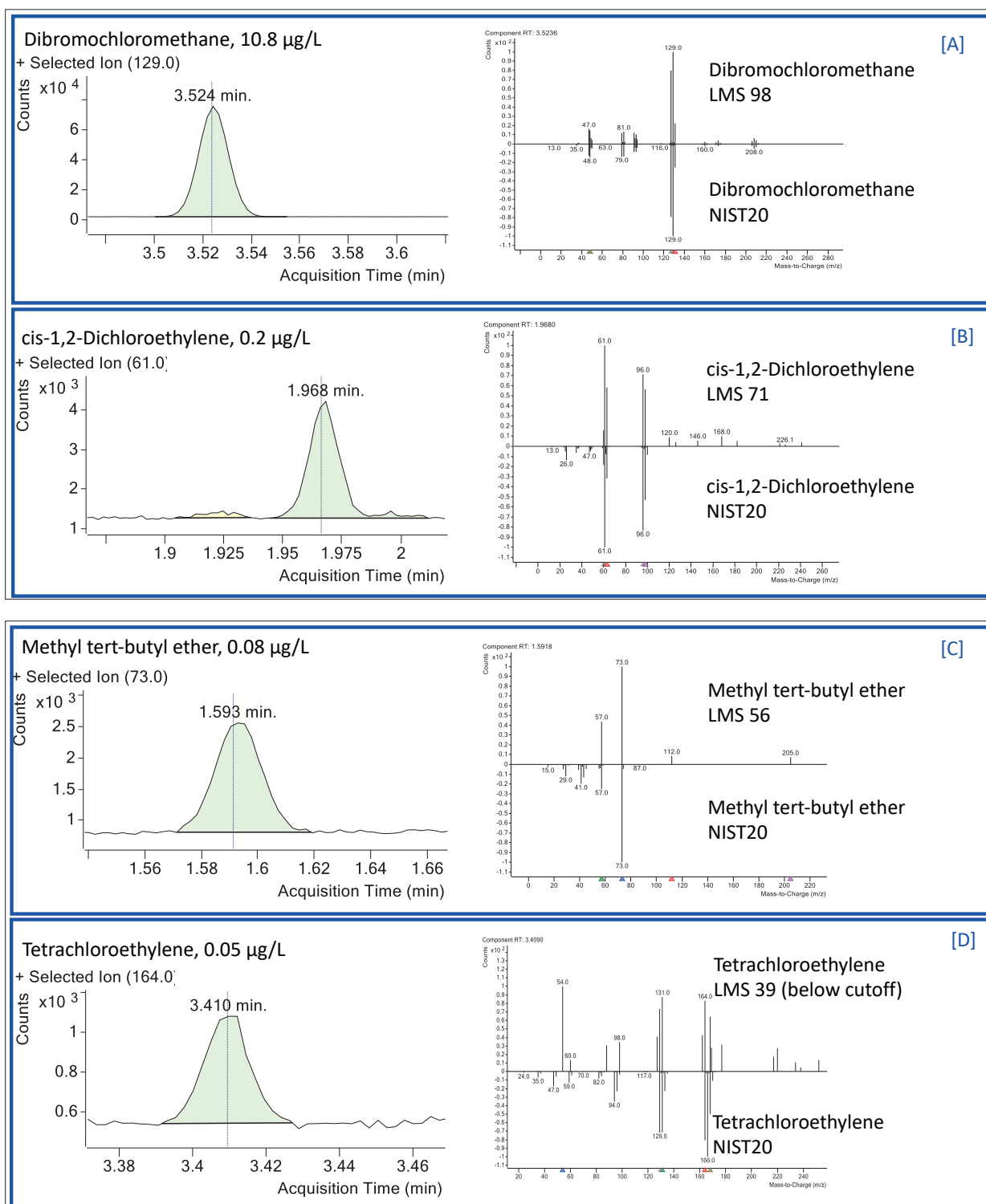


Figure 6. Quantifier ion extracted chromatograms from the SIM run and corresponding deconvoluted spectra from scan runs of the Eastern PA tap water sample

Table 4. Results from analysis of tap water samples.

Name	RT (min)	Eastern PA			Southeastern PA		
		Scan	Scan	SIM	Scan	Scan	SIM
		LMS NIST20	Conc. ($\mu\text{g/L}$)	Conc. ($\mu\text{g/L}$)	LMS NIST20	Conc. ($\mu\text{g/L}$)	Conc. ($\mu\text{g/L}$)
Methyl tert-butyl ether	1.592	56	0.08	0.08			
cis-1,2-Dichloroethylene	1.968	71	0.19	0.20			
Trichloromethane	2.087	98	43.47	44.08	97	21.03	20.90
Bromodichloromethane	2.785	98	21.81	22.07	92	4.82	4.85
Tetrachloroethylene	3.410			0.05			
Dibromochloromethane	3.524	98	11.34	10.80	68	0.69	0.69
Tribromomethane	4.266	97	3.97	3.71			0.02

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