Environmental

Adhering to U.S. EPA Method 524.2 for the analysis of volatile organic compounds in drinking water

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Goal

Demonstration of a routine analytical method that meets the requirements outlined in U.S. EPA 524.2 for the quantitation of volatile organic compounds (VOCs) in drinking water, using the Teledyne LABS Tekmar Lumin Purge and Trap (P&T) concentrator paired with the AQUATek LVA autosampler system along with a Thermo Scientific™ ISQ™ 7610 MS system coupled with a Thermo Scientific™ TRACE™ 1610 gas chromatograph (GC) and Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS). Method linearity, method detection limit (MDL), precision, and accuracy were assessed to evaluate method performance.

Introduction

Analytical testing labs play a crucial role in monitoring surface, ground, and drinking water for volatile organic compounds (VOCs). Common by-products in the processing of household and industrial products, VOCs can contaminate water sources, potentially harming the environment and public health. To safeguard against this, labs use the U.S. EPA Method 524.2[1] to test water for the presence of VOCs, including four trihalomethane disinfection by-products. This procedure utilizes Purge and Trap (P&T) procedures to remove VOCs with high volatility and low water solubility from water samples, followed by gas chromatography-mass spectrometry (GC-MS).

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U.S. EPA Method 524.2 has mandated criteria that environmental testing labs must adhere to, including detection limits, linearity, and precision. Labs must meet this criteria day in and day out to report their findings, hence having a robust and reproducible system is critical to reporting results on time.

The following evaluation describes the use of the ISQ 7610 MS system coupled coupled with a TRACE 1610 gas chromatograph (GC) and the Tekmar Lumin P&T concentrator paired with the AQUATek LVA autosampler for U.S. EPA Method 524.2.

Experimental

Sample preparation

A 50 µg/mL (parts per million or ppm) calibration working standard was prepared in purge and trap grade methanol (Honeywell/Burdick & Jackson, P/N 232-1L) from the following Restek™ standards: Drinking Water VOA MegaMix™ (P/N 30601), Ketone Mix (P/N 30602), and 502.2 Calibration Mix (P/N 30042). In total, the standards contained 83 compounds.

The calibration curve was prepared from 0.2 µg/L to 40 µg/L (parts per billion or ppb) for all compounds. The relative response factor (RF) was calculated for each compound using one Restek internal standard: fluorobenzene (P/N 30201). Surrogate standards from Restek consisted of 4-bromofluorobenzene and 1,2-dichlorobenzene-d4 (P/N 30201). Internal and surrogate standards were prepared in methanol from Restek standards at a concentration of 25 ppm, after which 5 µL was then mixed with each 25 mL sample for a resulting concentration of 10 ppb.

A total of seven standards at a concentration of 0.5 ppb were prepared in deionized water to calculate the MDL and precision calculations for all compounds. Also, seven standards with a concentration of 10 ppb were prepared to determine the accuracy and precision of recovery of each compound. All calibration, MDL, and recovery standards were analyzed with the Tekmar Lumin P&T and AQUATek LVA autosampler conditions in Table 1.

GC-MS conditions

A TRACE 1610 GC was coupled to the ISQ 7610 single quadrupole mass spectrometer equipped with the NeverVent™ vacuum probe interlock (VPI) and a Thermo Scientific™ ExtractaBrite™ ion source. A Thermo Scientific™ TraceGOLD™ TG-VMS, 30 m × 0.25 mm, 1.4 µm film column (P/N 26080-3320) was used for compound separation. The Thermo Scientific™ HeSaver-H$_2$Safer™ Split/Splitless injector was operated in split mode with a run time under 13 minutes. The ISQ 7610 mass spectrometer was operated in full scan mode, offering sufficient sensitivity to achieve the required limits of detection. Note: The instrument can also be operated in Selected Ion Monitoring (SIM) mode to increase selectivity. Expanded method parameters for the ISQ 7610 mass spectrometer are displayed in Table 2.

Instrument control and data processing

Data were acquired, processed, and reported using Chromeleon CDS, version 7.3. This software can control both the GC-MS system and the Tekmar Lumin P&T and AQUATek LVA autosampler. This allows a single software to be utilized for the full workflow simplifying the instrument operation. Figure 2 shows the Chromeleon CDS control of the Tekmar Lumin P&T and AQUATek LVA autosampler. The fully optimized method used within this application note is available for download in the Thermo Scientific™ AppsLab application note repository, which contains all the parameters needed to acquire, process, and report the analytical data for U.S EPA Method 524.2.[2]
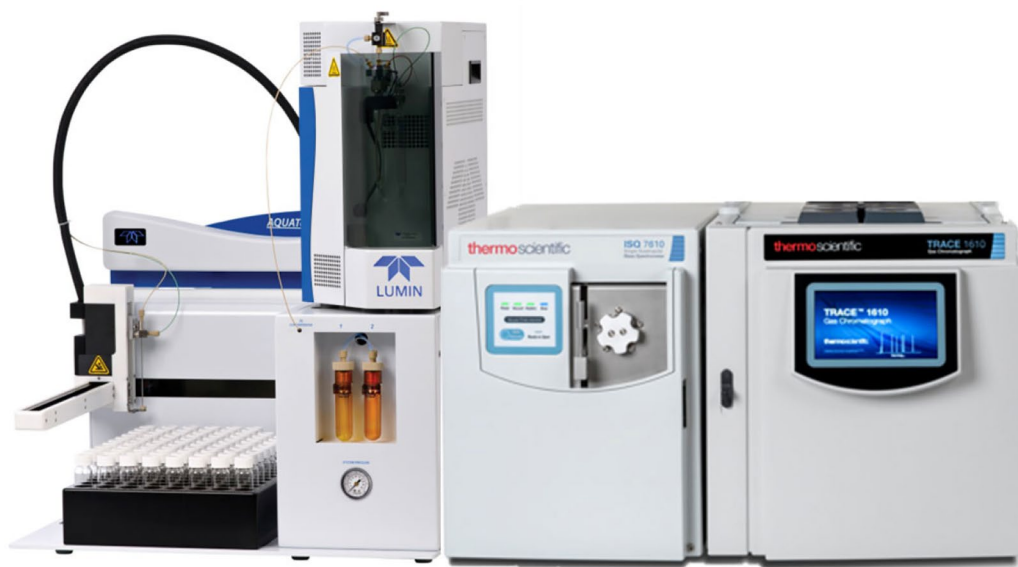

Figure 1. ISQ 7610 GC-MS coupled with the Tekmar Lumin P&T and AQUATek LVA autosampler

Table 1 (part 1). Teledyne Tekmar Lumin AQUATek LVA P&T water method conditions

Standby	Variable
Valve oven temp.	150 °C
Transfer line temp.	150 °C
Sample mount temp.	90 °C
Purge ready temp.	35 °C
MCS purge temp.	20 °C
Standby flow	10 mL/min
Purge	**Variable**
Purge temp.	20 °C
Purge time	11.00 min
Purge flow	40 mL/min
Dry purge temp.	20 °C
Dry purge time	1.0 min
Dry purge flow	100 mL/min
Sparge vessel heater	Off
Desorb	**Variable**
Desorb preheat temp.	245 °C
Desorb temp.	250 °C
Desorb time	4.00 min
Desorb flow	300 mL/min
GC start signal	Start_Only
Bake	**Variable**
Bake time	4.00 min
Trap bake temp.	270 °C
MCS bake temp.	180 °C
Bake flow	200 mL/min

Table 1 (part 2). Teledyne Tekmar Lumin AQUATek LVA P&T water method conditions

AQUATek LVA	Variable
Sample loop time	1.10 min
Sample transfer time	1.25 min
Rinse loop time	1.10 min
Sweek needle time	0.30 min
Presweep time	0.35 min
Water temperature	90 °C
Bake rinse cycles	1
Bake rinse drain time	0.60 min
Trap	9
Chiller tray	On
Purge gas	Helium

Table 2. GC-MS conditions

TRACE 1610 GC conditions	
Column	TraceGOLD TG-VMS, 30 m × 0.25 mm, 1.4 μm film (P/N 26080-3320)
Carrier gas	Helium, 1.8 mL/min
Oven profile	35 °C, 2 min; 15 °C/min to 100 °C; 30 °C/min to 225 °C; 2 min hold; Run time 12.5 min
HeSaver-H$_2$Safer Split/Splitless injector	200 °C, 30:1 split, purge flow 5.0 mL/min, 0.20 min helium delay
ISQ 7610 MS conditions	
Temperature	Transfer line 230 °C; ion source 280 °C
Scan	Range 35 amu to 260 amu, solvent delay 1.43 min, dwell/scan time 0.10 s
Current	Emission current 30 μA, gain 3.00E+005
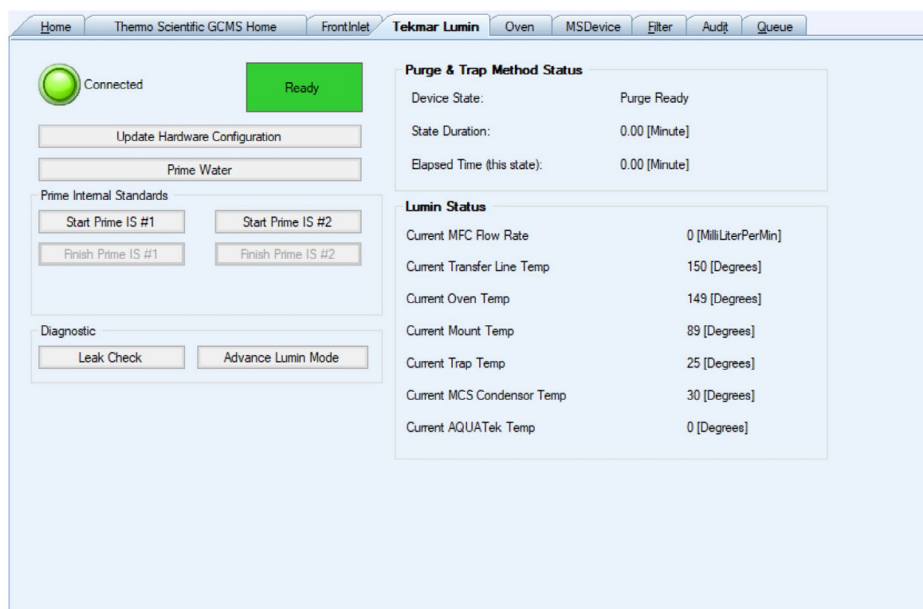
Figure 2. Chromeleon CDS control and monitoring of the Tekmar Lumin P&T and AQUATek LVA autosampler

Results and discussion

Chromatography

Employing the GC conditions outlined in Table 2, successful chromatographic resolution of all desired compounds was achieved. Minimal moisture entered the analytical column from the water samples, ensuring no adverse effects on peak shape. Consequently, even in lower concentration samples, the chromatography remained optimized. Figure 3 illustrates this consistent peak shape and separation using a 20 ppb VOC standard, showing minimal water interference.

Linearity and sensitivity

The calibration range of 0.2 ppb to 40 ppb was assessed for all compounds. Figure 4 demonstrates the quantitation of bromodichloromethane at 0.5 ppb in a VOC standard with excellent library spectral matching and calibration curve. Figure 5 demonstrates the same information for *trans*-1,3-dichloropropene.

20 ppb

18) *cis*-1,2-dichloroethane
19) 2,2-dichloropropane
20) Bromochloromethane
21) Chloroform
22) Carbon tetrachloride
23) Tetrahydrofuran
24) Methyl acrylate
25) 1,1,1-trichlorothane
26) 2-butanone
27) 1,1-dichloropropene
28) 1-chlorobutane
29) Benzene
30) Propionitrile
31) Methacrylonitrile
32) 1,2-dichlrorethane
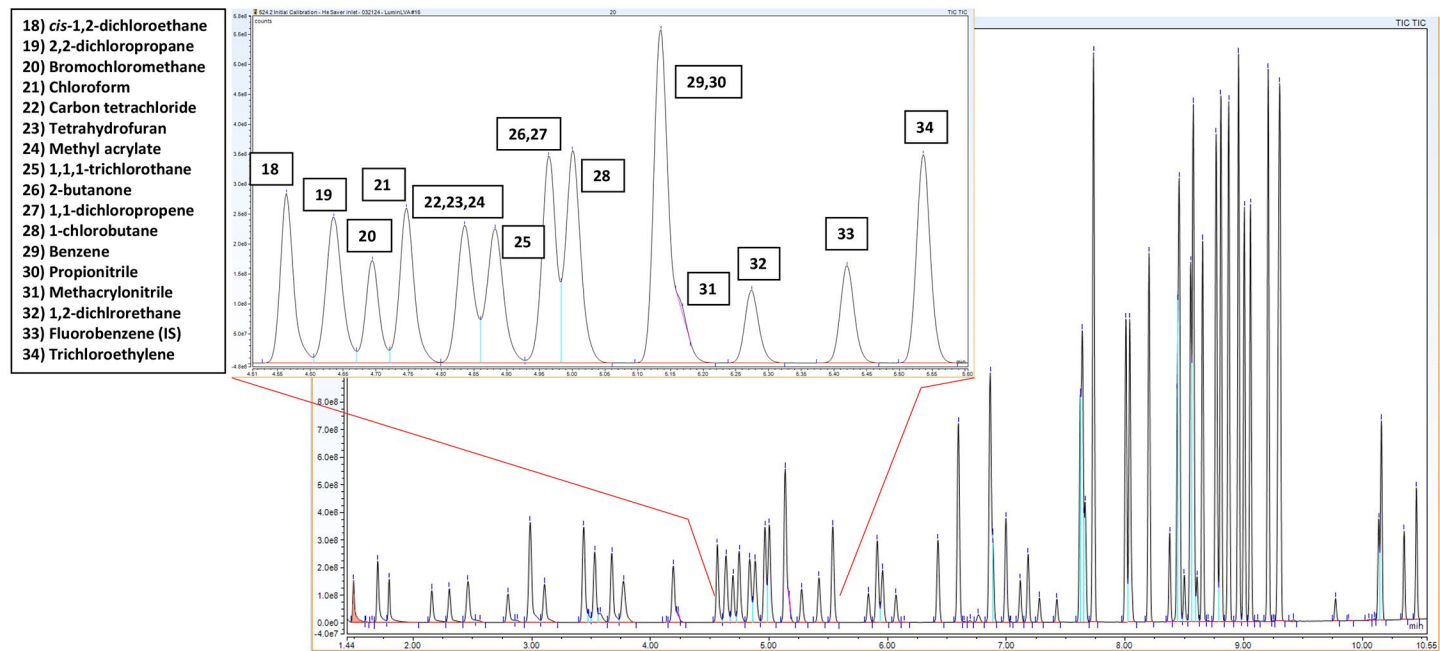33) Fluorobenzene (IS)
34) Trichloroethylene

Figure 3. Total ion chromatogram (TIC) of a 20 ppb VOC standard with an inset indicating consistent peak shapes and separation with minimal water interference
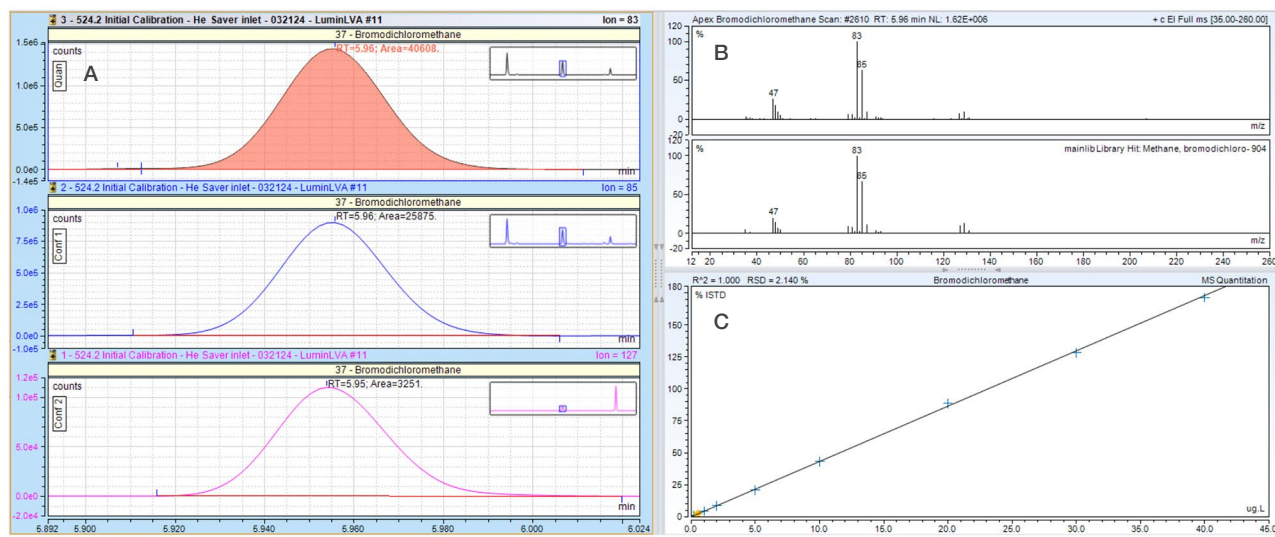

Figure 4. Chromeleon CDS results browser showing extracted ion chromatograms for bromodichloromethane in the 0.5 ppb water standard, quantitation ion (*m/z*= 83) and two confirming ions (*m/z* = 85, 127). (A) A matching measured spectrum to the NIST library and (B) a linear calibration over a concentration range of 0.2 ppb to 40 ppb (C).
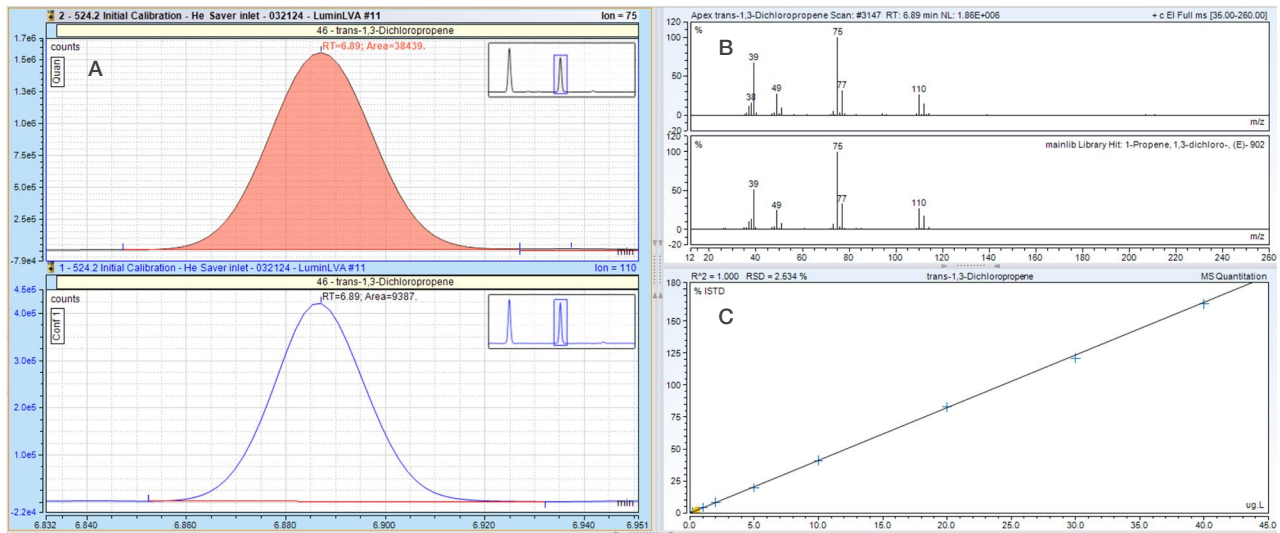
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Figure 5. Chromeleon CDS results browser showing extracted ion chromatograms for *trans*-1,3-dichloropropene in the 0.5 ppb water standard, quantitation ion (*m/z*= 75) and one confirming ion (*m/z* = 110). (A) A matching measured spectrum to the NIST library and (B) a linear calibration over a concentration range of 0.2 ppb to 40 ppb (C).

Appendix Table A1 displays the relative standard deviation (%RSD) of the response factors (RFs) which were <20% for all compounds, except for acetone, 1,1,2,2-tetrachloroethane, *trans*-1,4-dichloro-2-butene, and hexachloroethane, which used a quadratic regression calibration with r^2>0.995. The table also shows the MDL for each analyte calculated by injecting n=7 injections of the 0.5 ppb water standard. Figure 6 shows a subset of the MDL data with calculated MDLs and precision for 25 compounds.

Method robustness

To assess the stability of the method, which is essential for environmental testing labs, 10 ppb calibration check standards were injected at intervals 31 times over a sequence of 189 injections. This is equivalent to 3.5 days of uninterrupted analysis with no maintenance performed on the system. Figure 7 shows the reproducibility of 14 of the compounds over 189 injections with excellent percentage RSDs. RSDs for all compounds were under the 30% accuracy method requirements. Appendix Table A2 shows the reproducibility results for all compounds over the 189-injection sequence.
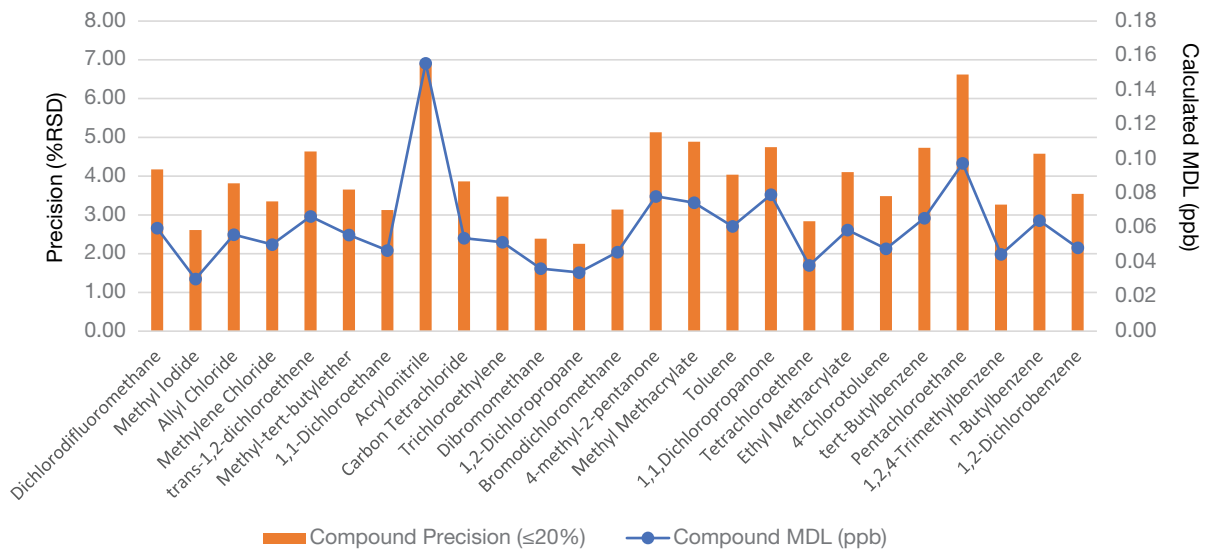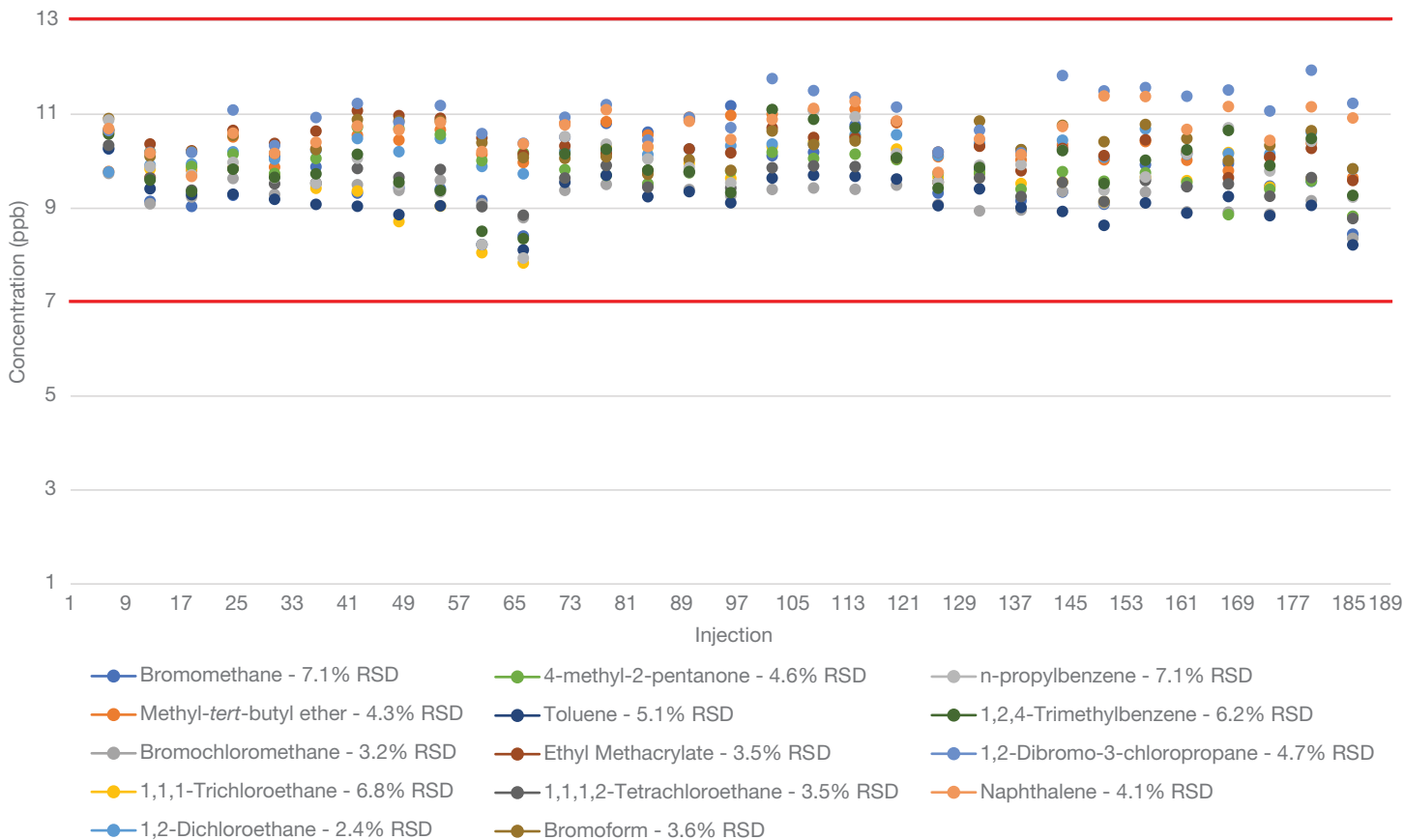

Figure 6. MDL and precision calculated for a subset of compounds (n=25) from n=7 injections of a 0.5 ppb standard

Figure 7. Repeatability of a 10 ppb VOC standard (n=31) (as concentration in ppb) assessed over n=189 consecutive injections. Red lines represent the ±30% accuracy as required by the method.

Conclusion

The TRACE 1610 GC, the ISQ 7610 system, and the Tekmar Lumin P&T with the AQUATek LVA autosampler system together offer benefits for executing U.S. EPA Method 524.2. The Tekmar Lumin P&T concentrator enhances sample throughput through efficient trap cooling and moisture control, thus reducing peak interference and extending GC column life. The ISQ 7610 system's VPI and ExtractaBrite ion source allow ionization source and analytical column replacement without venting the instrument, ensuring minimal downtime, and the XLXR™ detector offers extended linear dynamic range. The collective technology addresses routine VOC analysis challenges, ensuring robust sensitivity, maximized output, and consistent method compliance.

The ISQ 7610 system equipped with the VPI coupled with the Tekmar Lumin P&T and the AQUATek LVA autosampler exceeds all the requirements outlined in U.S. EPA Method 524.2 for analysis of VOCs in drinking water:

- Excellent linearity for all compounds was demonstrated with the %RSD of the calibration response factors passing all method requirements.

- MDL and precision for seven 0.5 ppb standards showed no interference from excessive water and produced very reproducible results. The average MDL result for all 83 target compounds was 0.06 ppb with a precision of 4.06%.

- The precision for n=31 samples over 189 injections displayed <30% RSD accuracy for all compounds as the method requires. The average precision for all 83 target compounds and 2 surrogates gave a %RSD of 6.43% with an accuracy of 98% recovering the compounds. Individually, 4-bromofluorobenzene and 1,2-dichlorobenzene-d4 had a 7.68% RSD with an accuracy of 98% and 4.95% RSD and an accuracy of 95%, respectively, over 189 injections and almost four days of uninterrupted analysis.

References

1. U.S. EPA Method 524.2. Measurement of purgeable organic compounds in water by capillary column gas chromatography/mass spectrometry. https://www.epa.gov/sites/production/files/2015-06/documents/epa-524.2.pdf
2. Thermo Scientific AppsLab: https://appslab.thermofisher.com/App/4373/epa-5242-compounds-drinking-water-by-gcms

Appendix

Table A1. U.S. EPA Method 524.2 calibration, accuracy, and precision data (part 1)

Compound	Calibration			Accuracy and precision (n=7, 0.5 ppb)			Mid-point check (n=7, 10 ppb)	
	Retention time	Quant ion	Relative SD (%RSD)	Average RF	MDL (ppb)	Precision (≤20%)	Precision (≤20%)	Accuracy (±20%)
Dichlorodifluoromethane	1.51	85	14.5	0.447	0.06	4.17	6.11	99
Chloromethane	1.71	50	14.3	1.01	0.06	3.86	6.12	87
Vinyl Chloride	1.81	62	8.16	0.509	0.05	3.34	5.66	92
Bromomethane	2.17	94	14.7	0.343	0.08	4.78	3.89	86
Chloroethane	2.32	64	8.68	0.407	0.05	3.52	5.10	81
Trichlorofluoromethane	2.47	101	10.4	0.487	0.05	3.86	4.45	95
Diethyl Ether	2.81	59	7.33	0.218	0.07	4.59	3.59	93
1,1-Dichloroethene	2.99	96	6.70	0.363	0.07	4.70	3.26	92
Carbon Disulfide	3.00	76	7.07	0.934	0.07	4.82	3.73	84
Methyl Iodide	3.11	142	12.9	0.652	0.03	2.61	2.87	98
Allyl Chloride	3.44	76	4.91	0.272	0.06	3.82	3.66	93
Methylene Chloride	3.54	84	7.16	0.404	0.05	3.35	2.25	90
Acetone[1]	3.60	43	1.00	0.174	0.13	7.37	10.7	98
trans-1,2-dichloroethene	3.68	96	6.88	0.416	0.07	4.64	2.61	89
Methyl-tert-butylether	3.78	73	4.32	0.657	0.06	3.66	2.31	95
1,1-Dichloroethane	4.20	63	6.71	0.853	0.05	3.13	3.30	92
Acrylonitrile	4.24	52	11.6	0.055	0.16	6.92	4.90	110
cis-1,2-Dichloroethene	4.57	96	5.59	0.428	0.05	3.07	2.88	91
2,2-Dichloropropane	4.64	77	7.36	0.560	0.07	4.43	5.96	94
Bromochloromethane	4.70	128	5.01	0.134	0.05	3.37	1.77	93
Chloroform	4.75	83	6.51	0.688	0.05	3.00	3.38	92
Methyl Acrylate	4.84	55	5.21	0.134	0.08	4.78	3.42	104
Carbon Tetrachloride	4.85	117	5.53	0.461	0.05	3.87	3.50	98
Tetrahydrofuran	4.86	71	11.5	0.021	0.09	4.77	4.50	109
1,1,1-Trichloroethane	4.89	97	5.77	0.537	0.05	3.27	3.73	95
2-Butanone	4.97	43	11.5	0.129	0.09	5.49	9.05	107
1,1-Dichloropropene	4.97	75	6.53	0.509	0.05	3.54	4.37	95
1-Chlorobutane	5.01	56	6.48	0.782	0.05	3.30	4.58	95
Benzene	5.14	78	5.95	1.68	0.04	2.87	3.36	93
Propionitrile	5.17	54	7.51	0.029	0.12	7.06	1.91	102
Methacrylonitrile	5.18	67	5.83	0.071	0.05	3.18	3.53	103
1,2-Dichloroethane	5.28	62	6.60	0.317	0.03	2.15	3.36	95
Fluorobenzene (ISTD)	5.43	96						
Trichloroethylene	5.54	95	7.36	0.424	0.05	3.47	2.99	92
Dibromomethane	5.84	93	5.14	0.139	0.04	2.39	1.99	95
1,2-Dichloropropane	5.92	63	5.56	0.423	0.03	2.26	3.11	94
Bromodichloromethane	5.96	83	2.14	0.433	0.05	3.14	2.73	96
4-methyl-2-pentanone	6.08	100	5.40	0.038	0.08	5.13	1.74	101
Methyl Methacrylate	6.08	69	3.54	0.109	0.07	4.89	2.53	102
cis-1,3-Dichloropropene	6.43	75	2.72	0.559	0.04	2.71	3.13	96
Toluene	6.60	92	7.10	1.08	0.06	4.04	2.52	92
Chloroacetonitrile	6.70	48	8.01	0.010	0.19	14.9	9.92	80
2-Nitropropane	6.77	43	7.55	0.110	0.09	5.04	4.28	109

Table A1. U.S. EPA Method 524.2 calibration, accuracy, and precision data (part 2)

Compound	Calibration			Accuracy and precision (n=7, 0.5 ppb)			Mid-point check (n=7, 10 ppb)	
	Retention time	Quant ion	Relative SD (%RSD)	Average RF	MDL (ppb)	Precision (≤20%)	Precision (≤20%)	Accuracy (±20%)
1,1,Dichloropropanone	6.87	43	8.13	0.233	0.08	4.75	4.96	105
Tetrachloroethene	6.87	166	6.11	0.949	0.04	2.84	4.27	92
trans-1,3-Dichloropropene	6.89	75	2.53	0.412	0.05	3.59	2.93	97
Ethyl Methacrylate	7.00	69	6.22	0.236	0.06	4.11	3.02	103
1,1,2-Trichloroethane	7.01	83	2.94	0.192	0.04	2.33	1.89	98
Dibromochloromethane	7.12	129	4.82	0.236	0.05	3.64	1.52	100
1,3-Dichloropropane	7.19	76	4.15	0.395	0.03	2.17	2.48	97
1,2-Dibromoethane	7.29	107	2.76	0.195	0.05	3.25	1.63	98
2-Hexanone	7.43	43	9.26	0.196	0.12	7.40	9.24	102
Chlorobenzene	7.63	112	3.45	1.17	0.05	3.67	2.09	95
Ethylbenzene	7.65	91	4.84	2.15	0.05	3.50	3.14	94
1,1,1,2-Tetrachloroethane	7.67	131	4.55	0.349	0.05	3.46	1.75	96
m,p-Xylene	7.74	106	3.80	0.905	0.09	3.29	2.84	93
o-Xylene	8.01	106	3.09	0.929	0.04	2.94	2.95	92
Styrene	8.05	104	7.41	1.37	0.05	3.61	2.54	95
Bromoform	8.06	173	16.7	0.168	0.04	3.52	0.76	101
Isopropylbenzene	8.21	105	4.17	2.43	0.06	4.16	3.95	96
4-Bromofluorobenzene (surr)	8.38	95	11.0	0.577		1.71	1.33	97
Bromobenzene	8.45	156	8.37	0.648	0.03	2.27	2.42	92
n-propylbenzene	8.46	91	7.03	3.23	0.05	3.46	3.61	99
1,1,2,2-Tetrachloroethane[1]	8.51	83	1.00	0.232	0.04	2.52	1.97	101
2-Chlorotoluene	8.56	91	4.80	2.20	0.05	3.55	3.43	95
1,3,5-Trimethylbenzene	8.58	105	7.11	2.51	0.05	3.55	3.37	97
1,2,3-Trichloropropane	8.59	75	10.3	0.233	0.05	3.60	3.47	103
trans-1,4-Dichloro-2-butene[1]	8.61	53	1.00	0.072	0.06	4.50	3.46	98
4-Chlorotoluene	8.66	91	7.06	2.10	0.05	3.48	3.31	94
tert-Butylbenzene	8.77	119	8.37	2.35	0.07	4.73	4.41	97
Pentachloroethane	8.79	117	17.8	0.249	0.10	6.62	6.64	99
1,2,4-Trimethylbenzene	8.81	105	6.74	2.62	0.04	3.27	3.42	99
sec-Butylbenzene	8.88	105	8.81	3.28	0.06	3.97	3.54	104
p-Isopropyltoluene	8.96	119	7.47	2.74	0.06	4.12	3.59	103
1,3-Dichlorobenzene	9.01	146	11.3	1.73	0.05	4.04	2.64	95
1,4-Dichlorobenzene	9.06	146	10.2	1.69	0.04	3.14	2.94	96
n-Butylbenzene	9.21	91	7.68	2.67	0.06	4.58	3.70	103
1,2-Dichlorobenzene-d4 (surr)	9.31	152	15.8	0.820		2.00	3.75	96
Hexachloroethane[1]	9.31	117	0.997	1.68	0.13	8.31	2.08	102
1,2-Dichlorobenzene	9.31	146	8.40	1.47	0.05	3.55	2.63	96
1,2-Dibromo-3-chloropropane	9.78	75	10.2	0.046	0.07	4.96	2.95	103
Nitrobenzene	10.11	123	12.9	0.005	0.05	3.44	9.66	84
Hexachlorobutadiene	10.14	225	10.1	0.048	0.08	5.57	3.20	103
1,2,4-Trichlorobenzene	10.17	180	7.42	0.595	0.06	4.21	1.99	101
Naphthalene	10.36	128	8.01	0.596	0.06	3.94	1.50	101
1,2,3-Trichlorobenzene	10.46	180	10.1	0.394	0.06	4.35	2.20	102

[1]Compounds used a quadratic regression calibration

Table A2. Repeatability of a 10 ppb VOC standard (n=31) (as absolute peak area counts) assessed over n=189 consecutive injections

Compound	Analyte recovery (10 ppb n=31, 191 injections)	
	Precision (≤20%RSD)	Accuracy (±30%)
Dichlorodifluoro-methane	14.4	120
Chloromethane	8.91	106
Vinyl Chloride	9.48	102
Bromomethane	7.10	98
Chloroethane	9.42	98
Trichlorofluoromethane	11.0	103
Diethyl Ether	5.18	104
1,1-Dichloroethene	10.1	96
Carbon Disulfide	11.3	92
Methyl Iodide	7.40	100
Allyl Chloride	7.80	98
Methylene Chloride	5.38	97
Acetone[1]	8.69	70
trans-1,2-dichloroethene	7.85	93
Methyl-tert-butylether	4.30	104
1,1-Dichloroethane	6.32	100
Acrylonitrile	6.17	124
cis-1,2-Dichloroethene	4.28	92
2,2-Dichloropropane	16.5	87
Bromochloromethane	3.21	93
Chloroform	3.78	97
Methyl Acrylate	4.35	109
Carbon Tetrachloride	7.82	97
Tetrahydrofuran	5.56	117
1,1,1-Trichloroethane	6.82	97
2-Butanone	5.36	74
1,1-Dichloropropene	7.59	96
1-Chlorobutane	7.38	97
Benzene	4.73	94
Propionitrile	4.05	112

Compound	Analyte recovery (10 ppb n=31, 191 injections)	
	Precision (≤20%RSD)	Accuracy (±30%)
Methacrylonitrile	4.07	108
1,2-Dichloroethane	2.42	102
Fluorobenzene (ISTD)		
Trichloroethylene	8.13	97
Dibromomethane	2.52	98
1,2-Dichloropropane	3.08	99
Bromodichloro-methane	2.76	100
4-methyl-2-pentanone	4.59	99
Methyl Methacrylate	4.00	103
cis-1,3-Dichloro-propene	4.16	96
Toluene	5.05	92
Chloroacetonitrile	9.16	81
2-Nitropropane	11.1	103
1,1,Dichloropropanone	4.83	86
Tetrachloroethene	7.24	93
trans-1,3-Dichloro-propene	3.72	98
Ethyl Methacrylate	3.50	104
1,1,2-Trichloroethane	2.71	102
Dibromochloro-methane	2.92	101
1,3-Dichloropropane	2.73	101
1,2-Dibromoethane	3.41	100
2-Hexanone	5.06	76
Chlorobenzene	4.20	94
Ethylbenzene	5.38	95
1,1,1,2-Tetrachloro-ethane	3.54	96
m,p-Xylene	5.92	91
o-Xylene	4.91	91
Styrene	4.42	93

Compound	Analyte recovery (10 ppb n=31, 191 injections)	
	Precision (≤20%RSD)	Accuracy (±30%)
Bromoform	3.63	103
Isopropylbenzene	6.13	94
4-Bromofluorobenzene (surr)	3.24	98
Bromobenzene	3.96	90
n-propylbenzene	7.15	99
1,1,2,2-Tetrachloro ethane[1]	9.19	94
2-Chlorotoluene	8.10	96
1,3,5-Trimethylbenzene	12.9	104
1,2,3-Trichloropropane	8.15	114
trans-1,4-Dichloro-2-butene[1]	6.39	99
4-Chlorotoluene	5.59	96
tert-Butylbenzene	7.87	94
Pentachloroethane	16.7	87
1,2,4-Trimethylbenzene	6.22	99
sec-Butylbenzene	8.56	103
p-Isopropyltoluene	8.17	102
1,3-Dichlorobenzene	5.81	95
1,4-Dichlorobenzene	5.18	95
n-Butylbenzene	9.08	106
1,2-Dichlorobenzene-d4 (surr)	7.52	99
Hexachloroethane[1]	4.11	101
1,2-Dichlorobenzene	4.80	96
1,2-Dibromo-3-chloropropane	4.71	110
Nitrobenzene	10.6	86
Hexachlorobutadiene	9.83	103
1,2,4-Trichlorobenzene	5.57	104
Naphthalene	4.09	107
1,2,3-Trichlorobenzene	5.20	107

[1]Compounds used a quadratic regression calibration

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