ThermoFisher
SCIENTIFIC

Environmental analysis

Uninterrupted analysis of volatile organic compounds in drinking water using single quadrupole GC-MS

Authors
Adam Ladak[1], Terry Jeffers[1], and Amy Nutter[2]

[1]Thermo Fisher Scientific, USA
[2]Teledyne Tekmar, Mason, OH, USA

Keywords
EPA, VOCs, phthalates, trace analysis, gas chromatography, single quadrupole mass spectrometry, selected ion monitoring, sensitivity, GRO, THM, volatiles, environmental lab, environmental sample analysis, analytical testing laboratories

Goal
Demonstration of a routine analytical method that meets the requirements outlined in U.S. EPA Method 524.2 for the quantitation of volatile organic compounds in drinking water, using the Teledyne Tekmar Atomx XYZ purge and trap (P&T) 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
It is essential that analytical testing laboratories monitor surface water, ground water, and drinking water for the presence of volatile organic compounds (VOCs). VOCs are human-made contaminants used and produced in the processing of, or as, paints, adhesives, petroleum products, pharmaceuticals, and refrigerants. If they are released into surface or ground water from industrial activities, they can have an adverse effect on natural environment, and ultimately the public. It is extremely important that analytical laboratories ensure both accurate and rapid detection and quantitation of VOCs to ensure public safety. U.S. EPA Method 524.2 is widely used in environmental analysis labs to test water samples for VOCs.[1] The method tests for a wide range of VOCs, including the four trihalomethane disinfection by-products that have sufficiently high volatility and low water solubility, so that they can be removed from water samples with P&T procedures.

thermo scientific

There are several challenges that analytical testing laboratories face when performing U.S. EPA Method 524.2. Laboratories must demonstrate the method acceptance criteria can be met, including detection limit requirements for an assortment of compounds over a wide range of concentrations. Another significant challenge is the management of the water sample matrix. Analysis of water samples can introduce moisture into the GC analytical column and cause damage if not properly managed. The resulting unproductive time of the analytical instrument can delay sample reporting, which could lead to public safety risks. The final challenge is to have a robust and reproducible method. If inconsistent results are produced with uncertainty, the samples will have to be reanalyzed, causing delays in sample reporting times.

This application note describes the use of the ISQ 7610 MS system coupled to a TRACE 1610 gas chromatograph (GC) and the Atomx XYZ P&T 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 81 compounds.

The calibration curve was prepared from 0.2 µg/L to 50 µg/L (parts per billion or ppb) for all compounds. The relative response factor (RRF) was calculated for each compound using one Restek internal standard: fluorobenzene (P/N 30030). Surrogate standards from Restek consisted of 4-bromofluorobenzene and 1,2-dichlorobenzene-d_4 (P/N 30607). 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 5 mL sample for a resulting concentration of 25 ppb.

A total of seven standards, each having a concentration of 0.2 µg/L, were prepared in deionized water to calculate the MDL and precision for all compounds. Also, seven standards containing 10 µg/L were prepared to determine the accuracy and precision of recovery of each compound. All calibration, MDL, and recovery standards were analyzed with the Atomx XYZ conditions in Table 1.

Table 1. Teledyne Tekmar Atomx XYZ Water method conditions

Standby	Variable	Desorb	Variable
Valve oven temp.	140 °C	Methanol needle rinse	Off
Transfer line temp.	140 °C	Water needle rinse volume	7.00 mL
Sample mount temp.	90 °C	Sweep needle time	0.25 min
Water heater temp.	90 °C	Desorb preheat temp.	245 °C
Sample cup temp.	20 °C	GC start signal	Begin desorb
Soil valve temp.	50 °C	Desorb time	4.00 min
Standby flow	10 mL/min	Drain flow	300 mL/min
Purge ready temp.	40 °C	Desorb temp.	250 °C
Purge	**Variable**	**Bake**	**Variable**
Sample equilibrate time	0.00 min	Methanol glass rinse	Off
Pre-sweep time	0.25 min	Water bake rinses	1
Prime sample fill volume	3.00 mL	Water bake rinse volume	7.00 mL
Sample volume	5.00 mL	Bake rinse sweep time	0.25 min
Sweep sample time	0.25 min	Bake rinse sweep flow	100 mL/min
Sweep sample flow	100 mL/min	Bake rinse drain time	0.40 min
Sparge vessel heater	Off	Bake time	2.00 min
Purge time	11.00 min	Trap bake temp.	260 °C
Purge flow	40 mL/min	MCS bake temp.	200 °C
Purge temp.	20 °C	Bake flow	200 mL/min
MCS purge temp.	20 °C		
Dry purge time	1.00 min	**Trap**	9
Dry purge flow	100 mL/min	**Chiller tray**	Off
Dry purge temp.	20 °C	**Purge gas**	Nitrogen

GC-MS conditions

A TRACE 1610 GC was coupled to the ISQ 7610 mass spectrometer equipped with the Thermo Scientific™ NeverVent™ vacuum probe interlock (VPI) and ExtractaBrite™ ion source. A Thermo Scientific™ TraceGOLD™ TG-VMS column, 20 m x 0.18 mm, 1 μm film (**P/N 26080-4950**), was used for compound separation. The injector was operated in split mode with a run time under 15 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.

Table 2. GC-MS conditions

TRACE 1610 GC conditions	
Column	TraceGOLD TG-VMS, 20 m x 0.18 mm, 1 μm film (**P/N 26080-4950**)
Carrier gas	Helium, 0.8 mL/min
Oven profile	35 ˚C, 3 min, 12 ˚C/min to 85 ˚C, 25 ˚C/min to 225 ˚C, 2 min hold, run time 14.767 min
Inlet	SSL at 200 ˚C, 50:1 Split, purge flow 0.5 mL/min
ISQ 7610 MS conditions	
Temp.	Transfer line 230 ˚C; ion source 280 ˚C
Scan	Range 35 amu to 260 amu, solvent delay 0.50 min, dwell/scan time 0.15 s
Current	Emission current 25 μA; gain 3.00E+005

Instrument control and data processing

Data were acquired, processed, and reported using Chromeleon CDS software, version 7.3. This software can control both the GC-MS system and the Atomx XYZ P&T. This allows a single software to be utilized for the full workflow, simplifying the instrument operation. Figure 1 shows the Chromeleon CDS control of the Atomx XYZ P&T. The fully optimized method used within this application note is available for download via AppsLab. AppsLab contains all the parameters needed to acquire, process, and report the analytical data for U.S. EPA Method 524.2.[2]

Results and discussion
Chromatography

Using the GC conditions described in Table 2, all compounds of interest were well resolved chromatographically. It is evident that there is minimal water transfer from the sample as there were no detrimental effects to peak shape due to moisture entering the analytical column. This resulted in optimized chromatography that was maintained in lower concentration samples. Figure 2 displays consistent peak shape and separation of a 10 ppb VOC standard with minimal water interference.

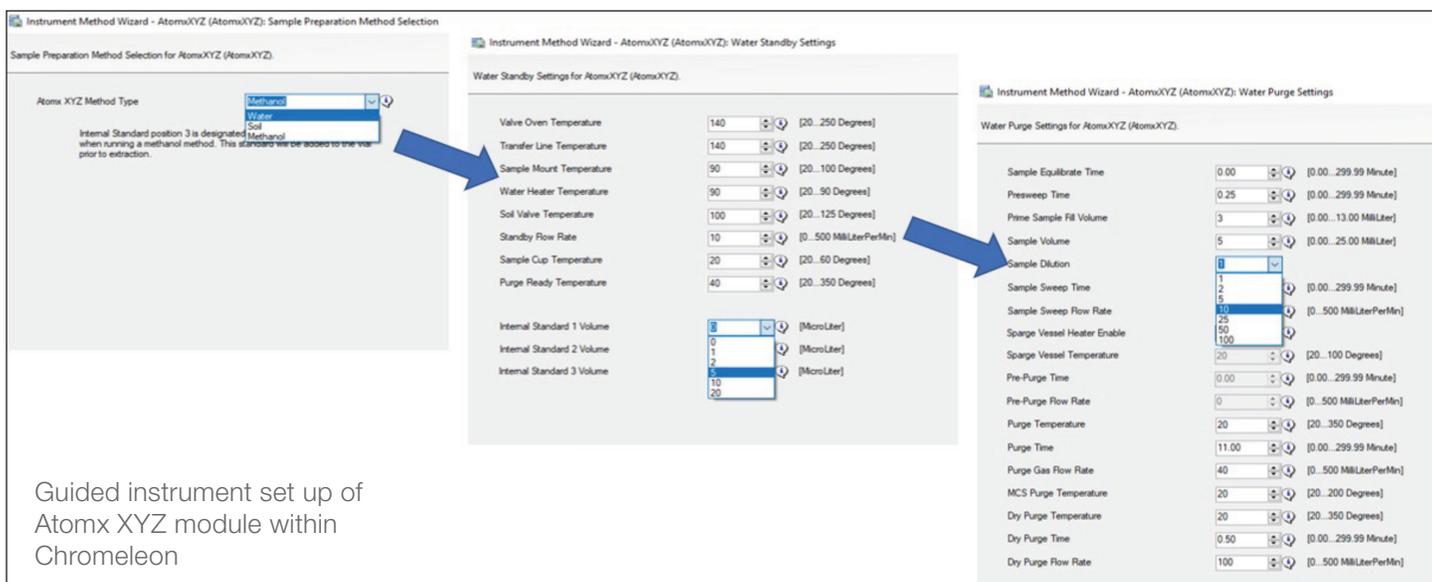Guided instrument set up of Atomx XYZ module within Chromeleon

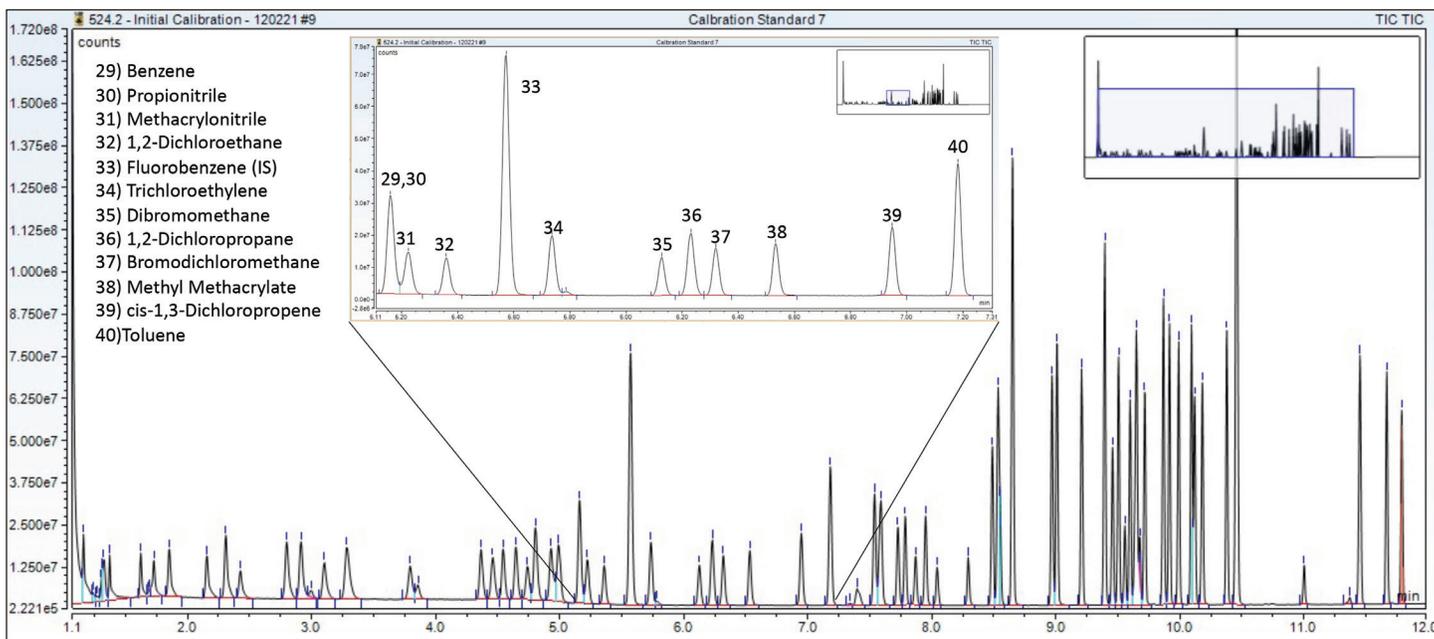Figure 1. Chromeleon control of the Atomx XYZ P&T

Figure 2. Total ion chromatogram (TIC) of a water method 10 ppb VOC standard with an inset indicating consistent peak shapes and separation with minimal water interference

Linearity and sensitivity

The calibration range of 0.2 ppb to 50 ppb was assessed for all compounds. Figure 3 demonstrates the quantitation of *o*-xylene at 0.2 ppb in a VOC standard with very good library spectral matching and calibration curve. Figure 4 demonstrates the same information for 1,3-dichloropropane. Appendix 1 displays the relative standard deviation (%RSD) of the response factors (RFs) which were less than 20% for all compounds, except for

acetone, 2-butanone, 2-nitropropane, hexachloroethane, and nitrobenzene, which used a linear calibration and achieved $R^2 > 0.99$ for these compounds. Appendix 1 also shows the MDL and precision (RSD%) for each analyte calculated by injecting n=7 injections of the 0.2 ppb water standard. Figure 3 shows a subset of the data with calculated MDLs and precision for 40 compounds.
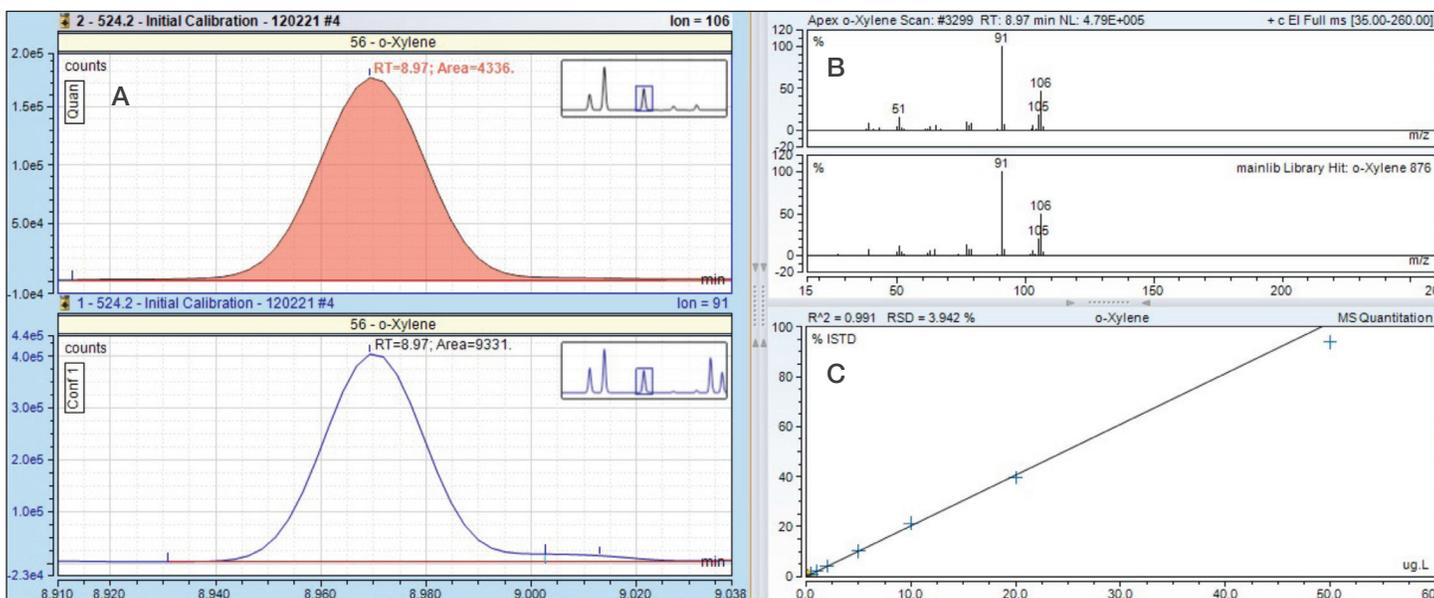

Figure 3. Chromeleon CDS results browser showing extracted ion chromatograms for *o*-xylene in the 0.2 ppb water standard, quantitation ion (*m/z* = 106), and one confirming ion (*m/z* = 91) (A), a matching measured spectrum to the NIST library (B), and a linear calibration over a concentration range of 0.2 ppb to 50 ppb (C)
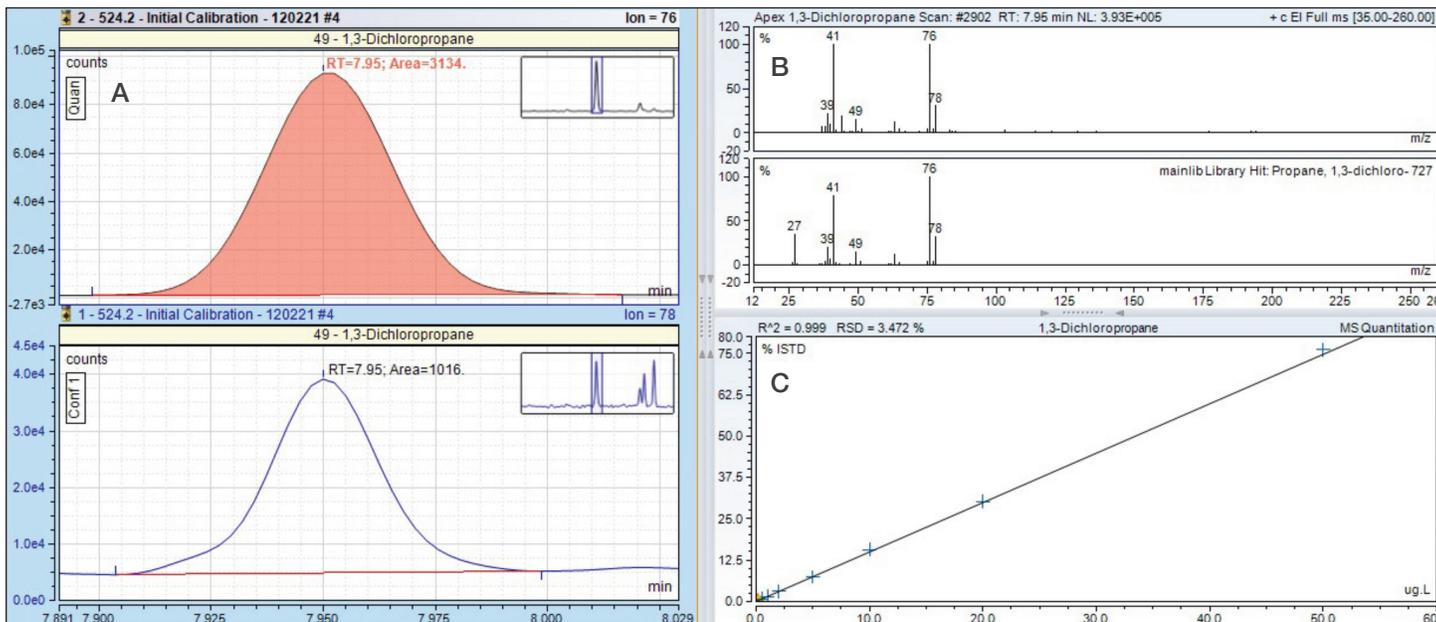
4

Figure 4. Chromeleon CDS results browser showing extracted ion chromatograms for 1,3-dichloropropane in the 0.2 ppb water standard, quantitation ion (*m/z* = 76) and one confirming ion (*m/z* = 78) (A), a matching measured spectrum to the NIST library (B), and a linear calibration over a concentration range of 0.2 ppb to 50 ppb (C)
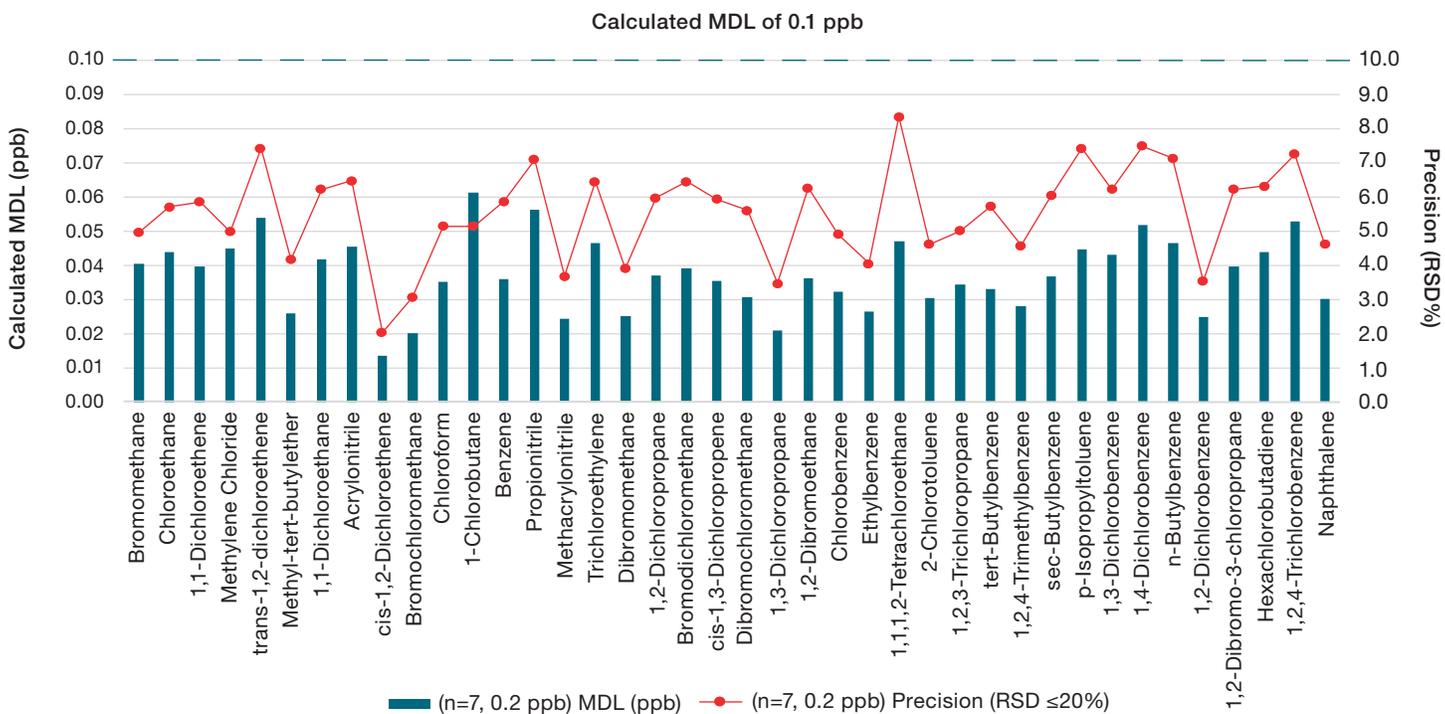
Figure 5. MDL and precision calculated for a subset of compounds (n=40) from n=7 injections of a 0.2 ppb water standard

Method robustness

Analytical testing labs must maximize the utilization of their GC-MS system to ensure results are delivered to customers in a timely manner. To assess the stability of the method, 10 ppb calibration check standards were injected at intervals 32 times over a sequence of 197 injections. This extended sequence is equivalent to 3 days of uninterrupted analysis. No maintenance

was performed on any part of the system during this extended test. Figure 6 shows the reproducibility of 6 of the compounds over 197 injections with excellent percentage RSDs. RSDs for all compounds were well below 30%, as required by the method. Appendix 2 shows the reproducibility results for all compounds over the 197-injection sequence.

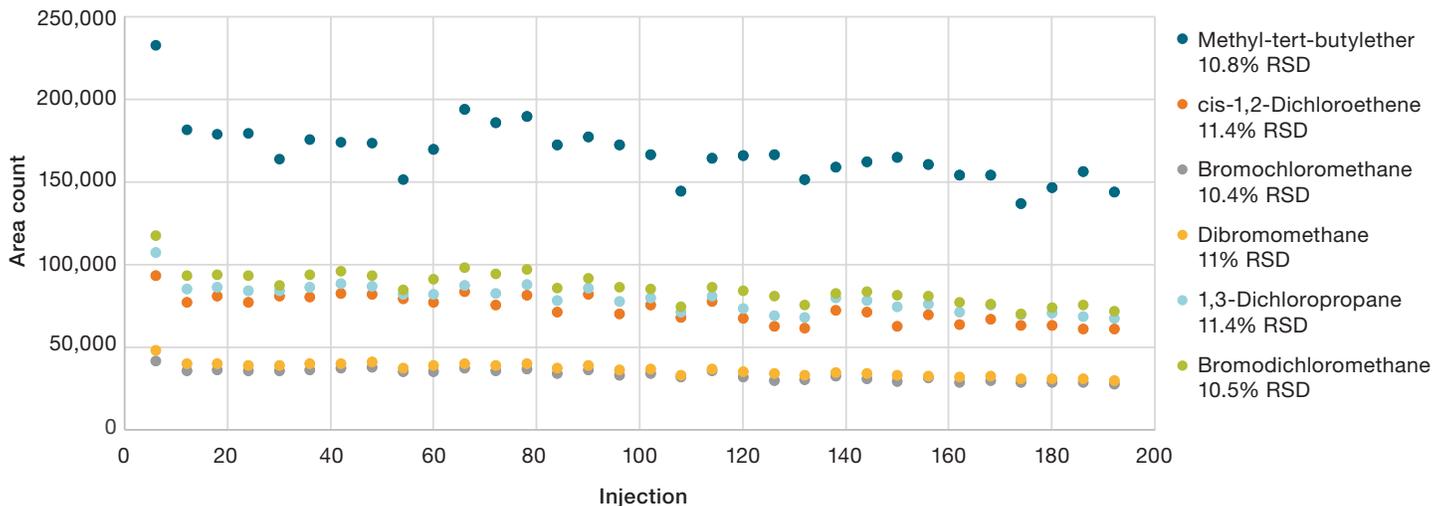**Figure 6. Repeatability of a 10 ppb VOC standard (n=32) (as absolute peak area counts) assessed over n=197 consecutive injections**

Legend:
- Methyl-tert-butylether 10.8% RSD
- cis-1,2-Dichloroethene 11.4% RSD
- Bromochloromethane 10.4% RSD
- Dibromomethane 11% RSD
- 1,3-Dichloropropane 11.4% RSD
- Bromodichloromethane 10.5% RSD

Conclusion

The combined solution of the TRACE 1610 GC coupled with the ISQ 7610 system and the Atomx XYZ P&T system provides clear advantages for U.S. EPA Method 524.2. The Atomx XYZ concentrator's efficient trap cooling design reduces sample cycle time, enabling an increase in sample throughput. The moisture control system improves water vapor removal, thereby reducing peak interference and increasing GC column life span. The ISQ 7610 VPI and ExtractaBrite ion source allow users to exchange ionization sources and analytical columns without venting the instrument, significantly reducing instrument downtime and minimizing sample analysis interruptions. The Thermo Scientific™ XLXR™ detection system on the ISQ 7610 mass spectrometer provides an extended linear dynamic range, allowing extended calibration curves to be run on the system. The detector also has an extended lifetime, which significantly reduces the need for replacement. Combined, these technologies effectively address the challenges of routine VOC analysis and provide a robust, sensitive solution needed for ensuring maximized instrument output and routine regulatory method compliance for U.S. EPA Method 524.2:

- The ISQ 7610 VPI coupled with the Teledyne Tekmar Atomx XYZ P&T exceeds all the requirements outlined in U.S. EPA Method 524.2 for analysis of VOCs in water.

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

- MDL, precision, and accuracy for seven 0.2 ppb standards showed no interference from excessive water and produced very reproducible results.

- The precision for n=32 samples over 197 injections displayed <30% RSD for all compounds as the method requires and an average recovery of 103%.

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 Application Note 65632: Routine Analysis of volatile organic compounds in drinking water using the Thermo Scientific ISQ 7000 MS system. **https://appslab.thermofisher.com/App/4373/epa-5242-compounds-drinking-water-by-gcms**

Appendix 1. U.S. EPA Method 524.2 calibration, accuracy, and precision data

Compound	Calibration				Accuracy and precision (n=7, 0.2 ppb)		Mid-point check (n=7, 10 ppb)	
	Retention time	Quant ion	Linearity (RRF %RSD)	Average RF	MDL (ppb)	Precision (RSD ≤20%)	Precision (≤20%)	Accuracy (±30%)
Dichlorodifluoromethane	1.16	85	8.6	0.335	0.06	8.7	6.2	109
Chloromethane	1.32	50	6.5	0.634	0.04	7.1	5.1	114
Vinyl chloride	1.37	62	8.0	0.330	0.06	8.2	5.9	115
Bromomethane	1.62	94	11.9	0.279	0.04	5.0	7.9	119
Chloroethane	1.73	64	18.8	0.229	0.04	5.7	4.9	115
Trichlorofluoromethane	1.85	101	7.9	0.443	0.05	7.6	5.5	114
Diethyl ether	2.16	59	4.5	0.217	0.09	14.4	3.2	119
Carbon disulfide	2.31	76	11.3	0.369	0.05	6.5	5.3	107
1,1-Dichloroethene	2.31	96	10.1	0.234	0.04	5.9	5.2	105
Methyl iodide	2.43	142	9.5	0.386	0.03	8.4	7.3	90
Allyl chloride	2.80	76	7.0	0.142	0.05	8.4	5.2	109
Methylene chloride	2.91	84	16.5	0.325	0.05	5.0	4.1	102
Acetone[1,2,5]	2.99	43	0.998	0.114	0.86	12.5	3.0	130
trans-1,2-dichloroethene	3.10	96	11.9	0.253	0.05	7.4	5.3	107
Methyl-tert-butylether	3.29	73	5.5	0.678	0.03	4.2	2.6	119
1,1-Dichloroethane	3.80	63	5.9	0.454	0.04	6.2	4.2	115
Acrylonitrile	3.86	52	8.4	0.100	0.05	6.5	3.6	113
cis-1,2-Dichloroethene	4.37	96	7.1	0.299	0.01	2.0	3.9	109
2,2-Dichloropropane	4.46	77	8.3	0.317	0.07	11.1	7.5	82
Bromochloromethane	4.54	128	7.3	0.142	0.02	3.1	3.8	107
Chloroform	4.65	83	8.5	0.470	0.04	5.2	4.2	114
Carbon tetrachloride	4.74	117	6.4	0.306	0.09	11.6	5.0	116
1,1,1-Trichloroethane	4.80	97	7.4	0.350	0.07	10.0	9.2	100
Methyl acrylate	4.80	55	5.4	0.204	0.05	7.8	6.8	111
Tetrahydrofuran[6]	4.80	71	12.9	0.046	0.14	8.5	5.2	112
1,1-Dichloropropene	4.93	75	7.3	0.269	0.05	7.5	5.3	111
2-Butanone[1,2,5]	4.97	43	0.997	0.195	0.57	6.3	6.6	114
1-Chlorobutane	4.99	56	9.0	0.405	0.06	5.2	4.5	113
Benzene	5.16	78	3.1	0.882	0.04	5.9	4.5	104
Propionitrile	5.20	54	7.7	0.045	0.06	7.1	6.3	108
Methacrylonitrile	5.22	67	6.3	0.120	0.02	3.7	3.6	106
1,2-Dichloroethane	5.36	62	4.0	0.288	0.02	3.2	2.9	120
Fluorobenzene (ISTD)	5.57	96	-	-	-	-	-	-
Trichloroethylene	5.73	95	5.8	0.247	0.05	6.5	4.8	115
Dibromomethane	6.13	93	5.1	0.170	0.03	3.9	4.1	106
1,2-Dichloropropane	6.23	63	3.5	0.255	0.04	6.0	3.5	112
Bromodichloromethane	6.32	83	3.6	0.330	0.04	6.5	3.2	112

Appendix 1 continued. U.S. U.S. EPA Method 524.2 calibration, accuracy, and precision data

Compound	Calibration				Accuracy and precision (n=7, 0.2 ppb)		Mid-point check (n=7, 10 ppb)	
	Retention time	Quant ion	Linearity (RRF %RSD)	Average RF	MDL (ppb)	Precision (RSD ≤20%)	Precision (≤20%)	Accuracy (±30%)
Methyl methacrylate	6.54	69	6.9	0.163	0.06	9.6	3.0	108
cis-1,3-Dichloropropene	6.95	75	2.7	0.371	0.04	5.9	3.6	106
Toluene	7.18	92	3.5	0.615	0.03	4.8	4.3	103
2-Nitropropane[1,7]	7.32		0.997	0.004	0.95	12.7	7.6	103
1,1,Dichloropropanone[3]	7.41	43	11.2	0.090	0.14	8.8	4.8	96
Tetrachloroethene	7.54	166	7.2	0.365	0.04	4.8	4.6	130
4-methyl-2-pentanone[3]	7.58	43	4.4	0.165	0.12	6.7	3.2	115
trans-1,3-Dichloropropene	7.59	75	5.1	0.341	0.04	6.6	2.9	107
1,1,2-Trichloroethane	7.73	83	3.8	0.212	0.03	5.5	3.3	109
Ethyl methacrylate	7.79	69	4.0	0.316	0.02	2.5	2.6	113
Dibromochloromethane	7.87	129	6.7	0.217	0.03	5.6	2.7	109
1,3-Dichloropropane	7.95	76	3.5	0.374	0.02	3.5	3.2	112
1,2-Dibromoethane	8.04	107	5.7	0.231	0.04	6.3	3.1	109
2-Hexanone[3]	8.30	43	10.1	0.133	0.14	8.3	2.7	112
Chlorobenzene	8.49	112	4.1	0.717	0.03	4.9	4.0	102
Ethylbenzene	8.54	91	6.0	1.202	0.03	4.1	4.1	107
1,1,1,2-Tetrachloroethane	8.55	131	6.7	0.195	0.05	8.4	3.9	110
m,p-Xylene	8.65	106	5.7	0.511	0.08	6.1	5.4	105
o-Xylene	8.97	106	3.9	0.508	0.03	4.4	3.7	102
Bromoform	9.01	173	11.8	0.148	0.01	2.5	3.0	116
Styrene	9.01	104	6.0	0.870	0.03	4.9	3.9	103
Isopropylbenzene	9.21	105	4.1	1.199	0.03	5.2	4.9	105
4-Bromofluorobenzene (surr)	9.40	95	5.4	0.439		3.6	1.1	102
Bromobenzene	9.46	156	5.2	0.345	0.03	4.6	2.5	105
n-propylbenzene	9.51	91	6.6	1.549	0.03	5.1	4.7	106
1,1,2,2-Tetrachloroethane	9.56	83	4.7	0.323	0.05	8.7	4.0	96
2-Chlorotoluene	9.60	91	5.9	0.937	0.03	4.6	4.5	108
1,2,3-Trichloropropane	9.64	75	4.9	0.258	0.03	5.0	3.5	112
1,3,5-Trimethylbenzene	9.65	105	4.8	1.108	0.03	4.5	5.4	109
trans-1,4-Dichloro-2-butene	9.68	53	3.7	0.113	0.06	8.9	4.1	112
4-Chlorotoluene	9.72	91	7.3	1.013	0.04	5.3	3.8	107
tert-Butylbenzene	9.87	119	4.5	0.990	0.03	5.7	5.2	99
1,2,4-Trimethylbenzene	9.92	105	4.8	1.141	0.03	4.6	4.9	109
sec-Butylbenzene	9.99	105	6.5	1.354	0.04	6.0	5.5	107
p-Isopropyltoluene	10.09	119	5.5	1.107	0.04	7.4	5.6	107

Appendix 1 continued. U.S. EPA Method 524.2 calibration, accuracy, and precision data

Compound	Calibration				Accuracy and precision (n=7, 0.2 ppb)		Mid-point check (n=7, 10 ppb)	
	Retention time	Quant ion	Linearity (RRF %RSD)	Average RF	MDL (ppb)	Precision (RSD ≤20%)	Precision (≤20%)	Accuracy (±30%)
1,3-Dichlorobenzene	10.12	146	7.7	0.701	0.04	6.2	4.5	104
1,4-Dichlorobenzene	10.18	146	10.6	0.725	0.05	7.5	4.9	102
n-Butylbenzene	10.38	91	8.3	1.152	0.05	7.1	6.3	105
1,2-Dichlorobenzene-d[4] (surr)	10.46	152	6.2	0.463		3.8	3.9	104
Hexachloroethane[1,4,7]	10.46	117	0.999	2.650	1.06	13.7	7.6	108
1,2-Dichlorobenzene	10.46	146	9.2	0.723	0.02	3.5	4.2	104
1,2-Dibromo-3-chloropropane	11.00	75	9.0	0.063	0.04	6.2	4.0	115
Nitrobenzene[1,4,8]	11.35	51	0.998	0.027	0.31	10.2	3.6	107
Hexachlorobutadiene	11.44	225	7.8	0.113	0.04	6.3	4.4	115
1,2,4-Trichlorobenzene	11.45	180	12.1	0.501	0.05	7.3	5.0	105
Naphthalene	11.67	128	6.5	1.338	0.03	4.6	5.0	104
1,2,3-Trichlorobenzene	11.79	180	7.3	0.494	0.04	6.0	4.9	107

[1]Compound used a linear regression calibration
[2]Calibration range 2.5–125 ppb
[3]Calibration range 0.5–125 ppb
[4]Calibration range 0.5–50 ppb
[5]MDL calculated using n=7, 2.5 ppb
[6]MDL calculated using n=7, 0.5 ppb
[7]MDL calculated using n=7, 2 ppb
[8]MDL calculated using n=7, 1 ppb

Appendix 2. Repeatability of a 5 ppb VOC standard (n=32) (as absolute peak area counts) assessed over n=197 consecutive injections

Compound	Analyte recovery (197 injections, n=32 samples, 10 ppb)	
	Precision (≤30%)	Accuracy (±30%)
Dichlorodifluoromethane	22.7	72
Chloromethane	18.7	80
Vinyl chloride	14.9	86
Bromomethane	10.0	90
Chloroethane	9.3	111
Trichlorofluoromethane	11.0	101
Diethyl ether	5.2	118
1,1-Dichloroethene	9.6	88
Carbon disulfide[1]	7.0	64
Methyl iodide	16.1	71
Allyl chloride	9.2	99
Methylene chloride	4.8	103
Acetone[2]	18.3	181
trans-1,2-dichloroethene	7.6	90
Methyl-tert-butylether	7.7	118
1,1-Dichloroethane	6.0	129
Acrylonitrile[3]	10.7	135

Appendix 2 continued. Repeatability of a 5 ppb VOC standard (n=32) (as absolute peak area counts) assessed over n=197 consecutive injections

Compound	Analyte recovery (197 injections, n=32 samples, 10 ppb)	
	Precision (≤30%)	Accuracy (±30%)
cis-1,2-Dichloroethene	6.3	116
2,2-Dichloropropane[1]	28.5	78
Bromochloromethane	5.2	112
Chloroform[3]	8.7	131
Carbon tetrachloride	10.3	115
1,1,1-Trichloroethane	10.4	115
Methyl acrylate	11.8	126
Tetrahydrofuran	10.8	98
1,1-Dichloropropene	8.5	106
2-Butanone[3]	13.5	146
1-Chlorobutane	8.7	117
Benzene	6.9	89
Propionitrile	9.4	113
Methacrylonitrile	7.2	93
1,2-Dichloroethane	5.5	124
Fluorobenzene (ISTD)	-	-
Trichloroethylene	7.9	106
Dibromomethane	4.7	102
1,2-Dichloropropane	5.5	109
Bromodichloromethane	7.1	115
Methyl methacrylate	10.3	77
cis-1,3-Dichloropropene	11.6	82
Toluene	11.1	80
2-Nitropropane	16.0	120
1,1,Dichloropropanone	16.8	85
Tetrachloroethene	6.2	118
4-methyl-2-pentanone	7.8	112
trans-1,3-Dichloropropene	9.8	94
1,1,2-Trichloroethane	7.4	113
Ethyl methacrylate	9.6	85
Dibromochloromethane	8.2	108
1,3-Dichloropropane	5.2	109
1,2-Dibromoethane	5.5	102
2-Hexanone	12.3	103
Chlorobenzene	6.9	90
Ethylbenzene	11.0	90
1,1,1,2-Tetrachloroethane	8.2	111
m,p-Xylene	9.6	91

Appendix 2 continued. Repeatability of a 5 ppb VOC standard (n=32) (as absolute peak area counts) assessed over n=197 consecutive injections

Compound	Analyte recovery (197 injections, n=32 samples, 10 ppb)	
	Precision (≤30%)	Accuracy (±30%)
o-Xylene	11.5	81
Bromoform	8.4	113
Styrene	8.0	92
Isopropylbenzene	12.5	88
4-Bromofluorobenzene (surr)	2.8	111
Bromobenzene	5.8	103
n-propylbenzene	10.9	97
1,1,2,2-Tetrachloroethane	13.3	93
2-Chlorotoluene	8.4	101
1,2,3-Trichloropropane	8.5	124
1,3,5-Trimethylbenzene	10.0	97
trans-1,4-Dichloro-2-butene	13.2	113
4-Chlorotoluene	8.3	104
tert-Butylbenzene	13.6	86
1,2,4-Trimethylbenzene	10.0	98
sec-Butylbenzene	12.2	98
p-Isopropyltoluene	13.1	90
1,3-Dichlorobenzene	7.0	106
1,4-Dichlorobenzene	6.8	100
n-Butylbenzene	14.1	94
1,2-Dichlorobenzene-d_4 (surr)	3.8	118
Hexachloroethane	11.1	123
1,2-Dichlorobenzene	6.2	107
1,2-Dibromo-3-chloropropane	8.0	101
Nitrobenzene	14.8	90
Hexachlorobutadiene	13.5	104
1,2,4-Trichlorobenzene	11.8	89
Naphthalene	9.8	84
1,2,3-Trichlorobenzene	7.7	101

[1]This is a highly reactive compound, therefore, only 17 samples were analyzed.
[2]The laboratory has contamination of this compound, therefore, it recovered high.
[3]This is a highly reactive compound that started to recover high.

Learn more at **thermofisher.com/ISQ7610**

thermo scientific