

## Environmental

# Sustainable uncompromised performance: analysis of volatile organic compounds in drinking water with the ISQ 7610 GC-MS using HeSaver-H<sub>2</sub>Safer technology

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## Keywords

Helium, HeSaver-H<sub>2</sub>Safer, EPA, EPA Method 524.4, VOCs, trace analysis, gas chromatography, single quadrupole mass spectrometry, volatiles, environmental sample analysis, analytical testing laboratories, ISQ 7610 GC-MS, TRACE 1610 GC

## Goal

Demonstration of a routine analytical method that meets the requirements outlined in U.S. EPA Method 524.4 for the quantitation of volatile organic compounds (VOCs) 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), equipped with the Thermo Scientific™ HeSaver-H<sub>2</sub>Safer™ technology for split splitless (SSL) injector, and Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS) software. Method linearity, method detection limit (MDL), precision, and MRL were assessed to evaluate method performance. A long-term study was performed to ensure the stability of this analytical method.

## Introduction

VOCs are analyzed widely in environmental laboratories that follow strict EPA regulations, including U.S. EPA Methods 524.2, 524.4, and 8260. VOCs are human-made contaminants, used and produced in the processing of, or as, paints, adhesives, petroleum products, pharmaceuticals, and refrigerants. When released into surface or ground water, they can have an adverse effect on the ecosystem. It is extremely important that analytical laboratories ensure both accurate and rapid detection and quantitation of VOCs to ensure public safety.

In a previous application note, the use of the ISQ 7610 MS system coupled with a TRACE 1610 GC and the Teledyne Tekmar Atomx XYZ P&T for U.S. EPA Method 524.4<sup>1</sup> was demonstrated. The method targets 75 VOCs and differs from U.S. EPA Method 524.2 as nitrogen is required as a purge gas and the method allows more flexibility with the parameters. Although the parameters are more flexible, U.S. EPA Method 524.4 has stricter QC requirements to ensure the method is fit for purpose. These QC requirements include the minimum reporting level (MRL), which is determining the upper and lower limits used to evaluate the continuing calibration checks. This is intended to minimize the occurrence of reporting false positive results. U.S. EPA Method 524.4 requires a linear or quadratic regression ( $r^2$ ) of 0.995 or better, where weighting of the individual calibration points may be used but forcing the calibration curve through zero cannot be applied. The lowest concentration in the curve must be within  $\pm 50\%$  of its true value, whereas all other points must be within  $\pm 30\%$ . The samples must also be chilled, which involves using the chiller tray upgrade for the Atomx XYZ P&T.

Helium is used as the carrier gas of choice for GC-MS analysis of VOCs; however, recently there have been several challenges in obtaining the helium supply for the analysis. Switching to alternative carrier gases, such as hydrogen, is a possible solution, but MS vacuum and detection performance are reduced, which may lead to issues with regulatory compliance. This highlights the need for helium conservation to maintain current system performance. The Thermo Scientific HeSaver-H<sub>2</sub>Safer carrier gas saving technology<sup>2</sup> offers an innovative approach to significantly reduce carrier gas consumption, even during GC operation. It consists of a modified Split Splitless (SSL) injector body connected to two gas lines: an inexpensive gas (e.g., nitrogen or argon) is used for inlet pressurization, analyte vaporization, and transfer to the analytical column, while the selected carrier gas (e.g., helium or hydrogen) is used only to supply the chromatographic column for the separation process, with a limited maximum flow rate. When used with helium as the carrier gas, the limited consumption allows mitigation of shortage issues while maintaining GC-MS performance without the need for method re-optimization, typically required when switching to a different carrier gas.

The following evaluation describes the use of the ISQ 7610 GC-MS system equipped with the HeSaver-H<sub>2</sub>Safer SSL inlet and the Atomx XYZ P&T for U.S. EPA Method 524.4.

## Experimental

### Sample preparation

A 50  $\mu\text{g}/\text{mL}$  (equivalent to 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: 524.3 VOA MegaMix™ (P/N 30013) and 524.3 Gas Calibration Mix (P/N 30014). In total, the standard contained 75 compounds.

The calibration curve was prepared to contain 0.2  $\mu\text{g}/\text{L}$  to 50  $\mu\text{g}/\text{L}$  (parts per billion or ppb) for all compounds. The relative response factor (RRF) was calculated for each compound using three Restek internal standard: 1,4-difluorobenzene, chlorobenzene-d<sub>5</sub>, and 1,4-dichlorobenzene-d<sub>4</sub> (P/N 30017). Surrogate standards from Restek consisted of methyl-*t*-butyl ether-d<sub>3</sub>, 4-bromofluorobenzene, and 1,2-dichlorobenzene (P/N 30017). Internal and surrogate standards were prepared in methanol at a concentration of 12.5 ppm, after which 5  $\mu\text{L}$  was then mixed with each 5 mL water sample for a resulting concentration of 12.5 ppb.

A total of seven standards at a concentration of 0.5 ppb were prepared in deionized water to determine the MDL and precision calculations for all compounds. Also, ten 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 Atomx XYZ using the conditions summarized in Table 1. Seven individual standards with a concentration of 1 ppb of each compound were prepared to determine the MRL.

### GC-MS conditions

A TRACE 1610 GC was coupled to the ISQ 7610 single quadrupole mass spectrometer equipped with the Thermo Scientific™ NeverVent™ vacuum probe interlock (VPI) and a Thermo Scientific™ ExtractaBrite™ ion source. A Thermo Scientific™ TraceGOLD™ TG-VMS column, 20 m x 0.18 mm, 1  $\mu\text{m}$  film (P/N 26080-4950) was used for compound separation. The injector was operated in split mode, and a sample turnover time of under 16 minutes was achieved. The HeSaver-H<sub>2</sub>Safer SSL inlet allows for most previous method parameters to remain the same, with the addition of new parameters to optimize the performance of the inlet. For example, the helium delay and nitrogen as the pressurizing gas allow for extended helium tank life. The ISQ 7610 single quadrupole mass spectrometer was operated in full scan mode, offering sufficient sensitivity to achieve the required limits of detection. The instrument can also be operated in Selected Ion Monitoring (SIM) mode to increase selectivity. Expanded method parameters for the ISQ 7610 GC-MS are displayed in Table 2.

**Table 1. Teledyne Tekmar Atomx XYZ water method conditions**

Standby	Variable
Valve oven temperature	140 °C
Transfer line temperature	140 °C
Sample mount temperature	90 °C
Water heater temperature	90 °C
Sample cup temperature	20 °C
Soil valve temperature	50 °C
Standby flow	10 mL/min
Purge ready temperature	40 °C
Purge	Variable
Sample equilibrate time	0.00 min
Pre-sweep time	0.25 min
Prime sample fill volume	3.00 mL
Sample volume	5.00 mL
Sweep sample time	0.25 min
Sweep sample flow	100 mL/min
Sparge vessel heater	Off
Purge time	8.00 min
Purge flow	55 mL/min
Purge temperature	20 °C
MCS purge temperature	20 °C
Dry purge time	0.5 min
Dry purge flow	100 mL/min
Dry purge temperature	20 °C
Desorb	Variable
Methanol needle rinse	Off
Water needle rinse volume	7.00 mL
Sweep needle time	0.25 min
Desorb preheat temperature	245 °C
GC start signal	Begin Desorb
Desorb time	1.00 min
Drain flow	300 mL/min
Desorb temperature	250 °C
Bake	Variable
Methanol glass rinse	Off
Water bake rinses	1
Water bake rinse volume	7.00 mL
Bake rinse sweep time	0.25 min
Bake rinse sweep flow	100 mL/min
Bake rinse drain time	0.40 min
Bake time	2.00 min
Trap bake temperature	270 °C
MCS bake temperature	200 °C
Bake flow	200 mL/min
<b>Trap</b>	Teledyne Tekmar #9 Proprietary U-shaped trap
<b>Chiller tray</b>	On
<b>Purge gas</b>	Nitrogen

**Table 2. GC-MS conditions**

TRACE 1610 GC conditions	
Column	TraceGOLD TG-VMS, 20 m × 0.18 mm, 1 µm film (P/N 26080-4950)
Carrier gas	Helium, 0.3 mL/min
Oven profile	35 °C, 4 min, 12 °C /min to 85 °C, 25 °C/min to 225 °C, 2 min hold, run time 15.767 min
Inlet	200 °C, 50:1 split, purge flow 5.0 mL/min, 0.40 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 1.55 min, dwell/scan time 0.10 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. The 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. 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 EPA Method 524.4.<sup>3</sup>

## Results and discussion

### Chromatography

Using the GC conditions described in Table 2, all compounds of interest were chromatographically well resolved. The chromatography was consistent with the results obtained with the standard split/splitless injector. The HeSaver-H<sub>2</sub>Safer inlet produces excellent results without any impact on chromatography. Figure 1 displays consistent peak shape and separation of a 10 ppb VOC standard with minimal water interference.

### Linearity and sensitivity

The calibration range of 0.2 ppb to 50 ppb was assessed for all compounds. Figure 2 demonstrates the quantitation of 4-chlorotoluene at 5 ppb in a VOC standard with excellent library spectral matching and calibration curve. Figure 3 shows the MDL and precision calculated for a subset of compounds and Appendix 1 displays the linear correlation ( $r^2$ ) and the MDL for each analyte calculated by injecting n=7 injections of the 0.5 ppb water standard. Also included is the MRL data, which was calculated by injecting n=7 of a 1 ppb standard.

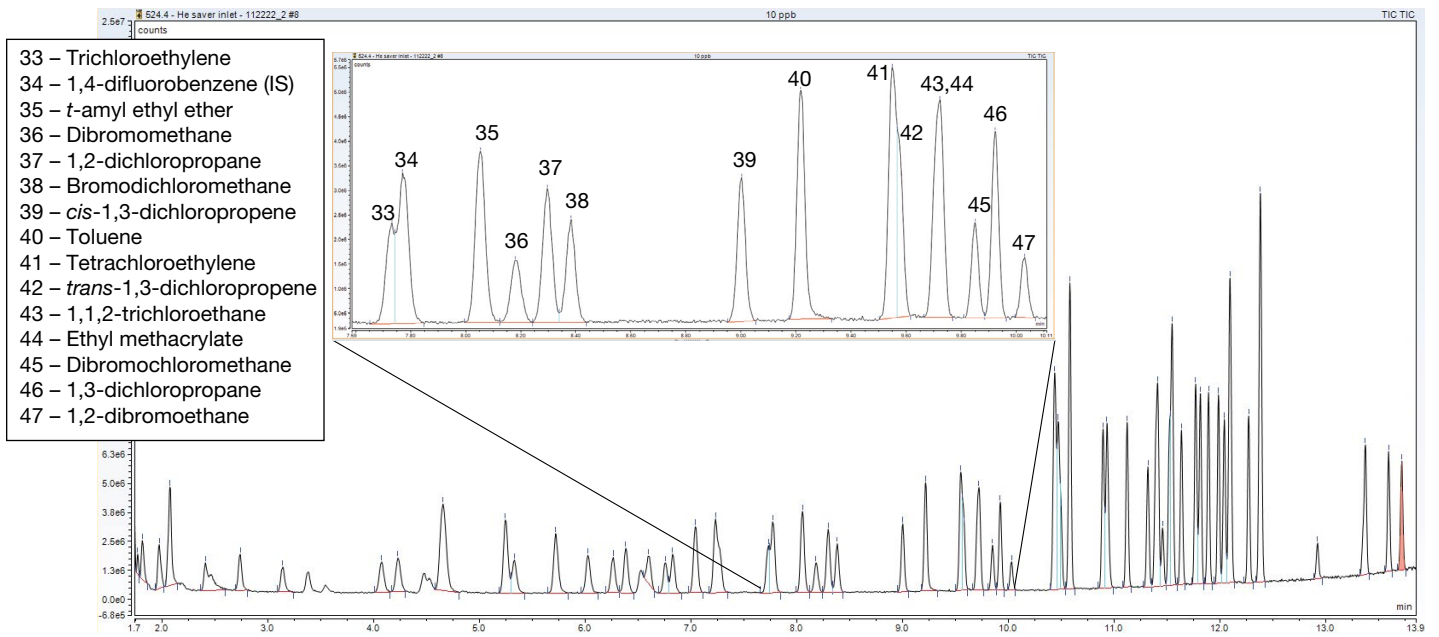


Figure 1. Total ion chromatogram (TIC) of a water method 10 ppb VOC standard with an inset indicating consistent peak shapes and separation with minimal water interference

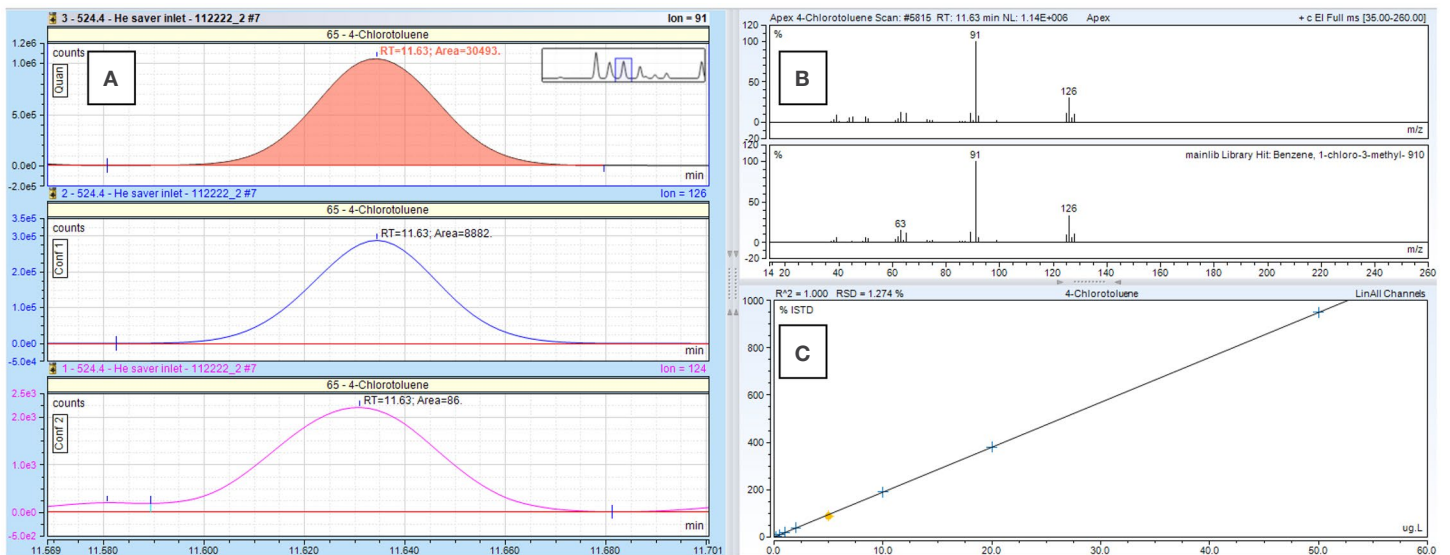


Figure 2. Chromleon CDS results browser showing extracted ion chromatograms for 4-chlorotoluene in the 5 ppb water standard, quantitation ion ( $m/z = 91$ ) and two confirming ions ( $m/z = 126, 124$ ) (A), a matching measured spectrum to the NIST library (B), and a linear calibration over a concentration range of 0.2 ppb to 50 ppb (C)

## 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 26 times over a sequence of 160 injections. This extended sequence is equivalent to two days of uninterrupted analysis. No maintenance

was performed on any part of the system during this extended test. Figure 4 shows the reproducibility of 12 of the compounds over 160 injections with excellent percentage RSDs. RSDs for all compounds were under the 30% method requirements. Appendix 2 shows the reproducibility results for all compounds over the 160-injection sequence.

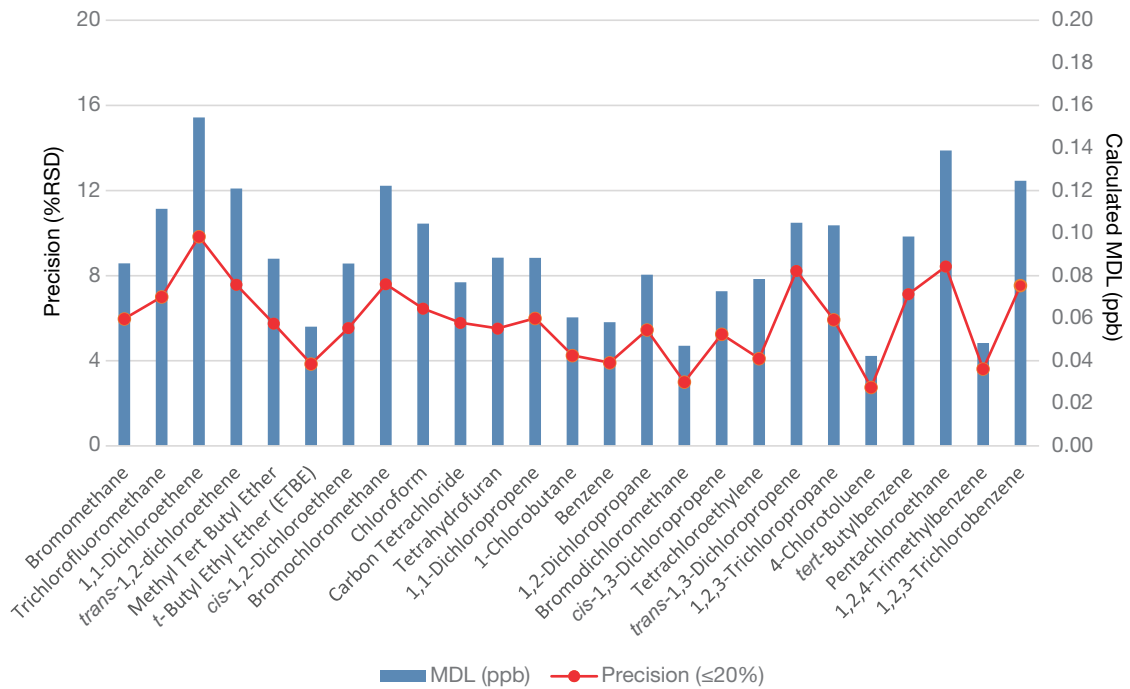


Figure 3. MDL and precision calculated for a subset of compounds (n=25) from n=7 injections of a 0.5 ppb water standard

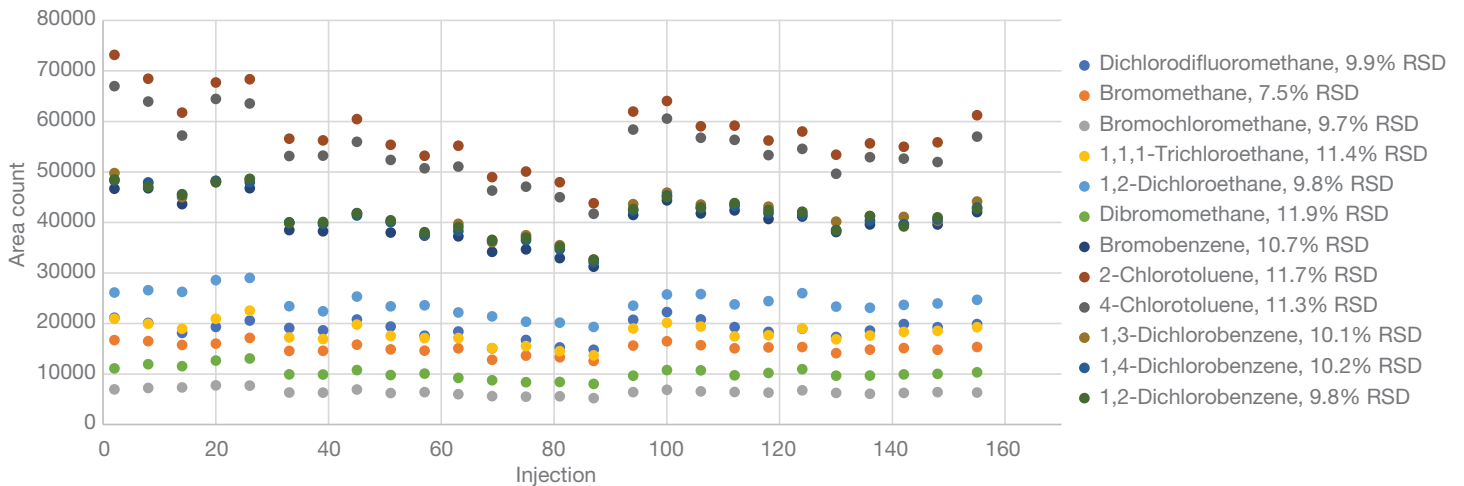


Figure 4. Repeatability of a 10 ppb VOC standard (n=26) (as absolute peak area counts) assessed over n=160 consecutive injections

### Reduced helium consumption and cost savings

The HeSaver-H<sub>2</sub>Safer technology offers significant gas savings not only when the GC is idle but during operation. This technology can extend helium/hydrogen cylinder lifetime from months to years, depending on instrument method parameters, usage, and the number of GCs supported by a given gas cylinder. The [Thermo Scientific™ Helium Saver Calculator](#) tool<sup>4</sup> offers an easy-to-use and intuitive interface to estimate helium consumption and cost impact on an individual laboratory's activities. GC parameters

regarding column dimensions, carrier gas and split flow settings, as well as helium and nitrogen costs are adjustable to reflect a given laboratory's methodology and regional gas cost to provide estimates on helium cylinder lifetime and cost savings (Figure 5). The usage of the HeSaver-H<sub>2</sub>Safer technology for the analysis of VOCs according to U.S. EPA Method 524.4 would allow the helium cylinder to last four times longer in comparison to the usage of a standard SSL injector.

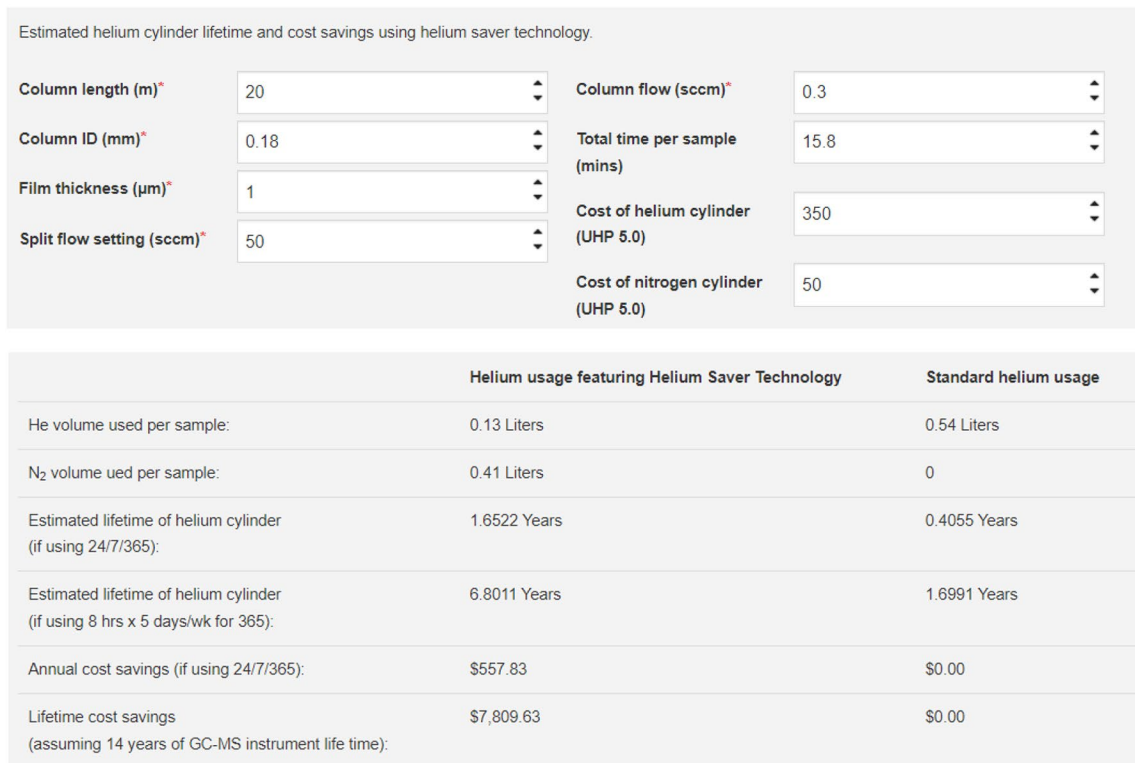


Figure 5. Helium saving calculator for U.S. EPA Method 524.4

## Conclusion

The combined solution of the TRACE 1610 GC equipped with HeSaver-H<sub>2</sub>Safer technology coupled with the ISQ 7610 MS and the Atomx XYZ P&T system provides clear advantages for EPA Method 524.4. 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 EPA Method 524.4.

- The ISQ 7610 VPI coupled with the Teledyne Tekmar Atomx XYZ P&T exceeds all the requirements outlined in EPA Method 524.4 for analysis of VOCs in water.
- Excellent linearity for all compounds was demonstrated with the  $r^2 > 0.995$ , passing all method requirements.
- MDL, precision, and accuracy for seven 0.5 ppb standards showed no interference from excessive water and produced very reproducible results.
- MRL passed all method requirements of the lower Prediction Interval of Results (PIR)  $\geq 50\%$  and the upper PIR  $\leq 150\%$ .

- Calibration standards meet the required  $\pm 50\%$  of the true value for first calibration standard and  $\pm 30\%$  of the true value for the rest of the calibration standards.
- The precision for  $n=26$  samples over 160 injections displayed  $< 30\%$  RSD for all compounds as the method requires and an average recovery of 92%.
- The helium consumption was reduced by a factor of 4 compared to a standard SSL inlet configuration, offering a concrete solution to support more sustainable operations and mitigate helium gas shortage issues.

## References

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3. Thermo Fisher Scientific AppsLab: <https://apps.thermofisher.com/>
4. Thermo Fisher Scientific Helium Saver Calculator, <https://www.thermofisher.com/it/en/home/industrial/chromatography/chromatography-learning-center/chromatography-consumables-resources/chromatography-tools-calculators/helium-saver-calculator.html>

## Appendix 1 (part 1). U.S. EPA Method 524.4 calibration, accuracy, and precision data

Compound	Retention time	Calibration			MDL (n=7, 0.5 ppb)		IDC (n=10, 10 ppb)		MRL confirmation (n=7, 1 ppb)	
		Cal type	Linearity (r <sup>2</sup> ≥0.995)	Avg. RF	MDL (ppb)	Precision (≤20% RSD)	Accuracy (±20%)	Precision (≤20% RSD)	LPIR (≥50%)	UPIR (≤150%)
Dichlorodifluoromethane	1.77	Lin	0.998	0.600	0.13	8.05	8.52	97	66	123
Chlorodifluoromethane	1.8	Lin	0.997	1.446	0.09	5.17	9.25	113	96	128
Chloromethane	1.97	Lin	0.997	1.369	0.07	3.83	9.01	111	88	129
Vinyl chloride	2.05	Lin	0.999	0.777	0.05	2.83	9.31	112	82	133
1,3-Butadiene	2.07	Lin	0.998	1.041	0.16	9.27	9.62	111	78	142
Bromomethane	2.4	Lin, WithOffset, 1/A	0.996	0.557	0.09	5.97	7.41	107	77	127
Trichlorofluoromethane	2.73	Lin	0.999	0.750	0.11	7.01	8.75	106	85	122
Diethyl ether	3.14	Lin	1.000	0.326	0.12	8.20	3.14	104	76	122
1,1-Dichloroethene	3.37	Lin	0.999	0.186	0.15	9.84	8.70	107	81	133
Carbon disulfide	3.39	Lin, WithOffset, 1/A	0.998	0.172	0.14	9.92	9.16	101	91	102
Methyl iodide <sup>1</sup>	3.55	Lin, WithOffset, 1/A	0.995	0.244	0.07	3.28	6.96	81	82	116
Allyl chloride	4.06	Lin	0.999	0.183	0.16	10.3	7.24	103	92	123
Methylene chloride	4.23	Lin, WithOffset, 1/A	0.997	0.952	0.12	8.35	5.71	110	87	114
<i>trans</i> -1,2-dichloroethene	4.47	Lin	0.999	0.408	0.12	7.58	7.21	108	78	128
Methyl acetate	4.55	Lin	0.998	0.582	0.16	9.38	3.97	105	78	136
Methyl- <i>t</i> -butyl ether-d <sub>3</sub> (surr)	4.64	AvgCalFact	2.11	1.195	-	4.33	2.15	100	97	105
Methyl tert butyl ether	4.67	Lin	1.000	1.320	0.09	5.75	4.02	99	88	117
<i>t</i> -Butyl alcohol (TBA)	5.24	Lin	1.000	0.158	0.12	8.13	4.10	103	88	127
Diisopropyl ether	5.25	Lin	1.000	1.978	0.09	5.98	4.98	99	88	117
1,1-Dichloroethane	5.33	Lin	0.999	0.871	0.11	6.68	6.75	111	92	124
<i>t</i> -Butyl ethyl ether (ETBE)	5.72	Lin	1.000	1.316	0.06	3.86	4.72	96	86	111
<i>cis</i> -1,2-Dichloroethene	6.03	Lin	1.000	0.432	0.09	5.54	6.11	105	87	120
Bromochloromethane	6.25	Lin	0.999	0.207	0.12	7.60	5.38	108	82	119
Chloroform	6.38	Lin	0.999	0.905	0.10	6.46	5.54	110	91	121
Carbon tetrachloride	6.53	Lin	0.999	0.404	0.08	5.79	7.22	107	73	119
1,1,1-Trichloroethane	6.6	Lin	0.999	0.546	0.27	17.6	8.18	107	95	112
Tetrahydrofuran	6.61	Lin	0.998	0.072	0.09	5.52	4.98	105	66	147
1,1-Dichloropropene	6.76	Lin	1.000	0.388	0.09	6.00	7.66	96	79	107
1-Chlorobutane	6.82	Lin	1.000	0.648	0.06	4.25	7.91	99	90	102
Benzene	7.04	Lin	1.000	1.411	0.06	3.91	5.99	99	85	113
<i>t</i> -Amyl methyl ether (TAME)	7.23	Lin	1.000	1.149	0.04	2.68	5.11	96	87	112
1,2-Dichloroethane	7.27	Lin	0.999	0.725	0.07	4.52	3.88	109	88	123
Trichloroethylene	7.73	Lin	0.997	0.429	0.22	14.0	6.00	116	71	147
1,4-Difluorobenzene (ISTD)	7.77	AvgCalFact	-	-	-	-	-	-	-	-
<i>t</i> -Amyl ethyl ether (TMEE)	8.05	Lin	1.000	1.065	0.06	4.14	4.98	101	92	112
Dibromomethane	8.18	Lin	0.999	0.317	0.11	7.39	4.61	107	82	121
1,2-Dichloropropane	8.29	Lin	1.000	0.552	0.08	5.45	5.13	102	83	116
Bromodichloromethane	8.38	Lin	0.999	0.722	0.05	3.00	4.92	107	79	121
<i>cis</i> -1,3-Dichloropropene	9	Lin	1.000	0.754	0.07	5.25	4.79	94	83	98
Toluene	9.22	Lin	1.000	1.683	0.24	12.5	5.97	100	104	141
Tetrachloroethylene	9.55	Lin	0.997	0.613	0.08	4.11	5.80	119	112	143

<sup>1</sup>Calibration from 0.5–50 ppb

## Appendix 1 (part 2). U.S. EPA Method 524.4 calibration, accuracy, and precision data

Compound	Retention time	Calibration			MDL (n=7, 0.5 ppb)		IDC (n=10, 10 ppb)		MRL confirmation (n=7, 1 ppb)	
		Cal type	Linearity (r <sup>2</sup> ≥0.995)	Avg. RF	MDL (ppb)	Precision (≤20% RSD)	Accuracy (±20%)	Precision (≤20% RSD)	LPIR (≥50%)	UPIR (≤150%)
<i>trans</i> -1,3-Dichloropropene	9.57	Lin	0.999	0.690	0.10	8.23	4.05	90	69	109
1,1,2-Trichloroethane	9.7	Lin	1.000	0.388	0.08	5.44	4.20	97	83	116
Ethyl methacrylate	9.72	Lin	1.000	0.624	0.12	8.48	4.07	96	85	116
Dibromochloromethane	9.85	Lin	0.999	0.404	0.06	4.63	4.28	93	66	111
1,3-Dichloropropane	9.92	Lin	0.999	0.816	0.05	3.87	3.38	96	86	106
1,2-Dibromoethane	10.03	Lin	1.000	0.400	0.11	7.71	4.69	94	80	104
Chlorobenzene-d <sub>5</sub> (ISTD)	10.43	AvgCalFact	-	-	-	-	-	-	-	-
Chlorobenzene	10.44	Lin	1.000	1.141	0.07	4.75	5.17	99	84	119
Ethylbenzene	10.47	Lin	1.000	1.861	0.06	3.78	5.97	95	82	111
1,1,1,2-Tetrachloroethane	10.49	Lin	0.999	0.361	0.07	5.06	5.08	95	83	101
<i>m,p</i> -Xylene	10.58	Lin	1.000	1.545	0.13	4.99	5.91	92	74	102
<i>o</i> -Xylene	10.89	Lin	1.000	1.649	0.06	4.09	5.74	93	74	105
Styrene	10.93	Lin	0.999	1.165	0.04	3.18	5.73	89	70	96
Bromoform	10.94	Lin	0.999	0.310	0.05	4.18	5.64	96	81	100
Isopropylbenzene	11.12	Lin	1.000	1.756	0.04	2.89	7.28	93	74	98
4-Bromofluorobenzene (surr)	11.31	AvgCalFact	3.57	0.904	-	2.80	2.08	97	93	108
Bromobenzene	11.39	Lin	1.000	1.766	0.06	3.59	5.31	104	91	126
<i>n</i> -Propylbenzene	11.41	Lin	1.000	3.408	0.06	3.88	7.35	97	84	114
1,1,2,2-Tetrachloroethane	11.45	Lin	0.998	0.716	0.09	6.80	5.16	91	70	107
2-Chlorotoluene	11.52	Lin	1.000	2.525	0.07	4.65	6.75	99	81	121
1,3,5-Trimethylbenzene	11.54	Lin	1.000	2.370	0.07	4.78	6.82	92	76	98
1,2,3-Trichloropropane	11.54	Lin	1.000	0.982	0.10	5.93	5.11	106	99	137
4-Chlorotoluene	11.63	Lin	1.000	2.394	0.04	2.75	6.80	98	80	113
<i>tert</i> -Butylbenzene	11.76	Lin	0.999	2.125	0.10	7.13	7.41	91	75	98
Pentachloroethane	11.76	Lin	1.000	0.294	0.14	8.44	8.09	99	66	131
1,2,4-Trimethylbenzene	11.81	Lin	0.999	2.456	0.05	3.62	5.67	92	72	99
<i>sec</i> -Butylbenzene	11.89	Lin	1.000	2.825	0.06	3.99	7.29	96	68	105
<i>p</i> -Isopropyltoluene	11.98	Lin	0.999	2.202	0.06	4.39	7.24	91	65	97
1,3-Dichlorobenzene	12.04	Lin	1.000	1.814	0.08	4.75	5.50	103	86	118
1,4-Dichlorobenzene-d <sub>4</sub> (ISTD)	12.08	AvgCalFact	-	-	-	-	-	-	-	-
1,4-Dichlorobenzene	12.09	Lin	1.000	1.799	0.10	6.07	5.46	102	82	124
<i>n</i> -Butylbenzene	12.26	Lin	0.998	2.252	0.08	5.42	7.38	90	69	102
Hexachloroethane	12.37	Lin	0.999	0.260	0.09	7.80	7.75	98	77	94
1,2-Dichlorobenzene (surr)	12.37	AvgCalFact	1.29	0.976	-	1.77	2.22	100	90	112
1,2-Dichlorobenzene	12.38	Lin	0.999	1.789	0.04	2.33	5.94	106	80	135
1,2-Dibromo-3-chloropropane	12.91	Lin	1.000	0.213	0.12	7.67	6.12	105	65	138
Hexachlorobutadiene	13.34	Lin	1.000	0.038	0.17	10.1	9.39	109	82	149
1,2,4-Trichlorobenzene	13.37	Lin	1.000	0.959	0.11	6.25	5.81	104	77	133
Naphthalene	13.59	Lin	0.999	2.143	0.07	4.52	4.73	94	77	119
1,2,3-Trichlorobenzene	13.71	Lin	1.000	0.813	0.12	7.54	5.84	104	78	123

<sup>1</sup>Calibration from 0.5–50 ppb



## Appendix 2. Repeatability of a 10 ppb VOC standard (n=26) (as absolute peak area counts) assessed over n=160 consecutive injections

Compound	Analyte recovery (10 ppb n=26, 160 injections)		Compound	Analyte recovery (10 ppb n=26, 160 injections)		Compound	Analyte recovery (10 ppb n=26, 160 injections)	
	Precision (≤20% RSD)	Accuracy (±30% RSD)		Precision (≤20% RSD)	Accuracy (±30% RSD)		Precision (≤20% RSD)	Accuracy (±30% RSD)
Dichlorodifluoromethane	9.1	104	1,1-Dichloropropene	6.4	86	Bromoform	11.7	86
Chlorodifluoromethane	9.3	116	1-Chlorobutane	5.4	89	Isopropylbenzene	7.5	84
Chloromethane	8.8	104	Benzene	4.3	94	4-Bromofluorobenzene (surr)	3.6	94
Vinyl chloride	8.7	105	<i>t</i> -Amyl methyl ether (TAME)	10.3	85	Bromobenzene	6.5	95
1,3-Butadiene	8.8	102	1,2-Dichloroethane	4.1	111	<i>n</i> -Propylbenzene	8.1	86
Bromomethane	7.0	104	Trichloroethylene	6.1	110	1,1,2,2-Tetrachloroethane	15.0	77
Trichlorofluoromethane	7.8	101	1,4-Difluorobenzene (ISTD)	-	-	2-Chlorotoluene	7.9	89
Diethyl ether	6.0	92	<i>t</i> -Amyl ethyl ether (TMEE)	7.3	90	1,3,5-Trimethylbenzene	12.5	76
1,1-Dichloroethene	6.4	92	Dibromomethane	3.2	108	1,2,3-Trichloropropane	12.2	92
Carbon disulfide	8.1	70	1,2-Dichloropropane	3.7	103	4-Chlorotoluene	7.4	87
Methyl iodide <sup>†</sup>	13.2	56	Bromodichloromethane	5.1	108	Pentachloroethane	7.1	89
Allyl chloride	6.0	96	<i>cis</i> -1,3-Dichloropropene	5.6	92	<i>tert</i> -Butylbenzene	9.4	80
Methylene chloride	6.6	111	Toluene	10.7	90	1,2,4-Trimethylbenzene	13.3	74
<i>trans</i> -1,2-dichloroethene	5.5	99	Tetrachloroethylene	7.1	109	<i>sec</i> -Butylbenzene	8.0	84
Methyl acetate	10.3	99	<i>trans</i> -1,3-Dichloropropene	9.6	82	<i>p</i> -Isopropyltoluene	10.4	76
Methyl- <i>t</i> -butyl ether- <i>d</i> <sub>3</sub> (surr)	5.7	95	1,1,2-Trichloroethane	8.3	91	1,3-Dichlorobenzene	6.0	95
Methyl <i>tert</i> butyl ether	8.4	91	Ethyl methacrylate	17.1	79	1,4-Dichlorobenzene- <i>d</i> <sub>2</sub> (ISTD)	-	-
Diisopropyl ether	5.2	92	Dibromochloromethane	8.9	87	1,4-Dichlorobenzene	6.4	92
<i>t</i> -Butyl alcohol (TBA)	6.1	98	1,3-Dichloropropane	8.1	88	<i>n</i> -Butylbenzene	10.4	75
1,1-Dichloroethane	8.2	109	1,2-Dibromoethane	10.7	86	Hexachloroethane	6.7	89
<i>t</i> -Butyl ethyl ether (ETBE)	7.8	87	Chlorobenzene- <i>d</i> <sub>2</sub> (ISTD)	-	-	1,2-Dichlorobenzene (surr)	2.0	100
<i>cis</i> -1,2-Dichloroethene	5.1	102	Chlorobenzene	6.7	91	1,2-Dichlorobenzene	6.3	96
Bromochloromethane	4.5	107	Ethylbenzene	7.4	86	1,2-Dibromo-3-chloropropane	16.1	86
Chloroform	5.6	114	1,1,1,2-Tetrachloroethane	7.6	89	Hexachlorobutadiene	11.4	92
Carbon tetrachloride	9.1	98	<i>m,p</i> -Xylene	7.3	84	1,2,4-Trichlorobenzene	11.4	86
Tetrahydrofuran	15.7	93	<i>o</i> -Xylene	6.5	86	Naphthalene	19.0	73
1,1,1-Trichloroethane	5.2	105	Styrene	7.8	81	1,2,3-Trichlorobenzene	13.4	85

<sup>†</sup>Reactive compound, compound degraded during analysis

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