

Analysis of volatile organic compounds in drinking water according to U.S. EPA Method 524.4

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Keywords

EPA, EPA 524.4, 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, ISQ 7610 MS, TRACE 1610 GC, GC-MS

Goal

Demonstration of an 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 Single Quadrupole 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

Volatile organic compounds, or VOCs, are human-made contaminants used and generated in the manufacturing of numerous products and have an adverse effect on the natural environment, and ultimately the public. Environmental testing laboratories must monitor VOCs and commonly follow U.S. EPA methods.¹ U.S. EPA Method 524.2 is one of the most common methods used for VOC testing in water and was described in a previous application note.² U.S. EPA Method 524.4 is another commonly used method for VOC analysis in water. The method targets 75 VOCs and differs from U.S. EPA Method 524.2 by allowing more flexibility with the method 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.

One of these QC requirements includes 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 $\rm r^2$ of 0.995 or better, weighting may be used, and zero cannot be forced. The lowest concentration in the curve must be within $\pm 50\%$ of its true value, all other points must be within $\pm 30\%$. The samples must also be chilled which involves using the chilled tray upgrade for the Atomx XYZ P&T.

There are a number of challenges that analytical testing laboratories face when performing U.S. EPA Method 524.4. Laboratories must ensure their conditions for the method are optimized and they can meet the method acceptance criteria including detection limit requirements for an assortment of compounds over a wide range of concentrations. A major challenge is to ensure the water matrix is managed correctly and limit the introduction of water into the GC-MS system, which can cause adverse effects. 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 method that produces consistent results to eliminate the need for reanalysis of samples.

The following evaluation describes the use of the ISQ 7610 MS system coupled with a TRACE 1610 Gas Chromatograph (GC) and the Atomx XYZ P&T for U.S. EPA Method 524.4.

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: 524.3 VOA MegaMix™ (P/N 30013) and 524.3 Gas Calibration Mix (P/N 30014). In total, the standards contained 75 compounds.

The calibration curve was prepared from 0.2 µg/L to 50 µg/L (parts per billion or ppb) for all compounds. The linear response was calculated for each compound using three Restek internal standards: 1,4-difluorobenzene, chlorobenzene-d $_{\rm s}$, and 1,4-dichlorobenzene-d $_{\rm d}$ (P/N 30017). Surrogate standards from Restek consisted of methyl-t-butyl ether-d $_{\rm s}$, 4-bromofluorobenzene, and 1,2-dichlorobenzene-d $_{\rm d}$ (P/N 30017). Internal and surrogate standards were prepared in methanol from Restek standards at a concentration of 20 ppm, after which 5 µL was then mixed with each 5 mL sample for a resulting concentration of 20 ppb.

Table 1. Teledyne Tekmar Atomx XYZ water method parameters

Standby	Variable
Valve oven temp.	140 °C
Transfer line temp.	140 °C
Sample mount temp.	90 °C
Water heater temp.	90 °C
Sample cup temp.	20 °C
Soil valve temp.	50 °C
Standby flow	10 mL/min
Purge ready temp.	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 temp.	20 °C
MCS purge temp.	20 °C
Dry purge time	0.5 min
Dry purge flow	100 mL/min
Dry purge temp.	20 °C
Dry purge temp. Desorb	20 °C Variable
Desorb	Variable
Desorb Methanol needle rinse	Variable Off
Desorb Methanol needle rinse Water needle rinse volume	Variable Off 7.00 mL
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time	Variable Off 7.00 mL 0.25 min
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp.	Variable Off 7.00 mL 0.25 min 245 °C
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp.	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off
Desorb Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse Water bake rinses	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off
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Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse Water bake rinses Water bake rinse volume Bake rinse sweep time Bake rinse sweep flow Bake rinse drain time	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off 1 7.00 mL 0.25 min 100 mL/min 0.40 min
Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse Water bake rinses Water bake rinse volume Bake rinse sweep time Bake rinse sweep flow Bake rinse drain time Bake time	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off 1 7.00 mL 0.25 min 100 mL/min 0.40 min 2.00 min
Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse Water bake rinses Water bake rinse volume Bake rinse sweep time Bake rinse sweep flow Bake rinse drain time Bake time Trap bake temp.	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off 1 7.00 mL 0.25 min 100 mL/min 0.40 min 2.00 min 260 °C
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Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse Water bake rinses Water bake rinse volume Bake rinse sweep time Bake rinse drain time Bake time Trap bake temp. Bake flow Trap	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off 1 7.00 mL 0.25 min 100 mL/min 0.40 min 2.00 min 260 °C 200 °C 200 mL/min
Methanol needle rinse Water needle rinse volume Sweep needle time Desorb preheat temp. GC start signal Desorb time Drain flow Desorb temp. Bake Methanol glass rinse Water bake rinses Water bake rinse volume Bake rinse sweep time Bake rinse drain time Bake time Trap bake temp. MCS bake temp. Bake flow	Variable Off 7.00 mL 0.25 min 245 °C Begin Desorb 2.00 min 300 mL/min 250 °C Variable Off 1 7.00 mL 0.25 min 100 mL/min 0.40 min 2.00 min 260 °C 200 °C 200 mL/min

A total of seven standards, each having a concentration of 0.5 ppb, were prepared in deionized water to calculate the MDL and minimum reporting level (MRL) for all compounds. Also, seven 10 ppb standards were prepared to determine the accuracy and precision of recovery of each compound. All calibration, MDL, MRL, and recovery standards were analyzed with the Atomx XYZ conditions in Table 1.

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 Thermo Scientific™ 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 compounds separation. The Thermo Scientific™ iConnect™ Split Splitless (SSL) injector was operated in split mode and the GC run time was 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 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 μ m 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

The 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.

Results and discussion

Chromatography

All compounds of interest were separated with good chromatographic resolution using the GC conditions described in Table 2. The good peak shapes of the compounds show that there is minimal water transfer from the samples. This resulted in optimized chromatography that was maintained in the lower concentration samples. 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 1,3-dichlorobennzene at 0.5 ppb in a VOC standard with excellent library spectral matching and calibration curve. Appendix 1 displays the linear value (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 0.5 ppb standard.

Appendix 1 also shows the initial demonstration of capability (IDC) for the method. This was determined by analyzing a 10 ppb standard seven times to ensure that the precision was under 20% variation and the accuracy was $\pm 20\%$. The average precision for all compounds was 3.4% and the average accuracy was 95%. This demonstrates that the method is fit for purpose. Figure 3 shows a subset of results for 20 compounds across the analytical range.

Method robustness

When performing VOC analysis, it is essential to produce consistent data to ensure sample results are delivered on time. To assess the stability of the method, 10 ppb calibration check standards were injected at intervals 40 times over a sequence of 245 injections. This extended sequence is equivalent to four days of uninterrupted analysis. No maintenance was performed on any part of the system during this extended test. Figure 4 shows the reproducibility of 10 of the compounds over 245 injections with excellent RSDs. RSDs for all compounds were under the 30% method requirements, and in fact gave an average of 9% RSD across the compounds. Appendix 2 shows the reproducibility results for all compounds over the 245-injection sequence.

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- 21. t-butyl ethyl ether
- 22. cis-1,2-dichloroethene
- 23. Bromochloromethane
- 24. Chloroform
- 25. Carbon tetrachloride
- 26. Tetrahydrofuran
- 27. 1,1,1-trichloroethane
- 28. 1,1-dichloropropene
- 29. 1-chlorobutane
- 30. Benzene
- 31. t-amyl methyl ether
- 32. 1,2-dichloroethane
- 33. Trichloroethylene
- 34. 1,4-dichluorobenzene (IS)
- 35. t-amyl ethyl ether
- 36. Dibromomethane
- 37. 1,2-dichloropropane
- 38. Bromodichloromethane

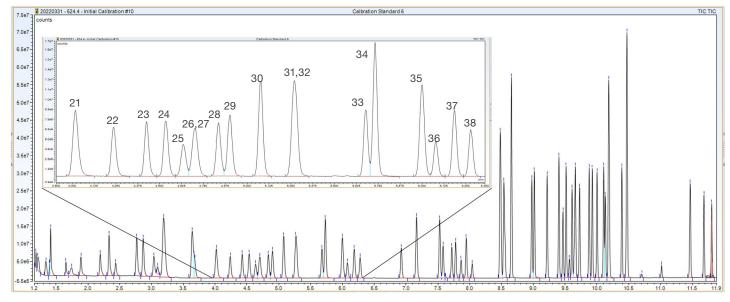


Figure 1. Total ion chromatogram (TIC) of a water method 10 ppb VOC standard with an inset indicating consistent peak shapes and separation with minimal water interference

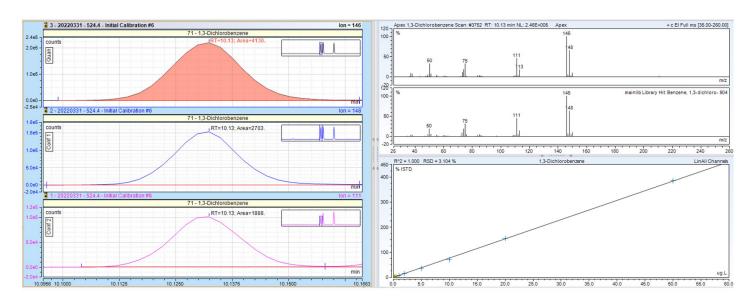


Figure 2. Chromeleon CDS results browser showing extracted ion chromatograms for 1,3-dichlorobennzene in the 0.5 ppb water standard, quantitation ion (m/z=146) and one confirming ions (m/z=148,111) (A), a matching measured spectrum to the NIST library (B), and a linear calibration over a concentration range of 0.2 ppb to 50 ppb (C)

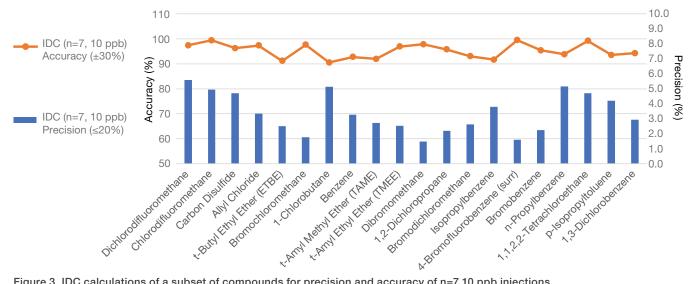


Figure 3. IDC calculations of a subset of compounds for precision and accuracy of n=7 10 ppb injections

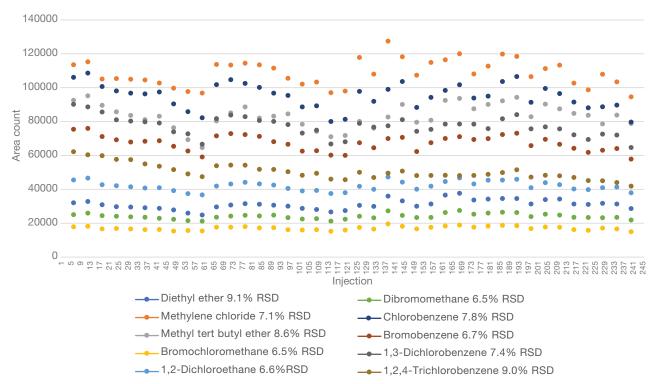


Figure 4. Repeatability of a 10 ppb VOC standard (n=40) (as absolute peak area counts) assessed over n=245 consecutive injections

Conclusion

The combined solution of the TRACE 1610 GC coupled with the ISQ 7610 MS and the Atomx XYZ P&T system effectively address the challenges of VOC analysis and provides a robust, sensitive solution needed for ensuring maximized instrument output and routine regulatory method compliance for U.S. EPA Method 524.4:

- Excellent linearity for all compounds was demonstrated with the $r^2 \ge 0.995$, 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.

The precision for n=40 samples over 245 injections displayed <30% RSD for all compounds as the method requires and an average recovery of 91%.

References

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- 2. Thermo Scientific Application Note 000525: Uninterrupted analysis of volatile organic compounds in drinking water using single quadrupole GC-MS. https://assets. thermofisher.com/TFS-Assets/CMD/Application-Notes/an-000525-gc-ms-volatileorganic-compounds-water-an000525-en.pdf

Appendix 1. U.S. EPA Method 524.4 calibration, accuracy, and precision data

Appendix 1, part 1

	Calibration (0.2–50 ppb)			MDL (n=7, 0.5 ppb)		IDC (n=7, 10 ppb)		MRL confirmation (n=7, 0.5 ppb)		
Compound	Retention time (min)	Confirming ion	Linearity (r² ≥0.995)	Avg. RRF	MDL (ppb)	Precision (≤20%)	Precision (≤20%)	Accuracy (±30%)	LPIR (≥50%)	UPIR (≤150%)
Dichlorodifluoromethane	1.18	85	1.000	0.468	0.17	11.5	5.6	97	52	139
Chlorodifluoromethane	1.21	51	1.000	1.05	0.13	8.7	4.9	99	62	127
Chloromethane	1.34	50	1.000	0.961	0.15	9.7	3.2	102	63	140
Vinyl chloride	1.40	62	1.000	0.400	0.14	9.0	4.6	98	61	130
1,3-Butadiene	1.42	39	1.000	0.848	0.10	5.9	8.8	99	83	133
Bromomethane ¹	1.66	94	0.999	0.396	0.17	11.5	3.3	108	51	138
Trichlorofluoromethane	1.89	101	1.000	0.666	0.14	9.9	5.3	95	55	125
Diethyl ether	2.19	59	1.000	0.383	0.06	3.7	2.3	97	81	109
Carbon disulfide	2.33	76	1.000	0.951	0.11	6.5	4.7	96	77	132
1,1-Dichloroethene	2.33	96	1.000	0.458	0.13	8.1	4.4	97	67	131
Methyl iodide ¹	2.44	142	0.997	0.558	0.07	3.7	2.8	88	99	133
Allyl chloride	2.76	76	1.000	0.273	0.12	8.3	3.3	97	63	125
Methylene chloride	2.87	49	1.000	1.32	0.11	6.5	1.5	103	78	133
trans-1,2-dichloroethene	3.04	61	1.000	0.593	0.10	6.7	3.2	100	72	124
Methyl acetate	3.10	43	1.000	0.774	0.10	6.8	2.4	93	71	122
Methyl-t-butyl ether-d ₃ (surr)	3.20	76	1.7 (%RSD)	1.00		1.7	0.7	99	90	103
Methyl tert butyl ether	3.21	73	0.999	1.13	0.04	3.0	2.3	94	80	102
t-Butyl alcohol (TBA)	3.39	59	1.000	0.038	0.17	10.0	3.2	90	65	149
Diisopropyl ether	3.65	45	1.000	2.58	0.04	2.6	2.6	94	77	95
1,1-Dichloroethane	3.67	63	1.000	0.764	0.11	7.3	2.3	99	70	126
t-Butyl ethyl ether (ETBE)	4.04	59	0.999	1.13	0.04	3.4	2.5	91	70	92
cis-1,2-Dichloroethene	4.24	96	1.000	0.499	0.12	7.6	1.6	95	67	125
Bromochloromethane	4.43	128	1.000	0.207	0.12	7.8	1.8	98	69	130
Chloroform	4.53	83	1.000	0.844	0.13	8.4	2.7	99	65	130
Carbon tetrachloride	4.64	117	0.999	0.435	0.07	5.9	4.0	91	60	96
Tetrahydrofuran	4.70	72	0.999	0.048	0.09	7.2	2.7	87	54	97
1,1,1-Trichloroethane	4.72	97	1.000	0.612	0.08	5.9	4.1	95	67	108
1,1-Dichloropropene	4.85	75	0.998	0.435	0.09	6.9	4.4	89	57	99
1-Chlorobutane	4.91	56	0.998	0.678	0.07	6.1	5.1	91	58	95
Benzene	5.08	78	0.999	1.45	0.06	4.9	3.3	93	66	98
t-Amyl methyl ether (TAME)	5.28	73	0.999	0.976	0.03	2.7	2.7	92	73	90
1,2-Dichloroethane	5.30	62	1.000	0.532	0.08	5.3	1.3	96	73	111
Trichloroethylene	5.68	95	1.000	0.535	0.09	6.0	4.1	108	76	123
1,4-Difluorobenzene (ISTD)	5.73	114								
t-Amyl ethyl ether (TMEE)	6.00	59	1.000	0.941	0.06	4.1	2.5	97	75	104
Dibromomethane	6.08	93	1.000	0.299	0.06	4.1	1.5	98	79	109
1,2-Dichloropropane	6.19	63	0.999	0.434	0.03	2.5	2.2	96	78	95
Bromodichloromethane	6.28	83	1.000	0.584	0.07	5.1	2.6	93	67	132
cis-1,3-Dichloropropene	6.93	75	0.998	0.594	0.05	4.5	1.8	89	62	131
Toluene	7.16	91	0.999	1.68	0.05	3.6	4.2	88	70	133
Tetrachloroethylene	7.53	164	1.000	0.545	0.09	5.6	3.6	99	80	125

¹Calibration range from 0.5 to 50 ppb

Appendix 1, part 2

	Calibration (0.2–50 ppb)				MDL (n=7, 0.5 ppb)		IDC (n=7, 10 ppb)		MRL confirmation (n=7, 0.5 ppb)	
Compound	Retention time (min)	Confirming ion	Linearity (r² ≥0.995)	Avg. RRF	MDL (ppb)	Precision (≤20%)	Precision (≤20%)	Accuracy (±30%)	LPIR (≥50%)	UPIR (≤150%)
trans-1,3-Dichloropropene	7.58	75	0.995	0.473	0.06	3.8	2.7	87	83	133
1,1,2-Trichloroethane	7.72	83	0.998	0.322	0.07	6.2	2.9	87	58	124
Ethyl methacrylate	7.78	69	0.999	0.431	0.02	1.9	2.3	88	63	122
Dibromochloromethane	7.86	129	1.000	0.287	0.05	4.5	2.4	94	64	103
1,3-Dichloropropane	7.95	76	0.998	0.557	0.03	2.7	2.5	87	66	102
1,2-Dibromoethane	8.04	107	0.999	0.340	0.06	5.0	2.7	88	60	149
Chlorobenzene-d ₅ (ISTD)	8.48	117								95
Chlorobenzene	8.49	112	1.000	1.09	0.03	2.4	3.8	92	82	126
Ethylbenzene	8.53	91	0.999	1.92	0.06	4.2	3.4	95	72	92
1,1,1,2-Tetrachloroethane	8.56	131	0.996	0.288	0.05	3.3	3.1	90	84	125
m,p-Xylene	8.66	91	0.999	1.58	0.13	5.1	3.6	97	65	130
o-Xylene	8.98	91	0.999	1.61	0.04	3.0	3.7	91	67	130
Bromoform	9.02	173	1.000	0.187	0.09	7.9	1.7	97	51	96
Styrene	9.02	104	0.999	1.17	0.06	4.6	2.5	92	62	97
Isopropylbenzene	9.22	105	0.999	1.75	0.07	6.4	3.8	92	55	108
4-Bromofluorobenzene (surr)	9.40	95	1.9 (%RSD)	1.08		1.7	1.6	99	94	99
Bromobenzene	9.47	77	1.000	1.29	0.03	2.2	2.2	95	88	95
n-Propylbenzene	9.52	91	1.000	4.01	0.06	4.2	5.1	94	72	98
1,1,2,2-Tetrachloroethane	9.58	83	1.000	0.463	0.10	6.9	4.7	99	64	112
2-Chlorotoluene	9.62	91	1.000	2.42	0.06	4.0	3.4	98	76	105
1,2,3-Trichloropropane	9.66	75	1.000	0.653	0.06	3.7	2.5	100	82	111
1,3,5-Trimethylbenzene	9.66	105	1.000	2.61	0.05	4.2	4.0	96	69	96
4-Chlorotoluene	9.73	91	1.000	2.57	0.07	4.7	4.1	97	73	107
tert-Butylbenzene	9.88	119	0.999	0.027	0.07	5.6	4.4	92	61	95
Pentachloroethane	9.88	167	1.000	2.09	0.14	9.4	13.6	97	59	128
1,2,4-Trimethylbenzene	9.93	105	0.999	2.64	0.07	5.4	3.9	99	64	99
sec-Butylbenzene	10.00	105	0.999	3.29	0.07	5.4	4.8	96	63	97
<i>p</i> -Isopropyltoluene	10.10	119	1.000	2.57	0.06	4.7	4.2	93	63	92
1,3-Dichlorobenzene	10.13	146	1.000	1.47	0.05	3.3	2.9	94	78	101
1,4-Dichlorobenzene-d, (ISTD)	10.18	152								
1,4-Dichlorobenzene	10.19	146	1.000	1.54	0.08	4.8	2.7	99	82	120
n-Butylbenzene	10.39	91	0.999	2.91	0.07	5.0	4.8	97	68	101
Hexachloroethane	10.46	201	0.996	0.199	0.10	7.2	5.1	100	66	119
1,2-Dichlorobenzene (surr)	10.47	152	1.4 (%RSD)	0.982		1.5	1.6	100	94	106
1,2-Dichlorobenzene	10.47	146	1.000	1.50	0.04	2.7	1.7	101	89	110
1,2-Dibromo-3-chloropropane	11.01	75	0.999	0.111	0.06	5.1	2.1	92	63	94
Hexachlorobutadiene	11.46	225	0.996	0.383	0.15	10.0	4.1	98	58	133
1,2,4-Trichlorobenzene	11.46	180	0.999	1.05	0.09	6.1	3.0	91	68	112
Naphthalene	11.68	128	0.999	2.62	0.05	4.3	2.4	87	62	87
1,2,3-Trichlorobenzene	11.80	180	0.998	1.04	0.07	4.7	3.4	91	72	105

Appendix 2. Repeatability of a 10 ppb VOC standard (n=40) (as absolute peak area counts) assessed over n=245 consecutive injections

	Analyte recovery (10 ppb n=40, 245 injections)				
Compound	Accuracy (%)	Precision (%)			
Dichlorodifluoromethane	10.8	89			
Chlorodifluoromethane	9.6	96			
Chloromethane	9.4	99			
Vinyl chloride	11.5	93			
1,3-Butadiene	11.7	95			
Bromomethane	12.0	113			
Trichlorofluoromethane	13.0	94			
Diethyl ether	7.2	97			
Carbon disulfide	15.4	91			
1,1-Dichloroethene	11.2	98			
Methyl iodide	10.3	80			
Allyl chloride	8.4	95			
Methylene chloride	6.0	105			
trans-1,2-dichloroethene	9.1	99			
Methyl acetate	8.0	95			
Methyl-t-butyl ether-d ₃ (surr)	4.0	98			
Methyl tert butyl ether	5.5	88			
t-Butyl alcohol (TBA)1	19.5	87			
Diisopropyl ether	4.7	85			
1,1-Dichloroethane	6.9	100			
t-Butyl ethyl ether (ETBE)	5.5	79			
cis-1,2-Dichloroethene	5.9	93			
Bromochloromethane	5.1	100			
Chloroform	5.8	98			
Carbon tetrachloride	10.9	85			
Tetrahydrofuran	9.9	78			
1,1,1-Trichloroethane	9.0	90			
1,1-Dichloropropene	10.1	80			
1-Chlorobutane	9.8	83			
Benzene	7.1	89			
t-Amyl methyl ether (TAME)	5.9	78			
1,2-Dichloroethane	4.0	94			
Trichloroethylene	8.0	96			
1,4-Difluorobenzene (ISTD)	-	-			
t-Amyl ethyl ether (TMEE)	7.5	80			
Dibromomethane	4.7	97			
1,2-Dichloropropane	4.6	94			
Bromodichloromethane	4.5	90			
' 10 B' 11					
cis-1,3-Dichloropropene	5.4	78			
Toluene	5.4 8.2	78 81			

	Analyte recovery (10 ppb n=40, 245 injections)			
Compound	Accuracy (%)	Precision (%)		
1,1,2-Trichloroethane	7.4	83		
Ethyl methacrylate	8.3	76		
Dibromochloromethane	6.6	88		
1,3-Dichloropropane	7.1	82		
1,2-Dibromoethane	7.3	83		
Chlorobenzene-d ₅ (ISTD)	-	-		
Chlorobenzene	5.8	89		
Ethylbenzene	7.7	87		
1,1,1,2-Tetrachloroethane	6.9	84		
m,p-Xylene	7.5	91		
o-Xylene	6.5	84		
Bromoform	8.4	89		
Styrene	5.5	87		
Isopropylbenzene	7.9	84		
4-Bromofluorobenzene (surr)	4.6	101		
Bromobenzene	10.5	94		
n-Propylbenzene	11.4	88		
1,1,2,2-Tetrachloroethane ²	19.0	102		
2-Chlorotoluene	11.0	93		
1,2,3-Trichloropropane	14.3	97		
1,3,5-Trimethylbenzene	11.6	91		
4-Chlorotoluene	10.6	93		
tert-Butylbenzene	10.5	87		
Pentachloroethane ³	19.8	106		
1,2,4-Trimethylbenzene	10.9	94		
sec-Butylbenzene	10.9	90		
p-Isopropyltoluene	10.8	87		
1,3-Dichlorobenzene	9.9	91		
1,4-Dichlorobenzene-d ₄ (ISTD)	-	-		
1,4-Dichlorobenzene	9.3	95		
n-Butylbenzene	10.1	86		
Hexachloroethane	17.1	103		
1,2-Dichlorobenzene (surr)	3.3	102		
1,2-Dichlorobenzene	9.6	97		
1,2-Dibromo-3-chloropropane	19.4	93		
Hexachlorobutadiene	11.4	93		
1,2,4-Trichlorobenzene	8.0	82		
Naphthalene	9.9	79		
1,2,3-Trichlorobenzene	7.6	84		

¹Reactive compound, compound analyzed n=35 samples

 $^{^{2}}$ Reactive compound, compound analyzed n=30 samples

 $^{^{3}}$ Reactive compound, compound analyzed n=25 samples



Additional resources

- AN000525: Uninterrupted analysis of volatile organic compounds in drinking water using single quadrupole GC-MS (US EPA 524.2)
- AN001018: Uninterrupted analysis of VOCs according to U.S. EPA Method 8260C using purge and trap and single quadrupole GC-MS technology
- AN000305: Analysis of volatile organic compounds in water using purge and trap coupled to single quadrupole GC-MS
- AN000377: Analysis of volatile organic compounds in soil using purge and trap coupled to single quadrupole GC-MS



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