Optimized Volatile Organic Compound Analysis Using Agilent VOC Application Solution

ENVIRONMENTAL ANALYSIS

The Agilent 5975C GC/MS is the perfect tool for VOC analysis. The Agilent VOC Solution provides all the keys to jumpstart the application.

The quality of drinking water is a global health concern and efforts to monitor water quality have been at the forefront of public policy for several decades. In particular, contamination from volatile organic compounds (VOC) has been a high priority of environmental protection agencies around the world. VOCs are used in a diverse assortment of materials such as fuels, personal care products, household goods, and industrial products. Improper use, storage, or disposal of these products can potentially lead to the introduction of VOCs into drinking water supplies. Exposure can cause a multitude of chronic and acute health related conditions, justifying a demand for a reliable, accurate, and sensitive method for their detection.

In many regions of the world, the primary methods for VOC analysis are based on US EPA 524.2 and 8260B. The Agilent 5975C GC/MS has a very successful legacy of implementing these methods that goes back several decades. With improvements to instrumentation, many of the commonly used parameters and method conditions require reoptimization. The Agilent VOC Solution optimizes these instrument conditions to provide the best sensitivity, robustness and stability while meeting all of the required method quality control elements. The Agilent VOC Application Kit (p/n G7022A) describes the optimizations and includes tips to ensure a successful analysis. The solution includes updated software, hardware and methods, and has been installed in numerous private and government VOC laboratories with great success, as shown by these quotes from a couple of early adopters of the Application Kit.

> "Increased sensitivity, stability and analyte linearity have all been greatly improved."
>
> "We have found the new BFB Autotune program to be very stable and easy to use. The chromatography looks great and sensitivity is good."

Key Benefits

- Increased tune stability allows for longer time in between tuning
- Median MDL of 0.05 ug/L for 524.2 compound list; for details see Table 1
- Median MDL of 0.06 ug/L for 8260B compound list; for details see Table 2
- All calibrations used average response factor with an average RSD of 8% for 524.2 and 6.1% for 8260B

One of the key changes included in the solution is a tuning algorithm named BFB Autotune, found in ChemStation E.02.02 SP1. The tune is specifically designed to be more stable and provide an increased sensitivity than previous versions of the BFB tune. By increasing the stability of the tune, the number of failed spectral tune evaluations was reduced by more than half. Additionally, internal checks have been added to the tune to preemptively catch and warn of problems that may arise in the system. The increase in sensitivity allows for one or two additional ICAL levels lower than what is prescribed in the published method. Additionally, tune evaluation has been improved with a new BFB evaluation macro included in the software service pack. The updated macro is better at identifying BFB and allows for the option to average the spectra over the entire chromatographic peak.

The Agilent VOC Application Kit provides a powerful solution for accurate, sensitive and robust VOC analysis.

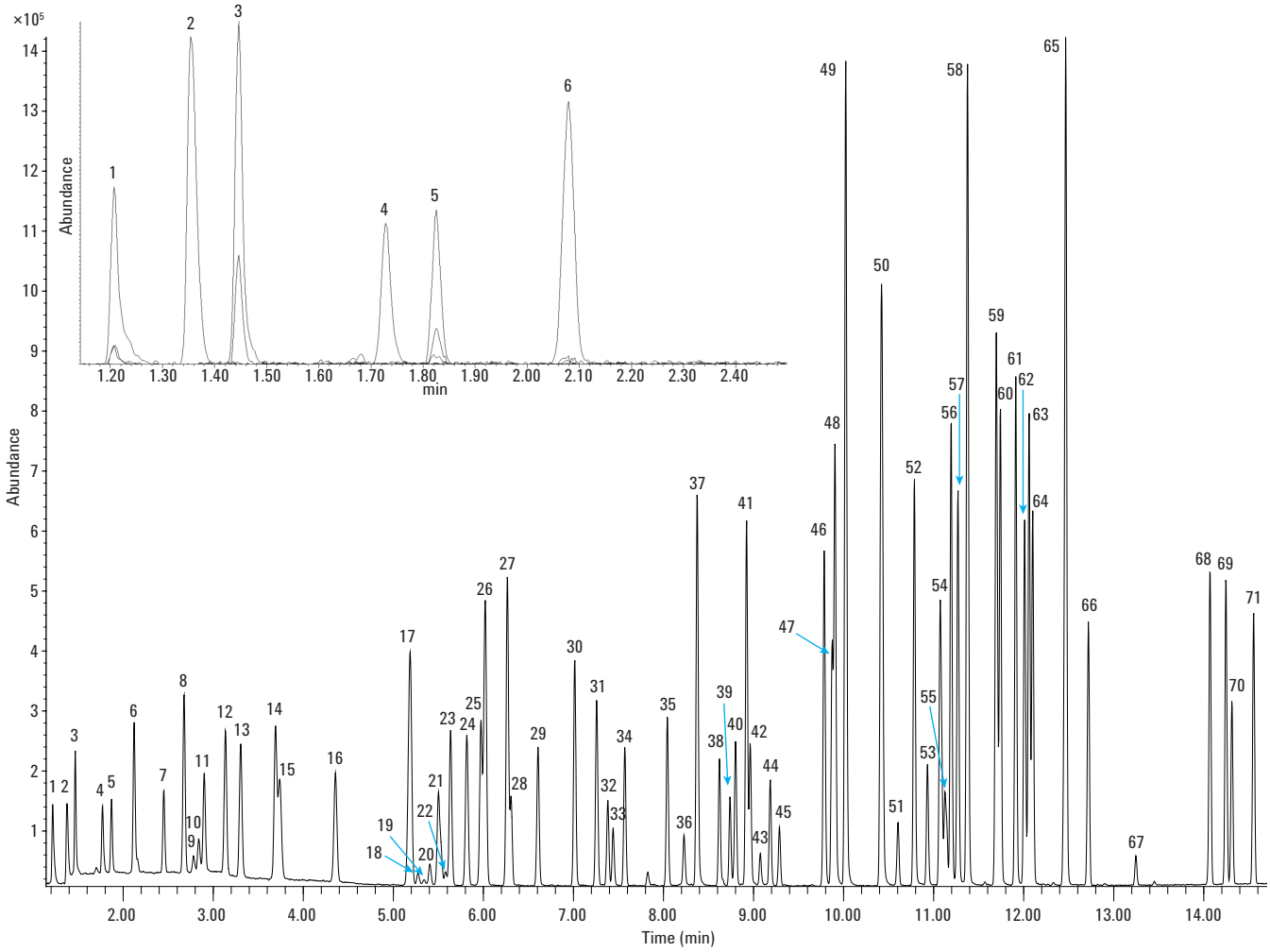

Figure 1. Total Ion Chromatogram of Method 524.2 ICAL standard. Inset: extracted ion chromatogram of the gases from left to right: dichlorodifluoromethane (85 m/z), chloromethane (50 m/z), vinyl chloride (62 m/z), bromomethane (94 m/z), chloroethane (64 m/z), and trichlorofluoromethane (101 m/z) in order of their elution. Peak numbers correlate to compound names in Table 1.

1. J.S. Hollis, H. Prest, Volatile Organic Compound analysis Using Purge and Trap, Agilent Application Manual 5991-0029E (2012).
2. J.W. Munch, T.A Bellar, J.W. Eichelberger, W.L. Budde, R.W. Slater, Jr., A. Alford-Stevens, Method 524.2 – Measurement of Purgeable Organic Compounds In Water by Capillary Column Gas Cromatography/Mass Spectrometry – Revision 4.1.

Table 1. MDL and Average Relative Response Factors for 524.2. Bracketed Numbers Correspond to Peaks in Figure 1

	Calibration			Method detection limit		
	Range (µg/L)	**Avg RRF**	**% RSD**	**Spike (µg/L)**	**Avg (µg/L)**	**MDL (µg/L)**
Dichlorodifluoromethane {1}	0.25–50	0.090	11.3	0.25	0.29	0.08
Chloromethane {2}	0.25–50	0.159	10.4	0.25	0.29	0.04
Vinyl chloride {3}	0.25–50	0.153	7.3	0.25	0.26	0.06
Bromomethane {4}	0.25–50	0.066	9.8	0.25	0.29	0.06
Chloroethane {5}	0.25–50	0.083	5.0	0.25	0.24	0.06
Trichlorofluoromethane {6}	0.25–50	0.169	9.2	0.25	0.27	0.05
Diethyl ether {7}	0.25–50	0.074	8.6	0.25	0.28	0.03
1,1-Dichloroethene {8}	0.25–50	0.181	7.5	0.25	0.28	0.06
Acetone {9}	5–50	0.018	14.0	2.0	2.87	0.43
Iodomethane {10}	0.25–50	0.066	15.0	0.25	0.24	0.15
Carbon disulfide {11}	0.25–50	0.282	7.7	0.25	0.26	0.04
Allyl chloride {12}	0.25–50	0.198	4.2	0.25	0.26	0.05
Methylene chloride {13}	0.25–50	0.157	9.5	0.25	0.29	0.07
trans-1,2-Dichloroethene {14}	0.25–50	0.166	7.0	0.25	0.29	0.07
Methyl *tert*-butyl ether (MTBE) {15}	0.25–50	0.244	12.5	0.25	0.27	0.03
1,1-Dichloroethane {16}	0.25–50	0.220	6.6	0.25	0.24	0.06
2,2-Dichloropropane {17}	0.25–50	0.165	10.4	0.25	0.18	0.16
cis-1,2-Dichloroethene {17}	0.25–50	0.200	4.3	0.25	0.28	0.06
2-Butanone(MEK) {18}	5–50	0.025	6.9	1.0	0.99	0.22
Bromochloromethane {21}	0.25–50	0.086	6.2	0.25	0.3	0.06
Chloroform {23}	0.25–50	0.202	4.4	0.25	0.23	0.04
1,1,1-Trichloroethane {24}	0.25–50	0.180	4.5	0.25	0.25	0.05
1-Chlorobutane {25}	0.25–50	0.253	5.9	0.25	0.28	0.05
Carbon Tetrachloride {26}	0.25–50	0.158	5.5	0.25	0.23	0.05
1,1-Dichloro-1-propene {26}	0.25–50	0.167	7.4	0.25	0.28	0.06
Benzene {27}	0.25–50	0.494	4.1	0.25	0.29	0.02
1,2-Dichloroethane {28}	0.25–50	0.118	5.7	0.25	0.29	0.08
Fluorobenzene (ISTD) {29}	N/A		4.0	N/A		
Trichloroethene {30}	0.25–50	0.130	8.7	0.25	0.25	0.04
1,2-Dichloropropane {31}	0.25–50	0.129	9.3	0.25	0.34	0.11
Dibromomethane {32}	0.25–50	0.049	3.8	0.25	0.25	0.06
Bromodichloromethane {34}	0.25–50	0.148	4.8	0.25	0.23	0.03
cis-1,3-Dichloropropene {35}	0.25–50	0.173	6.8	0.25	0.25	0.04
4-methyl-2-pentanone (MIBK) {36}	5–50	0.077	4.0	0.25	0.32	0.16
Toluene {37}	0.25–50	0.527	6.4	0.25	0.24	0.02
trans-1,3-Dichloropropene {38}	0.25–50	0.128	9.2	0.25	0.25	0.07
1,1,2-Trichloroethane {40}	0.25–50	0.076	12.4	0.25	0.35	0.05
Tetrachloroethene {41}	0.25–50	0.142	13.6	0.25	0.32	0.15
1,3-Dichloropropane {42}	0.25–50	0.132	8.8	0.25	0.29	0.04
2-Hexanone {43}	5–50	0.041	2.5	1.0	0.81	0.13
Dibromochloromethane {44}	0.25–50	0.094	6.8	0.25	0.25	0.04
1,2-Dibromoethane (EDB) {45}	0.25–50	0.070	13.6	0.25	0.29	0.1
Chlorobenzene {46}	0.25–50	0.311	5.6	0.25	0.24	0.02
1,1,1,2-Tetrachloroethane {47}	0.25–50	0.111	7.8	0.25	0.24	0.05

Table 1. MDL and Average Relative Response Factors for 524.2 (continued)

	Calibration			Method detection limit		
	Range (µg/L)	**Avg RRF**	**% RSD**	**Spike (µg/L)**	**Avg (µg/L)**	**MDL (µg/L)**
Ethylbenzene {48}	0.25–50	0.571	6.3	0.25	0.25	0.04
m+*p*-Xylene {49}	0.25–50	0.436	7.2	0.5	0.5	0.05
o-Xylene {50}	0.25–50	0.430	4.8	0.25	0.25	0.03
Styrene {50}	0.25–50	0.331	4.8	0.25	0.37	0.05
Bromoform {51}	0.25–50	0.052	10.6	0.25	0.28	0.07
Isopropylbenzene {52}	0.25–50	0.479	7.3	0.25	0.26	0.05
Bromofluorobenzene (Surr) {53}	0.25–50	0.330	2.9	1.0	1.03	0.06
Bromobenzene {54}	0.25–50	0.211	6.3	0.25	0.29	0.04
1,1,2,2-Tetrachloroethane {54}	0.25–50	0.095	14.0	0.25	0.3	0.05
1,2,3-Trichloropropane {55}	0.25–50	0.023	18.3	0.25	0.31	0.17
n-Propylbenzene {56}	0.25–50	0.375	6.0	0.25	0.28	0.04
2-Chlorotoluene {57}	0.25–50	0.377	6.5	0.25	0.27	0.02
1,3,5-Trimethylbenzene {58}	0.25–50	0.460	9.0	0.25	0.26	0.02
4-Chlorotoluene {58}	0.25–50	0.432	8.6	0.25	0.26	0.04
tert-Butylbenzene {59}	0.25–50	0.446	9.2	0.25	0.25	0.05
1,2,4-Trimethylbenzene {60}	0.25–50	0.452	7.7	0.25	0.26	0.03
sec-Butylbenzene {61}	0.25–50	0.604	11.5	0.25	0.28	0.03
1,3-Dichlorobenzene {62}	0.25–50	0.239	8.4	0.25	0.26	0.05
p-Isopropyltoluene {63}	0.25–50	0.472	12.7	0.25	0.27	0.02
1,4-Dichlorobenzene {64}	0.25–50	0.236	8.1	0.25	0.26	0.04
1,2-Dichlorobenzene-d4 (SURR) {65}	0.25–50	0.287	3.1	1.0	1.1	0.05
1,2-Dichlorobenzene {65}	0.25–50	0.207	8.5	0.25	0.3	0.04
n-Butylbenzene {65}	0.25–50	0.482	12.5	0.25	0.29	0.05
Hexachloroethane {66}	0.25–50	0.095	9.8	0.25	0.25	0.02
1,2-Dibromo-3-chloropropane (DBCP) {67}	0.25–50	0.013	12.0	0.25	0.29	0.13
1,2,4-Trichlorobenzene {68}	0.25–50	0.158	11.5	0.25	0.28	0.04
Hexachlorobutadiene {69}	0.25–50	0.101	15.3	0.25	0.29	0.06
Naphthalene {70}	0.25–50	0.252	13.1	0.25	0.32	0.04
1,2,3-Trichlorobenzene {71}	0.25–50	0.133	10.0	0.25	0.28	0.04

Table 2. MDL and Average Relative Response Factors for 8260B

	Calibration			Method detection limit		
	Range (µg/L)	Avg RRF	% RSD	Spike (µg/L)	Avg (µg/L)	MDL (µg/L)
1,1,1,2-Tetrachloroethane	0.25-80	0.3638	4.1	0.25	0.269	0.061
1,1,1-Trichloroethane	0.25-80	0.5747	5.6	0.25	0.246	0.06
1,1,2,2-Tetrachloroethane	0.25-80	0.9389	4.5	0.25	0.264	0.067
1,1,2-Trichloroethane	0.5-80	0.2912	6.4	0.25	0.269	0.045
1,1-Dichloroethane	0.25-80	0.6702	5.3	0.25	0.248	0.071
1,1-Dichloroethene	0.25-80	0.3236	8.3	0.25	0.257	0.094
1,1-Dichloropropene	0.25-80	0.5417	9.8	0.25	0.254	0.077
1,2,3-Trichlorobenzene	0.25-80	0.7801	9.0	0.25	0.238	0.081
1,2,3-Trichloropropane	0.25-80	0.3245	8.1	0.25	0.279	0.072
1,2,4-Trichlorobenzene	0.25-80	0.8484	8.3	0.25	0.245	0.095
1,2,4-Trimethylbenzene	0.25-80	2.5387	3.4	0.25	0.264	0.024
1,2-Dibromo-3-chloropropane	0.25-80	0.2728	13.7	0.25	0.31	0.168
1,2-Dibromoethane	0.25-80	0.3503	3.5	0.25	0.257	0.083
1,2-Dichlorobenzene	0.25-80	1.3153	2.5	0.25	0.246	0.039
1,2-Dichloroethane	0.25-80	0.4572	5.2	0.25	0.249	0.062
1,2-Dichloroethane-d4	0.5-80	0.3790	8.1			
1,2-Dichloroethene (total)	0.25-80	0.3943	8.7			
1,2-Dichloropropane	0.25-80	0.3547	3.5	0.25	0.262	0.053
1,3,5-Trimethylbenzene	0.25-80	2.6269	2.7	0.25	0.256	0.057
1,3-Dichlorobenzene	0.25-80	1.4055	2.8	0.25	0.273	0.037
1,3-Dichloropropane	0.25-80	0.5321	5.7	0.25	0.252	0.059
1,4-Dichlorobenzene	0.25-80	1.4309	4.7	0.25	0.266	0.041
1,4-Dioxane	0.5-60	0.0063	14.0	0.25	5.107	3.531
1-Chlorohexane	0.5-80	0.5254	7.3	0.25	0.311	0.094
2,2-Dichloropropane	0.25-80	0.5231	9.9	0.25	0.257	0.11
2-Butanone	1-80	0.3475	11.7	0.25	0.558	0.197
2-Chloroethyl vinyl ether	0.25-80	0.2386	3.0	0.25	0.261	0.092
2-Chlorotoluene	0.25-80	2.1159	2.7	0.25	0.27	0.036
2-Hexanone	0.5-80	0.4861	8.7	0.25	0.283	0.064
4-Bromofluorobenzene	0.5-80	0.4751	5.9			
4-Chlorotoluene	0.25-80	2.4325	2.8	0.25	0.265	0.044
4-Methyl-2-pentanone	0.25-80	0.5944	6.3	0.25	0.248	0.081
Acetone	4-80	0.1953	4.0	2	2.38	0.509
Acrylonitrile	0.25-80	0.2351	3.7	2.5	2.371	0.388
Benzene	0.25-80	1.4414	3.5	0.25	0.246	0.029
Bromobenzene	0.25-80	0.7458	3.7	0.25	0.268	0.059
Bromochloromethane	1-80	0.1922	5.7	0.25	0.276	0.093
Bromodichlorornethane	0.25-80	0.4627	4.9	0.25	0.242	0.049
Bromoform	0.25-80	0.3102	3.7	0.25	0.226	0.054
Bromomethane	0.5-80	0.2256	14.3	0.25	0.29	0.243
Carbon disulfide	0.25-80	1.0005	6.2	0.25	0.295	0.083
Carbon tetrachloride	0.25-80	0.5297	6.3	0.25	0.26	0.083
Chlorobenzene	0.25-80	0.9817	3.1	0.25	0.25	0.045

Table 2. MDL and Average Relative Response Factors for 8260B (continued)

	Calibration			Method detection limit		
	Range (µg/L)	**Avg RRF**	**% RSD**	**Spike (µg/L)**	**Avg (µg/L)**	**MDL (µg/L)**
Chloroethane	0.25-80	0.2199	6.7	0.25	0.249	0.204
Chloroform	0.5-80	0.6293	3.9	0.25	0.254	0.05
Chloromethane	0.25-80	0.4123	11.2	0.25	0.231	0.099
cis-1,2-Dichloroethene	0.25-80	0.4298	11.9	0.25	0.261	0.031
cis-1,3-Dichloropropene	0.25-80	0.5437	7.3	0.25	0.234	0.028
Dibromochloromethane	0.25-80	0.3671	4.6	0.25	0.247	0.063
Dibromofluoromethane	0.5-80	0.3620	8.7			
Dibromomethane	0.25-80	0.2397	9.7	0.25	0.24	0.055
Dichlorodifluoromethane	0.25-80	0.3762	11.5	0.25	0.189	0.059
Ethylbenzene	0.25-80	0.5501	7.2	0.25	0.262	0.03
Hexachlorobutadiene	0.25-80	0.4819	7.6	0.25	0.244	0.156
Isopropylbenzene	0.25-80	1.7766	3.2	0.25	0.246	0.039
Methylene chloride	0.25-80	0.3450	5.8	0.25	0.28	0.124
Methyl-*t*-butyl-ether	0.25-80	0.9668	5.5	0.25	0.253	0.041
Naphthalene	0.25-80	2.7184	6.3	0.25	0.244	0.081
n-Butylbenzene	0.25-80	2.6290	4.3	0.25	0.245	0.054
n-Propylbenzene	0.25-80	3.8186	2.5	0.25	0.262	0.043
p-Isopropyltoluene	0.25-80	2.8715	4.7	0.25	0.255	0.033
sec-Butylbenzene	0.25-80	3.4331	2.9	0.25	0.257	0.038
Styrene	0.25-80	1.0517	2.8	0.25	0.247	0.039
t-Butanol	0.25-80	0.1255	8.7	6.25	6.191	1.033
t-Butylbenzene	0.25-80	2.2963	4.0	0.25	0.258	0.05
Tetrachloroethene	0.25-80	0.4324	5.1	0.25	0.259	0.044
Toluene	0.25-80	0.8833	4.5	0.25	0.263	0.045
Toluene-d8	0.5-80	1.3329	3.8			
trans-1,2-dichloroethene	0.25-80	0.3589	9.6	0.25	0.274	0.033
trans-1,3-Dichloropropene	0.25-80	0.4816	7.4	0.25	0.235	0.054
Trichloroethene	0.25-80	0.3991	3.7	0.25	0.257	0.066
Trichlorofluoromethane	0.25-80	0.5389	6.7	0.25	0.236	0.074
Trichlorotrifluoroethane	0.25-80	0.3015	7.0	0.25	0.185	0.23
Trifluorotoluene	0.5-80	0.6530	6.3			
Vinyl acetate	0.5-80	0.7542	6.3	0.25	0.248	0.055
Vinyl chloride	0.25-80	0.3782	6.9	0.25	0.205	0.125
Xylene (o)	0.25-80	0.6415	3.4	0.25	0.262	0.062
Xylenes (m,p)	0.25-80	0.6775	2.2	0.5	0.513	0.067
Xylenes (total)	0.5-80	0.6655	2.6			

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