ICx Technologies
Detection Division
3000 Kent Avenue
West Lafayette, IN 47906

P: 1.888.775.1701
E: griffin450@icxt.com

Detection of Volatile Organic Compounds (VOCs) in Water Using a Mobile GC/MS/MS

INTRODUCTION

Sensitive and selective detection of chemical species, including chemical warfare (CW) agents, explosives, pesticides, and other toxic industrial compounds and materials (TICs/TIMs) has become a necessity in many applications. Although mass spectrometry has long been considered the gold-standard in laboratory analysis, its field potential remains largely underdeveloped. Field-deployable sensors conserve valuable time, resources, and chemical information by performing analyses directly on-site, rather than retrieving samples to be studied at a later time in the laboratory. Griffin's family of compact, mobile, tandem mass spectrometers based on the Cylindrical Ion Trap (CIT) mass analyzer[1,2] fulfill this need (see Figure 1).

This application note demonstrates the detection of Volatile Organic Compounds (VOCs) in water using the Griffin 450™ Mobile GC/MS/MS system (the Griffin 400™ may also be used to perform this analysis). A manual headspace sampler was used for sample preparation. The manual headspace sampler (Figure 1) is a compact, easy to operate, convenient accessory for water sample analysis using field-ready Gas Chromatography/Mass Spectrometery (GC/MS).

Figure 1. The Griffin 450 Mobile GC/MS/MS with Headspace Sampler

INSTRUMENTATION

- Griffin 450 with Griffin System Software 3.5.

Gas Chromatograph and Conditions:

Temperature Program: 40 °C hold for 1 min, then increase at 5 °C per minute to 130 °C, hold for 1.5 min	
Column:	Low Thermal Mass-Gas Chromatograph (LTM-GC) Rtx-5ms, 30m X 0.25mm X 0.25µm
Carrier Gas:	1 mL/minute helium
Sample:	100 ppb VOC mixture in water was prepared by diluting 8260 volatiles calibration mix (Supelco®, 2000 µg/mL in methanol) with LC/MS grade water.

Mass Spec Conditions:

ALC enabled with maximum ionization time at 150 ms.	
Mass Scan Range:	m/z 40-350
Detector Temp:	150 °C
Injector Temp:	200 °C

Manual Headspace Sampler:

Teknokroma 2t® Static Headspace Sampler	
Furnace Temp:	75 °C
Equilibrium time:	30 minutes
Sampled volume:	0.7 mL

RESULTS AND DISCUSSION

Figure 2 shows the chromatograph for the headspace sample of 100 ppb VOC's in water. All 52 components in the VOC mixture were detected in less than 18 min. Table 1 lists the 52 components in the order of elution time.

CONCLUSIONS

The Griffin 450 system identified all 52 compounds in the 8260 VOC mix in water. When utilized in tandem, the compact, easy to operate manual Headspace sampler and Griffin 450 provide a convenient field-ready solution for field analysis of water and soil samples. The Griffin 450 solution is ideal for a wide range of applications including water treatment analysis, environmental monitoring, and site-contamination clean-up efforts.

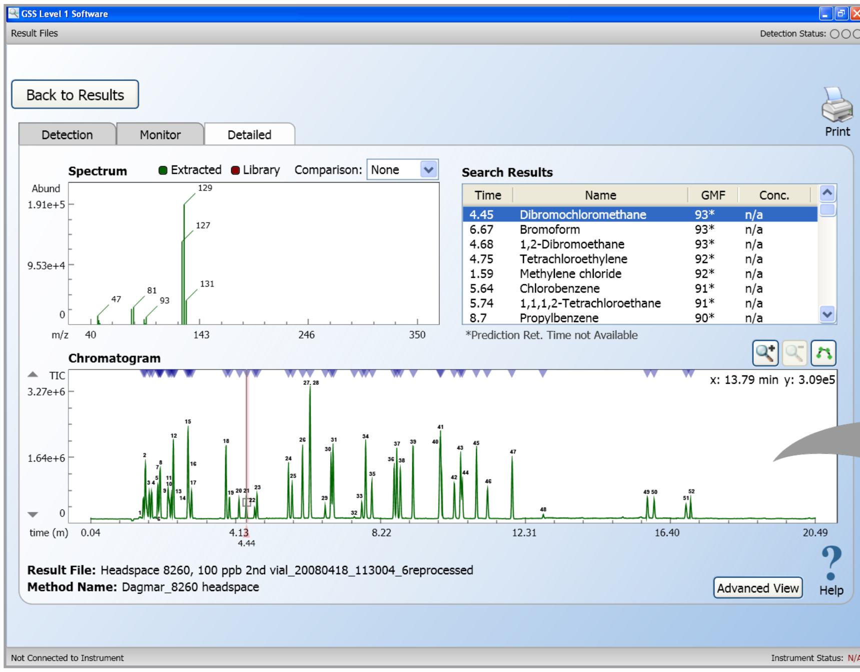
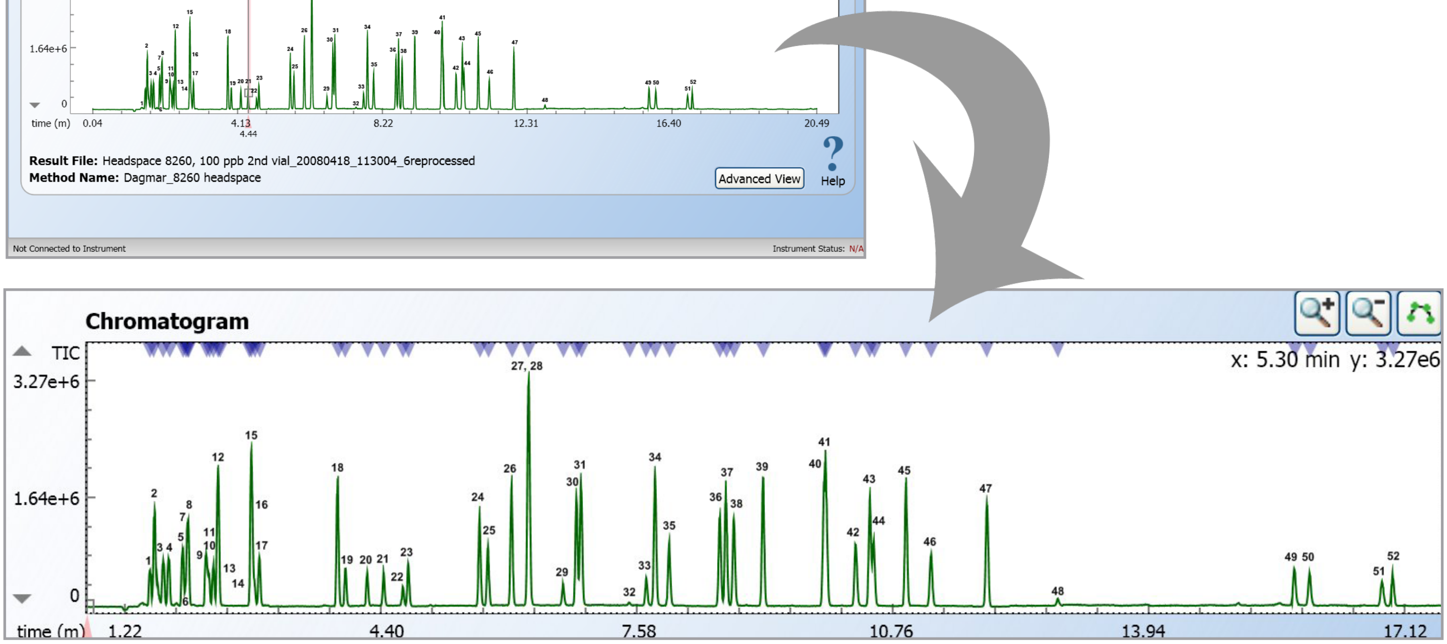


Figure 2.
Chromatograph and Mass Spectrum of 100 ppb VOC's in water.



#	Component	Ret. Time (min)	#	Component	Ret. Time (min)	#	Component	Ret. Time (min)	#	Component	Ret. Time (min)
Table 1. List of components identified in the 8260 volatiles calibration mix.											
1	1,1 dicholoroethylene	1.54	14	1, 2 –dichloropropane	2.78	27	o-Xylene	6.24	40	Tert-butylbenzene	9.91
2	methylene chloride	1.59	15	trichloroethylene	2.80	28	m-Xylene	6.24	41	1, 2, 4-trimethylbenzene	9.93
3	trans-1, 2-dicholoroethylene	1.71	16	dibromomethane	2.84	29	bromoform	6.67	42	1, 3-dichlorobenzene	10.31
4	1,1-dichlororethane	1.79	17	bromodichloromethane	2.90	30	styrene	6.84	43	sec-butylbenzene	10.48
5	cis-1, 2-dichloroethylene(Z)	1.96	18	toluene	3.88	31	p-Xylene	6.90	44	1, 4-dichlorobenzene	10.54
6	2, 2-dichloropropane	1.99	19	1, 1, 2-trichloroethane	3.97	32	1, 1, 2, 2-tetrachloroethane	7.50	45	p-isopropyltoluene	10.93
7	bromodichloromethane	2.01	20	1, 3-dichloropropane	4.24	33	1, 2, 3-trichloropropane	7.71	46	1, 2-dichlorobenzene	11.24
8	chloroform	2.02	21	dibromochloromethane	4.45	34	isopropylbenzene	7.82	47	butylbenzene	11.93
9	1, 1, 1-tricholoroethane	2.24	22	1, 2-dibromoethane	4.68	35	bromobenzene	7.99	48	1, 2-dibromo-3-chloropropane	12.82
10	1, 2-dichloroethane	2.28	23	tetrachloroethylene	4.75	36	2-chlorotoluene	8.61	49	1, 2, 4-trichlorobenzene	15.76
11	1,1-dichloropropene	2.33	24	chlorobenzene	5.64	37	propylbenzene	8.70	50	napthalene	15.95
12	benzene	2.39	25	1, 1, 1, 2-tretrachloroethane	5.74	38	4-chlorotoluene	8.79	51	1, 2, 3-trichlorobenzene	16.85
13	carbon tetrachloride	2.42	26	ethylbenzene	6.04	39	1, 3, 5-trimethylbenzene	9.16	52	hexachlorobutadiene	16.98

These data represent typical results.

REFERENCES

(1) Wells, J.M.; Badman, E.R.; Cooks, R.G. Anal. Chem. 1998, 70, 438-444.
(2) Patterson, G.E.; Guymon, A.J.; Riter, L.S.; Everly, M.; Griep-Raming, J.; Laughlin, B.C.; Ouyang, Z.; Cooks, R.G. Anal. Chem. 2002, 74, 6145-6153.