

INTRODUCTION

Sensitive and selective detection of chemical species, including chemical warfare agents (CWAs), 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. The ICx family of compact, mobile, tandem mass spectrometers are based on the Cylindrical Ion Trap (CIT) mass analyzer^{1, 2}.

This technical 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 is a compact, easy-to-operate, convenient accessory for water sample analysis using field ready Gas Chromatography/Mass Spectrometry (GC/MS).

INSTRUMENTATION

- Griffin 450
- Griffin System Software

Gas Chromatograph and Conditions

Temperature Program: 40°C hold for 1 min, then increase at 5°C/minute to 130°C, hold for 1.5 min	
Column	Low Thermal Mass-Gas Chromatograph (LTM-GC)
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 Temperature	150°C
Injector Temperature	200°C

Manual Headspace Sampler

Teknokroma 2t® Static Headspace Sampler	
Furnace Temperature	75°C
Equilibrium Time	30 minutes
Sampled Volume	0.7 mL

RESULTS AND DISCUSSION

Figure 1 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 minutes.

Table 1 lists the 52 components in the order of elution time.

CONCLUSIONS

The Griffin 450 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 is ideal for a wide range of applications including water treatment analysis, environmental monitoring and site-contamination cleanup efforts.

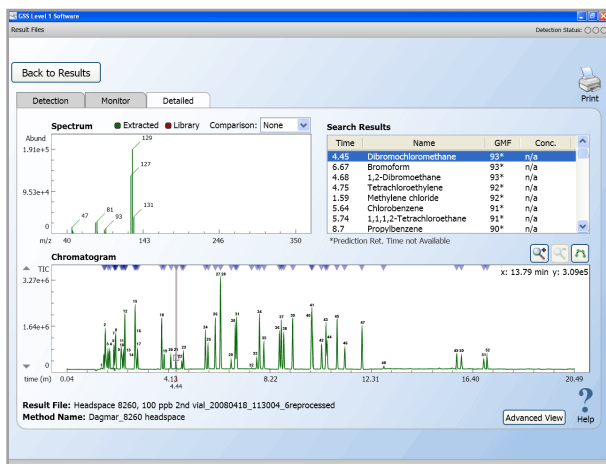


Figure 1: Chromatograph and Mass Spectrum of 100 ppb VOCs in water

#	Component	Ret. Time (min.)	#	Component	Ret. Time (min.)
1	1,1 dichloroethylene	1.54	27	o-Xylene	6.24
2	Methylene chloride	1.59	28	m-Xylene	6.24
3	Trans-1, 2-dichloroethylene	1.71	29	Bromoform	6.67
4	1,1-dichloroethane	1.79	30	Styrene	6.84
5	Cis-1, 2-dichloroethylene (Z)	1.96	31	p-Xylene	6.90
6	2, 2-dichloropropane	1.99	32	1, 1, 2, 2-tetrachloroethane	7.50
7	Bromochloromethane	2.01	33	1, 2, 3-trichloropropane	7.71
8	Chloroform	2.02	34	Isopropylbenzene	7.82
9	1, 1, 1-trichloroethane	2.24	35	Bromobenzene	7.99
10	1, 2-dichloroethane	2.28	36	2-chlorotoluene	8.61
11	1, 1-dichloropropene	2.33	37	Propylbenzene	8.70
12	Benzene	2.39	38	4-chlorotoluene	8.79
13	Carbon tetrachloride	2.42	39	1, 3, 5-trimethylbenzene	9.16
14	1,2- dichloropropane	2.78	40	Tert-butybenzene	9.91
15	Trichloroethylene	2.80	41	1, 2, 4-trimethylbenzene	9.93
16	Dibromomethane	2.84	42	1, 3-dichlorobenzene	10.31
17	Bromodichloromethane	2.90	43	Sec-butylbenzene	10.48
18	Toluene	3.88	44	1, 4-dichlorobenzene	10.54
19	1, 1, 2-trichloroethane	3.97	45	p-isopropyltoluene	10.93
20	1, 3-dichloropropane	4.24	46	1, 2-dichlorobenzene	11.24
21	Dibromochloromethane	4.45	47	Butylbenzene	11.93
22	1, 2-dibromomethane	4.68	48	1, 2-dibromo-3-chloropropane	12.82
23	Tetrachloroethylene	4.75	49	1, 2, 4-trichlorobenzene	15.76
24	Chlorobenzene	5.64	50	Naphthalene	15.95
25	1, 1, 1, 2-tetrachloroethane	5.74	51	1, 2, 3-trichlorobenzene	16.85
26	Ethylbenzene	6.04	52	Hexachlorobutadiene	16.9

Table 1: List of components identified in the 8260 volatiles calibration mix

References

- Wells, J.M.; Badman, E.R.; Cooks, R.G. Anal. Chem. 1998, 70, 438-444.
- 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.

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