INFICON

APPLICATION NOTE

HAPSITE® Portable GC/MS with SituProbe™: Calibration Curves for 68 Volatile Organic Compounds in Water

INTRODUCTION

The ability to identify and quantify volatile organic compound (VOC) contaminants can be vital to determining the health and safety of a water supply. Data must be as accurate as possible, particularly when determining the safety of drinking water. The HAPSITE portable gas chromatograph/mass spectrometer (GC/MS), with the SituProbe (SP) sampling accessory can accurately determine VOC concentrations in water by utilizing stored analytical methods with carefully designed calibration curves. As a result, actionable laboratory quality data can be generated at the site quickly and accurately. Additionally, the SituProbe and HAPSITE GC/MS system can be set up to monitor a water supply 24 hours a day, 7 days a week.

CALIBRATION CURVES

Response data for each of the 68 analytes (Figure 1) was collected from a 25-minute run at each concentration level. A Tri-Bed carbon based concentrator was used to pre-concentrate the sample before analysis. A 1-minute sample collection time was used for each calibration point. The system automatically injects the HAPSITE Internal Standards with each sample, providing the benefits of internal standard calibration without the need for sample preparation.

Linear calibration curves were created from six calibration standards (0.2, 0.4, 1, 2, 4, and 10 ppb) with low linear curve fit standard deviations. Adjusting the sample collection time on the concentrator can modify the sensitivity range.

Table 1 is a list of the sixty-eight analytes in the calibration library including CAS number, quantitation ion, retention time, calibration range, and %RSD of the curve fit for each analyte. The HAPSITE was equipped with the standard Rtx-1MS (30 m, 0.32 mm i.d., 1.0 µm df) analytical GC column for separating the analytes prior to MS detection. A minimum MS qualitative fit of 75% was required for positive compound identification.

WATER MONITORING

The HAPSITE / SituProbe system can be used to monitor water supplies for extended periods of time. Potential contaminants can be calibrated prior to system deployment for quantitative on-site monitoring.

With automated internal standard injection and data collection and analysis, the timely health and safety monitoring of water supplies can be accomplished without manual sample collection and traditional laboratory analysis.

Figure 1: Response Data

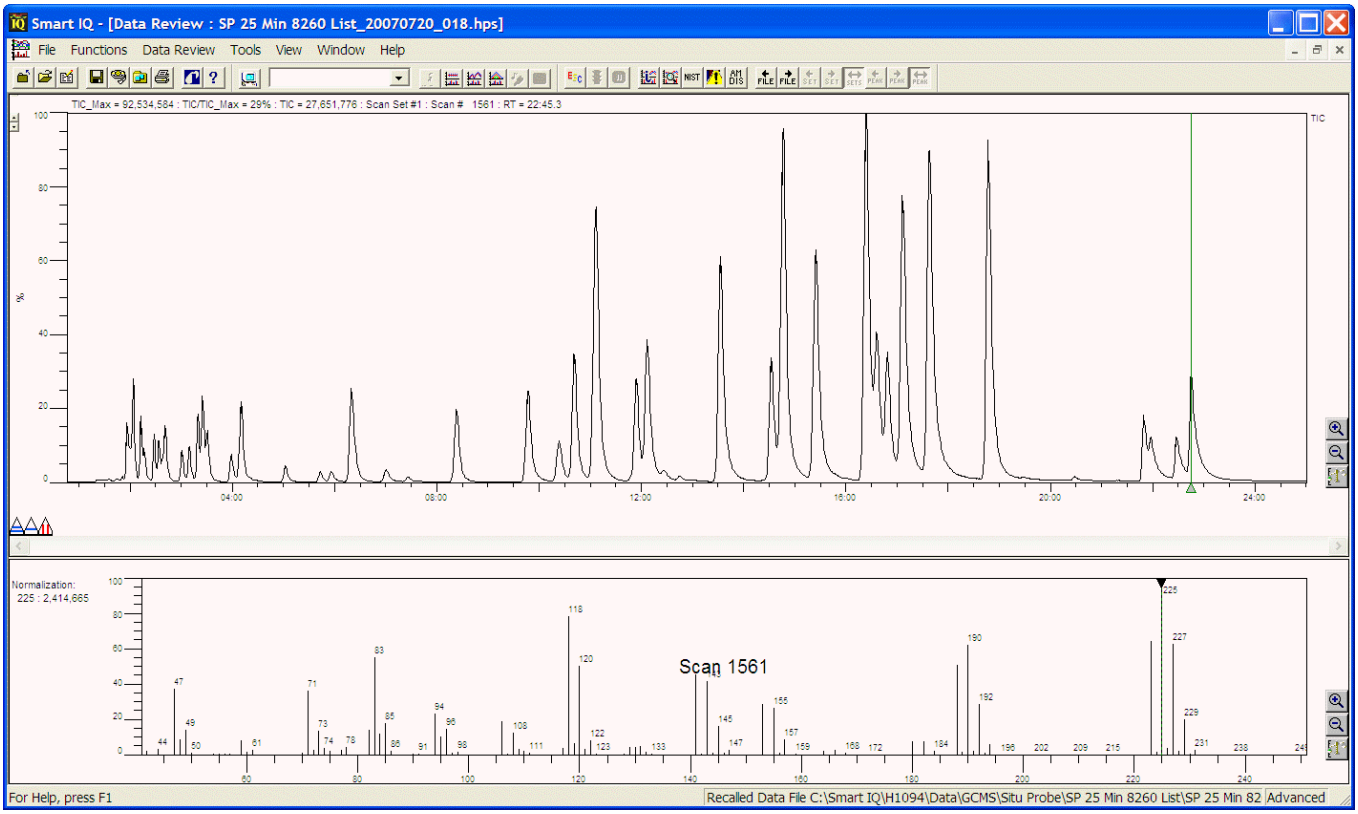

Table 1: List of Analytes

No.	Analyte name	CAS#	Q Ion	Ret Time	Curve Range (ppb)	%RSD
1	Ethyl Ether	60-29-7	74	1:52	0.2-10	6.3
2	1,1-Dichloroethylene	75-35-4	61	1:57	0.2-10	9.5
3	Iodomethane	74-88-4	142	1:57	0.2-4	2.7
4	Methylene chloride	75-09-2	84	1:59	0.2-10	13.2
5	Allyl chloride	107-05-1	76	2:00	0.2-10	15.4
6	1,1,2-Trichlorotrifluoroethane	76-13-1	101	2:02	0.2-10	3.5
7	Carbon disulfide	75-15-0	76	2:04	0.2-10	0.9
8	Propionitrile	107-12-0	54	2:09	1-10	6.8
9	trans-1,2-Dichloroethene	156-60-5	61	2:13	0.2-10	8.2
10	1,1-Dichloroethane	75-34-3	63	2:17	0.2-10	7.4
11	Methacrylonitrile	126-98-7	67	2:23	0.2-10	13.8
12	2-Chloro-1,3-butadiene	126-99-8	88	2:29	0.2-10	2.5
13	cis-1,2-Dichloroethene	156-59-2	61	2:34	0.2-10	8.0
14	Bromochloromethane	74-97-5	130	2:39	0.4-10	6.9
15	Trichloromethane	67-66-3	83	2:41	0.2-10	2.7
16	2,2-Dichloropropane	594-20-7	77	2:42	0.2-10	2.0
17	Tetrahydrofuran	109-99-9	72	2:53	0.2-10	17.6

Table 1: List of Analytes (Continued)

No.	Analyte name	CAS#	Q Ion	Ret Time	Curve Range (ppb)	%RSD
18	1,2-Dichloroethane	107-06-2	62	3:02	0.2-10	11.9
19	1,1,1-Trichloroethane	71-55-6	97	3:10	0.2-10	19.2
20	1,1-Dichloro-1-propene	563-58-6	75	3:20	0.2-10	22.5
21	Benzene	71-43-2	78	3:26	0.2-10	15.9
22	Carbon tetrachloride	56-23-5	117	3:31	0.2-10	4.4
23	2-Nitropropane	79-46-9	43	3:46	0.2-10	9.1
24	Dibromomethane	74-95-3	174	3:58	0.2-10	4.5
25	1,2-Dichloropropane	78-87-5	63	4:00	0.2-10	10.9
26	Bromodichloromethane	75-27-4	83	4:09	0.2-10	7.0
27	Trichloroethylene	79-01-6	130	4:11	0.2-10	1.8
28	Methyl methacrylate	80-62-6	69	4:22	0.2-10	13.2
29	cis-1,3-Dichloro-1-propene	10061-01-5	75	5:03	0.2-10	4.6
30	trans-1,3-Dichloro-1-propene	10061-02-6	75	5:44	0.2-10	5.0
31	1,1,2-Trichloroethane	79-00-5	97	5:57	0.2-10	6.4
32	Toluene	108-88-3	91	6:20	0.2-10	16.2
33	1,3-Dichloropropane	142-28-9	76	6:24	0.2-10	10.1
34	Ethyl methacrylate	97-63-2	69	0:00	0.2-10	11.3
35	Dibromochloromethane	124-48-1	129	7:01	0.2-10	6.9
36	1,2-Dibromoethane	106-93-4	107	7:27	0.2-10	5.2
37	Tetrachlorothylene	127-18-4	166	8:24	0.4-10	23.3
38	1,1,1,2-Tetrachloroethane	630-20-6	131	9:47	0.2-10	14.6
39	Chlorobenzene	108-90-7	112	9:47	0.2-10	16.4
40	Ethylbenzene	100-41-4	91	10:42	0.2-10	21.0
41	Bromoform	75-25-2	173	11:05	0.2-10	17.1
42	m,p-Xylene	108-38-3, 106-42-3	91	11:07	0.4-8	15.7
43	cis-1,4-Dichloro-2-butene	1476-11-5	75	11:49	0.2-10	13.1
44	Styrene	100-42-5	104	11:54	0.2-10	18.4
45	o-Xylene	95-47-6	91	12:07	0.2-10	25.2
46	1,1,2,2-Tetrachloroethane	79-34-5	83	12:10	0.2-10	8.1
47	1,2,3-Trichloropropane	96-18-4	75	12:27	0.2-10	7.7
48	trans-1,4-Dichloro-2-butene	110-57-6	75	12:46	0.2-4	13.1
49	Bromobenzene	108-86-1	77	13:32	0.2-10	4.7
50	Isopropylbenzene	98-82-8	105	13:33	0.2-10	2.7
51	2-Chlorotoluene	95-49-8	91	14:33	0.2-10	7.9
52	4-Chlorotoluene	106-43-4	126	14:47	0.2-4	1.9
53	Propylbenzene	103-65-1	120	14:47	0.2-4	16.2
54	Pentachloroethane	76-01-7	117	15:23	0.2-10	6.1
55	1,3,5-Trimethylbenzene	108-67-8	105	15:25	0.2-10	3.8
56	t-Butylbenzene	98-06-6	119	16:23	0.2-10	3.2

Table 1: List of Analytes (Continued)

No.	Analyte name	CAS#	Q Ion	Ret Time	Curve Range (ppb)	%RSD
57	1,2,4-Trimethylbenzene	95-63-6	105	16:25	0.2-10	2.8
58	1,3-Dichlorobenzene	541-73-1	146	16:37	0.2-10	5.0
59	1,4-Dichlorobenzene	106-46-7	146	16:49	0.2-10	3.7
60	sec-Butylbenzene	135-98-8	105	17:07	0.2-10	3.8
61	4-Isopropyltoluene	99-87-6	119	17:37	0.2-10	6.5
62	1,2-Dichlorobenzene	95-50-1	146	17:40	0.2-10	9.1
63	Butylbenzene	104-51-8	91	18:48	0.2-10	2.5
64	1,2-Dibromo-3-chloropropane	96-12-8	157	18:55	0.2-10	16.5
65	1,2,4-Trichlorobenzene	120-82-1	180	21:50	0.2-10	18.6
66	Naphthalene	91-20-3	128	21:58	0.2-10	11.3
67	1,2,3-Trichlorobenzene	87-61-6	180	22:28	0.2-10	18.9
68	Hexachloro-1,3-butadiene	87-68-3	225	22:45	0.2-10	23.5