EPA Method 8270 for SVOC Analysis on the 5977A Series GC/MSD

Application Note

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Introduction

Several environmental agencies in the world use the methodology described by the United States Environment Protection Agency (USEPA) in Method 8270, which utilizes gas chromatography/mass spectrometry (GC/MS) to analyze solid, liquid and gaseous samples for semi-volatile organic compounds. Method 8270 presents several analytical challenges due to the requirement for simultaneous measurement of acid, base, and neutral compounds over a wide concentration range.

Many laboratories strictly follow the method and typically analyze more than 70 compounds in a single analytical run, at a working concentration range between 20–160 parts per million (ppm), while a growing number of laboratories are pushing for lower detection limits and a wider dynamic range. New instrumentation, technologies and techniques are constantly evolving to meet these analytical demands.

Agilent Technologies

This Application Note describes the use of the highly inert and sensitive Agilent 5977A Series GC/MSD, coupled to the Agilent 7890B GC, to meet the performance requirements of the USEPA 8270 method over a working range of 0.2–100 ppm (Figure 1). The inert Extractor EI source, which has an operational temperature of up to 350 °C, plays a major role in delivering improved sensitivity. While Agilent MassHunter Workstation software was used for data acquisition and analysis, the 5977A Series GC/MSD continues to be compatible with the GC/MSD ChemStation data analysis software.

Experimental

Reagents and Standards

EPA 8270 GC-MS tuning solution containing benzidine, 4,4′- dichlorodiphenyltrichloroethane (DDT), decafluorotriphenylphosphine (DFTPP), and pentachlorophenol was used to evaluate the tuning of the 5977A Series GC/MSD. The calibration and performance evaluation standards were spiked with internal standard at a concentration of 5 ppm.

Instruments

This method was developed on the Agilent 5977A GC/MSD coupled to the Agilent 7890B Gas Chromatograph using a split/splitless inlet and the Agilent G1544-8070 liner. The instrument conditions used are shown in Table 1. MassHunter Workstation software was used for data acquisition and processing.

Table 1. Agilent 7890 GC and Agilent 5977A Series GC/MSD Instrument Conditions

GC run conditions	
Analytical column	DB-UI 8270D 30 m × 250 µm, 0.25 µm column (p/n 122-9732)*
Injection volume	1 µL
Inlet temperature	Isothermal at 250 °C
Injection mode	Pulsed splitless
Oven temperature gradient	0.5 minute hold at 40 °C
	40 °C to 100 °C at 10 °C/min, hold for 0 minutes
	100 °C to 260 °C at 25 °C/min, hold for 0 minutes
	260 °C to 280 °C at 5 °C/min, hold for 0 minutes
	280 °C to 320 °C at 40 °C/min, hold for 2 minutes
Carrier gas	Helium, constant flow at 9.1473 mL/min
Transfer line temperature	280 °C
Run time	21.6 minutes
MS conditions	
Ion source temperature	300 °C
Quadrupole temperature	150 °C
Ionization	EI mode
Scan mode	Full scan, *m/z* 35–500
EMV mode	Gain factor
Gain factor	0.30
Resulting EM voltage	1,259.3 V
Solvent delay	2.5 minutes

*This column is used in the 0.2 to 100 ppm detection range, and the DB-UI 8270D 30 m × 250 µm, 0.50 µm column (p/n 122-9736) is used in the 20 to 160 ppm detection range.

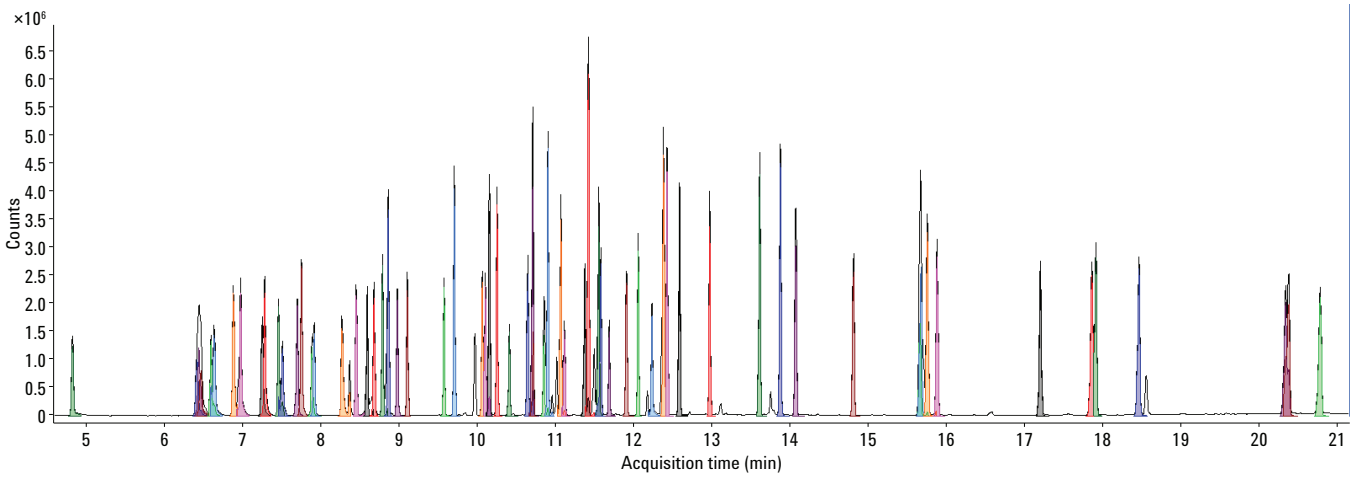


Figure 1. Total compound chromatogram (TCC) of 20 ppm standard.

Results and Discussion

Instrument Tuning

The 5977A Series GC/MSD was tuned using both Atune and Etune automatic tuning algorithms. The Etune algorithm provides the optimal condition for stability and sensitivity for the 5977A Series GC/MSD system. A voltage is applied to the extractor lens and ion body which accelerates and focuses the ions from the ionization volume. This provides higher ion transfer into the quadrupole and in turn improves the instrument sensitivity. This increase in sensitivity favors higher masses and, therefore, produces a DFTPP spectrum with a tilt different than the tuning criteria outlined in Method 8270 (Table 2). However, Method 8270B does allow for alternative tuning criteria if published and recommended by a manufacturer (§11.3.1).

The system tune performance for both tuning algorithms was evaluated using a 1-µL injection of a 50 µg/mL DFTPP solution. For Etune, the obtained DFTPP spectrum was compared to that of the NIST library, and it demonstrated a proper tune by meeting a match factor score of greater than 90 (Figure 2).

Atune was evaluated using the traditional DFTPP criteria set forth by the USEPA as listed in Table 2. MassHunter Quantitative Analysis was used to determine if the DFTPP ions produced by the tuned system met the EPA criteria. Both Etune and Atune passed their respective evaluative criteria.

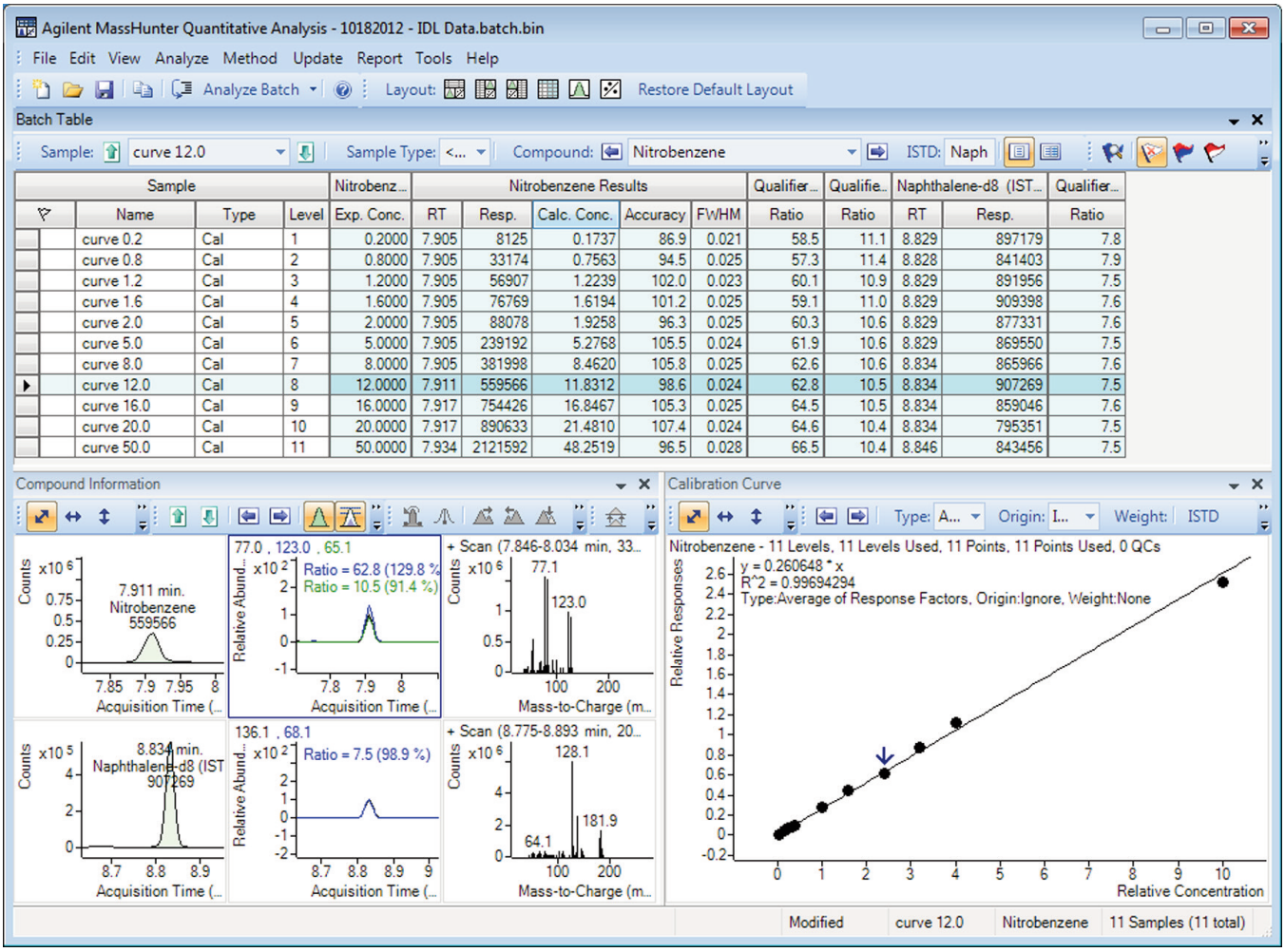
Table 2. USEPA Tuning Criteria for DFTTP

Mass (*m/z*)	Ion abundance criteria
51	10-80% of Base peak
68	<2% of mass 99
70	<2% of mass 69
127	10-80% of Base peak
197	<2% of mass 198
198	Base peak, or >50% of mass 442
199	5-9% of mass 198
275	10-60% of Base peak
365	>1% of mass 198
441	Present but <24% of mass 442
442	Base peak, or >50% of mass 198
443	15-24% of mass 442

Figure 2. Evaluation of the instrument performance by spectral matching DFTPP to the NIST library.

Initial Calibration

A multipoint calibration was run and the relative response factor was determined for each concentration of each component of the calibration standard (Figure 3). The mean response factor was then calculated across all of the average relative response factors for the calibration curve of each compound, along with its relative standard deviation (RSD). Table 3 displays the mean response factor and RSD. Due to the large number of compounds analyzed by this method, some compounds may fail to meet the Method 8270 relative response factor criterion of an RSD less than 20%. In such cases, an alternate curve fit algorithm is employed (in this case linear). When a linear curve fit is used, it is noted with a (-------) in the %RSD column in Table 3 and the calibration coefficient (R^2) of the fit is displayed instead of the RSD.



Sample				Nitrobenz...	Nitrobenzene Results					Qualifier...	Qualifie...	Naphthalene-d8 (IST...		Qualifier...
	Name	Type	Level	Exp. Conc.	RT	Resp.	Calc. Conc.	Accuracy	FWHM	Ratio	Ratio	RT	Resp.	Ratio
	curve 0.2	Cal	1	0.2000	7.905	8125	0.1737	86.9	0.021	58.5	11.1	8.829	897179	7.8
	curve 0.8	Cal	2	0.8000	7.905	33174	0.7563	94.5	0.025	57.3	11.4	8.828	841403	7.9
	curve 1.2	Cal	3	1.2000	7.905	56907	1.2239	102.0	0.023	60.1	10.9	8.829	891956	7.5
	curve 1.6	Cal	4	1.6000	7.905	76769	1.6194	101.2	0.025	59.1	11.0	8.829	909398	7.6
	curve 2.0	Cal	5	2.0000	7.905	88078	1.9258	96.3	0.025	60.3	10.6	8.829	877331	7.6
	curve 5.0	Cal	6	5.0000	7.905	239192	5.2768	105.5	0.024	61.9	10.6	8.829	869550	7.5
	curve 8.0	Cal	7	8.0000	7.905	381998	8.4620	105.8	0.025	62.6	10.6	8.834	865966	7.6
▶	curve 12.0	Cal	8	12.0000	7.911	559566	11.8312	98.6	0.024	62.8	10.5	8.834	907269	7.5
	curve 16.0	Cal	9	16.0000	7.917	754426	16.8467	105.3	0.025	64.5	10.5	8.834	859046	7.6
	curve 20.0	Cal	10	20.0000	7.917	890633	21.4810	107.4	0.024	64.6	10.4	8.834	795351	7.5
	curve 50.0	Cal	11	50.0000	7.934	2121592	48.2519	96.5	0.028	66.5	10.4	8.846	843456	7.5

Figure 3. Evaluation of calibration using Agilent MassHunter Quantitative Analysis, in this case using the nitrobenzene component of the 8270 test mix.

Table 3. Calibration Curve Data for 84 Compounds Specified by Method 8270

	Average response factor determined at each of 11 points on the calibration curve													
Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**Mean RF***	**%RSD**	**R^2**
N-Nitrosodimethylamine	0.704	0.690	0.751	0.690	0.638	0.759	0.718	0.700	0.697	0.727	0.660	0.703	5.1	-----
2-Fluorophenol	1.212	1.149	1.326	1.233	1.121	1.254	1.267	1.203	1.224	1.295	1.178	1.224	5.0	-----
Aniline	1.655	1.648	1.916	1.800	1.680	1.886	1.706	1.679	1.682	1.886	1.646	1.744	6.1	-----
Phenol-d5	1.651	1.513	1.770	1.721	1.503	1.736	1.674	1.505	1.556	1.692	1.570	1.626	6.1	-----
Phenol	1.583	1.698	1.975	1.904	1.678	1.923	1.790	1.667	1.697	1.858	1.641	1.765	7.4	-----
bis(2-Chloroethyl)ether	1.374	1.221	1.412	1.360	1.246	1.384	1.308	1.242	1.280	1.355	1.266	1.313	5.1	-----
2-Chlorophenol	1.531	1.372	1.577	1.433	1.358	1.544	1.451	1.413	1.462	1.540	1.431	1.465	5.0	-----
1,3-Dichlorobenzene	1.650	1.599	1.741	1.674	1.552	1.733	1.619	1.576	1.613	1.646	1.470	1.625	4.8	-----
1,4-Dichlorobenzene	1.828	1.734	1.865	1.824	1.716	1.891	1.790	1.633	1.669	1.786	1.600	1.758	5.4	-----
Benzyl alcohol	0.879	0.834	0.919	0.907	0.819	0.887	0.859	0.821	0.837	0.876	0.736	0.852	6.0	-----
1,2-Dichlorobenzene	1.670	1.591	1.782	1.736	1.587	1.704	1.644	1.539	1.566	1.629	1.327	1.616	7.5	-----
2-Methylphenol	1.210	1.145	1.288	1.281	1.159	1.322	1.243	1.098	1.190	1.279	1.092	1.210	6.6	-----
bis(2-Chloroisopropyl)ether	1.380	1.375	1.509	1.476	1.314	1.477	1.405	1.233	1.295	1.341	1.183	1.363	7.6	-----
4-Methylphenol	1.286	1.237	1.379	1.355	1.208	1.379	1.337	1.157	1.251	1.335	1.210	1.285	6.0	-----
N-Nitroso-di-propylamine	0.893	0.739	0.785	0.788	0.708	0.791	0.764	0.663	0.701	0.713	0.648	0.745	9.3	-----
Hexachloroethane	0.499	0.471	0.507	0.504	0.469	0.519	0.502	0.443	0.467	0.490	0.415	0.481	6.5	-----
Nitrobenzene--d5	0.225	0.233	0.245	0.247	0.234	0.260	0.264	0.248	0.271	0.275	0.256	0.251	6.4	-----
Nitrobenzene	0.226	0.247	0.265	0.264	0.251	0.275	0.276	0.257	0.274	0.280	0.252	0.261	6.2	-----
Isophorone	0.557	0.575	0.586	0.577	0.553	0.602	0.575	0.525	0.557	0.565	0.558	0.566	3.6	-----
2-Nitrophenol	0.087	0.088	0.097	0.098	0.093	0.121	0.127	0.127	0.146	0.150	0.167	0.118	-----	0.9957
2,4-Dimethylphenol	0.222	0.219	0.235	0.225	0.215	0.258	0.252	0.224	0.248	0.261	0.244	0.237	7.0	-----
bis(2-Chloroethoxy)methane	0.432	0.402	0.436	0.435	0.414	0.422	0.420	0.384	0.398	0.411	0.376	0.412	4.9	-----
Benzoic Acid	0.095	0.060	0.046	0.044	0.039	0.069	0.067	0.239	0.266	0.281	0.263	0.133	-----	0.9947
2,4-Dichlorophenol	0.301	0.284	0.311	0.317	0.294	0.315	0.313	0.287	0.301	0.317	0.297	0.303	3.9	-----
1,2,4-Trichlorobenzene	0.341	0.318	0.360	0.359	0.331	0.345	0.327	0.303	0.319	0.330	0.284	0.329	6.9	-----
Naphthalene	1.106	1.070	1.196	1.190	1.091	1.154	1.089	0.974	1.005	1.021	0.823	1.065	10.1	-----
4-Chloroaniline	0.415	0.404	0.439	0.452	0.425	0.455	0.431	0.397	0.418	0.438	0.384	0.423	5.4	-----
Hexachlorobutadiene	0.168	0.158	0.175	0.174	0.152	0.171	0.162	0.149	0.162	0.161	0.140	0.161	6.8	-----
4-Chloro-3-methylphenol	0.289	0.279	0.292	0.289	0.262	0.282	0.271	0.262	0.283	0.281	0.250	0.276	4.9	-----
2-Methylnaphthalene	0.640	0.658	0.704	0.705	0.620	0.659	0.636	0.573	0.601	0.597	0.464	0.623	10.8	-----
Hexachlorocyclopentadiene	0.111	0.118	0.142	0.125	0.115	0.153	0.180	0.166	0.188	0.212	0.243	0.159	-----	0.9989
2,4,6-Trichlorophenol	0.394	0.363	0.419	0.373	0.347	0.397	0.396	0.362	0.389	0.406	0.408	0.387	5.8	-----
2,4,5-Trichlorophenol	0.411	0.385	0.447	0.406	0.376	0.431	0.438	0.414	0.410	0.428	0.397	0.413	5.3	-----
2-Fluorobiphenyl	1.655	1.532	1.722	1.572	1.438	1.538	1.510	1.354	1.346	1.337	1.172	1.471	10.9	-----
2-Chloronaphthalene	1.500	1.399	1.566	1.415	1.331	1.381	1.357	1.240	1.193	1.249	1.132	1.342	9.7	-----
2-Nitroaniline	0.225	0.244	0.303	0.290	0.281	0.353	0.360	0.383	0.398	0.420	0.454	0.337	-----	0.9976
Dimethyl phthalate	1.585	1.434	1.632	1.477	1.386	1.422	1.398	1.330	1.326	1.379	1.338	1.428	7.1	-----
Acenaphthylene	2.329	2.273	2.576	2.339	2.091	2.234	2.137	1.863	1.905	1.875	1.594	2.110	13.3	-----
2,6-Dinitrotoluene	0.140	0.157	0.200	0.192	0.176	0.239	0.244	0.233	0.252	0.264	0.283	0.216	-----	0.9979
3-Nitroaniline	0.185	0.215	0.273	0.283	0.267	0.314	0.291	0.317	0.324	0.349	0.376	0.290	19.1	-----
Acenaphthene	1.524	1.398	1.586	1.540	1.396	1.441	1.381	1.262	1.233	1.234	1.004	1.363	12.4	-----
2,4-Dinitrophenol	0.018	0.018	0.020	0.019	0.018	0.030	0.027	0.038	0.043	0.050	0.083	0.033	-----	0.9997
4-Nitrophenol	0.120	0.058	0.073	0.068	0.068	0.074	0.060	0.074	0.075	0.082	0.092	0.077	-----	0.9991
Dibenzofuran	1.986	1.841	2.079	1.980	1.737	1.817	1.796	1.673	1.657	1.691	1.400	1.787	10.6	-----
2,4-Dinitrotoluene	0.163	0.184	0.250	0.261	0.228	0.322	0.332	0.366	0.371	0.401	0.414	0.299	-----	0.9986
Fluorene	1.588	1.453	1.671	1.610	1.437	1.400	1.289	1.216	1.171	1.181	0.912	1.357	16.8	-----
Diethyl phthalate	1.622	1.239	1.395	1.341	1.201	1.217	1.126	1.150	1.153	1.195	1.061	1.245	12.6	-----

Table 3. Calibration Curve Data for 84 Compounds Specified by Method 8270 (continued)

	Average response factor determined at each of 11 points on the calibration curve													
Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**Mean RF***	**%RSD**	**R^2**
4-Chlorophenyl-phenylether	0.726	0.668	0.761	0.745	0.656	0.635	0.595	0.565	0.545	0.550	0.427	0.625	16.2	-----
4-Nitroaniline	0.188	0.181	0.251	0.250	0.241	0.273	0.215	0.285	0.276	0.326	0.351	0.258	-----	0.9933
4,6-Dinitro-2-methylphenol	0.032	0.031	0.036	0.032	0.031	0.048	0.046	0.066	0.069	0.083	0.116	0.054	-----	0.9991
N-Nitrosodiphenylamine	0.603	0.529	0.591	0.573	0.528	0.547	0.549	0.525	0.494	0.488	0.420	0.532	9.7	-----
Azobenzene	0.183	0.166	0.184	0.182	0.165	0.175	0.180	0.174	0.169	0.168	0.164	0.174	4.4	-----
2,4,6-Tribromophenol	0.095	0.091	0.101	0.097	0.082	0.105	0.113	0.119	0.118	0.122	0.130	0.107	14.1	-----
4-Bromophenylphenyl ether	0.226	0.219	0.243	0.235	0.205	0.225	0.226	0.217	0.209	0.200	0.214	0.220	5.8	-----
Hexachlorobenzene	0.296	0.259	0.288	0.283	0.248	0.261	0.267	0.247	0.247	0.240	0.234	0.261	7.9	-----
Pentachlorophenol	0.086	0.084	0.090	0.086	0.073	0.106	0.108	0.122	0.122	0.132	0.157	0.106	-----	0.9997
Phenanthrene	1.277	1.131	1.265	1.232	1.088	1.132	1.072	0.991	0.937	0.958	0.806	1.081	13.7	-----
Anthracene	1.228	1.070	1.243	1.192	1.053	1.075	1.030	0.998	0.960	0.935	0.756	1.049	13.5	-----
Di-n-butylphthalate	1.305	1.207	1.313	1.333	1.159	1.302	1.186	1.108	1.086	1.088	0.876	1.178	11.6	-----
Fluoranthene	1.225	1.096	1.290	1.189	1.070	1.185	1.062	0.977	0.968	0.964	0.800	1.075	13.3	-----
Pyrene	1.724	1.645	1.641	1.488	1.244	1.431	1.533	1.359	1.295	1.333	1.010	1.428	14.6	-----
d14-Terphenyl	0.958	0.917	0.964	0.862	0.752	0.859	0.844	0.802	0.728	0.765	0.611	0.824	12.9	-----
Butylbenzylphthalate	0.512	0.507	0.549	0.505	0.432	0.537	0.554	0.557	0.532	0.560	0.516	0.524	7.0	-----
Benzo(a)anthracene	1.073	0.946	1.078	1.042	0.939	1.001	0.969	0.934	0.897	0.932	0.786	0.963	8.8	-----
3,3'-Dichlorobenzidine	0.299	0.250	0.323	0.319	0.330	0.329	0.340	0.326	0.338	0.361	0.316	0.321	8.8	-----
Chrysene	1.154	1.025	1.176	1.173	0.989	1.081	1.068	0.936	0.980	1.013	0.786	1.035	11.2	-----
bis(2ethylhexyl)phthalate	0.870	0.804	0.823	0.816	0.665	0.863	0.861	0.831	0.827	0.840	0.774	0.816	7.0	-----
Di-n-octyl phthalate	1.459	1.379	1.490	1.487	1.283	1.783	1.659	1.871	1.632	1.862	1.619	1.593	12.1	-----
Benzo(b)fluoranthene	1.246	1.086	1.292	1.284	1.110	1.258	1.229	1.239	1.197	1.369	1.289	1.236	6.6	-----
Benzo(k)fluoranthene	1.176	1.108	1.280	1.282	1.133	1.269	1.326	1.271	1.121	1.369	1.290	1.239	7.2	-----
Benzo(a)pyrene	1.063	0.962	1.149	1.144	1.034	1.244	1.171	1.166	1.106	1.229	1.171	1.131	7.4	-----
Indeno(1,2,3-cd)pyrene	0.932	0.791	0.996	0.944	1.029	1.104	1.185	1.107	1.102	1.267	1.159	1.056	12.7	-----
Dibenzo(a,h)anthracene	0.691	0.581	0.764	0.737	0.822	0.888	0.976	0.899	0.913	1.074	0.943	0.844	16.8	-----
Benzo(g,h,i)perylene	0.848	0.730	0.888	0.862	0.859	0.968	0.977	0.945	0.932	1.102	0.940	0.914	10.3	-----

*Mean response factor calculated across all of the average response factors

Method Reproducibility Study

Ten replicates of the 8270 low standard, 0.2 ppm, were run to illustrate system reproducibility and accuracy (Table 4). More than 80% of the compounds exhibited RSDs below 6%, with several below 2%.

Table 4. Ten Replicate Determinations of 0.2 ppm Samples of Each of 84 Analytes

	Replicate number											
	1	**2**	**4**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**Average**	**%RSD**
N-Nitrosodimethylamine	0.173	0.183	0.155	0.161	0.160	0.170	0.157	0.163	0.169	0.158	0.165	5.1
2-Fluorophenol (surr1)	0.178	0.164	0.165	0.162	0.166	0.163	0.143	0.161	0.148	0.158	0.161	5.7
Phenol-d5 (surr2)	0.179	0.191	0.182	0.183	0.187	0.182	0.183	0.179	0.180	0.176	0.182	2.5
Phenol	0.178	0.188	0.188	0.182	0.188	0.183	0.181	0.183	0.182	0.178	0.183	2.1
Aniline	0.151	0.162	0.162	0.163	0.169	0.164	0.168	0.171	0.170	0.164	0.164	3.3
bis(2-Chloroethyl)ether	0.171	0.181	0.181	0.175	0.185	0.179	0.180	0.185	0.177	0.172	0.178	2.7
2-Chlorophenol	0.178	0.179	0.183	0.181	0.181	0.176	0.175	0.157	0.176	0.176	0.176	4.0
1,3-Dichlorobenzene	0.189	0.190	0.181	0.182	0.187	0.181	0.185	0.188	0.188	0.182	0.185	1.8
1,4-Dichlorobenzene	0.186	0.187	0.181	0.176	0.178	0.182	0.177	0.181	0.187	0.176	0.181	2.3
Benzyl Alcohol	0.151	0.160	0.142	0.151	0.150	0.150	0.147	0.153	0.148	0.138	0.149	4.1
1,2-Dichlorobenzene	0.197	0.207	0.201	0.199	0.202	0.202	0.193	0.202	0.195	0.195	0.199	2.1
2-Methylphenol	0.192	0.198	0.192	0.187	0.196	0.197	0.192	0.188	0.186	0.180	0.191	3.0
bis(2-Chloroisopropyl)ether	0.198	0.207	0.201	0.198	0.200	0.198	0.202	0.202	0.195	0.192	0.199	2.1
4-Methylphenol	0.177	0.182	0.166	0.170	0.170	0.174	0.169	0.169	0.163	0.161	0.170	3.7
N-Nitroso-di-propylamine	0.149	0.154	0.150	0.151	0.154	0.150	0.149	0.143	0.147	0.143	0.149	2.6
Hexachloroethane	0.189	0.192	0.196	0.189	0.204	0.190	0.189	0.192	0.191	0.193	0.192	2.3
Nitrobenzene--d5 (surr3)	0.181	0.179	0.163	0.156	0.158	0.152	0.149	0.148	0.146	0.144	0.158	8.6
Nitrobenzene	0.172	0.174	0.169	0.165	0.168	0.160	0.159	0.155	0.155	0.149	0.163	5.2
Isophorone	0.148	0.153	0.153	0.150	0.146	0.152	0.149	0.146	0.140	0.141	0.148	3.1
2-Nitrophenol	1.230	1.227	1.224	1.226	1.222	1.228	1.223	1.218	1.217	1.221	1.224	0.3
2,4-Dimethylphenol	0.166	0.164	0.166	0.164	0.170	0.162	0.155	0.157	0.156	0.161	0.162	2.9
bis(2-Chloroethoxy)methane	0.199	0.202	0.199	0.202	0.199	0.204	0.203	0.197	0.199	0.201	0.201	1.2
2,4-Dichlorophenol	0.152	0.147	0.146	0.144	0.147	0.148	0.139	0.141	0.141	0.130	0.143	4.6
1,2,4-Trichlorobenzene	0.212	0.208	0.206	0.214	0.209	0.213	0.213	0.206	0.212	0.209	0.210	1.3
Naphthalene	0.209	0.205	0.209	0.208	0.205	0.205	0.207	0.206	0.206	0.208	0.207	0.8
4-Chloroaniline	0.132	0.145	0.148	0.160	0.155	0.162	0.157	0.168	0.148	0.167	0.154	6.4
Hexachlorobutadiene	0.187	0.208	0.201	0.202	0.184	0.198	0.202	0.201	0.205	0.205	0.199	3.6
4-Chloro-3-methylphenol	0.127	0.162	0.132	0.141	0.148	0.153	0.136	0.143	0.146	0.127	0.141	8.4
2-Methylnaphthalene	0.197	0.215	0.206	0.205	0.202	0.208	0.206	0.205	0.206	0.205	0.206	2.1
Hexachlorocyclopentadiene	1.549	1.552	1.551	1.546	1.549	1.551	1.551	1.548	1.548	1.547	1.549	0.1
2,4,6-Trichlorophenol	0.067	0.063	0.069	0.061	0.062	0.060	0.063	0.058	0.055	0.054	0.061	8.0
2,4,5-Trichlorophenol	0.061	0.055	0.053	0.051	0.051	0.053	0.053	0.049	0.047	0.042	0.052	11.0
2-Fluorobiphenyl (surr4)	0.214	0.220	0.221	0.216	0.219	0.218	0.217	0.217	0.214	0.215	0.217	1.1
2-Chloronaphthalene	0.210	0.217	0.221	0.219	0.219	0.223	0.218	0.217	0.219	0.218	0.218	1.4
2-Nitroaniline	1.044	1.035	1.034	1.026	1.026	1.027	1.025	1.024	1.024	1.022	1.029	0.7
Dimethyl phthalate	0.192	0.186	0.189	0.179	0.190	0.195	0.188	0.192	0.188	0.184	0.188	2.2
Acenaphthylene	0.214	0.213	0.213	0.215	0.215	0.212	0.209	0.213	0.210	0.210	0.212	1.0
3-Nitroaniline	1.024	1.012	1.006	1.001	1.003	0.995	0.998	0.994	0.994	0.994	1.002	0.9
Acenaphthene	0.225	0.222	0.221	0.225	0.220	0.222	0.218	0.222	0.216	0.222	0.221	1.2
Dibenzofuran	0.224	0.221	0.224	0.224	0.222	0.221	0.221	0.219	0.216	0.215	0.221	1.4
2,4-Dinitrotoluene	0.961	0.947	0.944	0.944	0.942	0.939	0.939	0.938	0.938	0.934	0.943	0.8
Diethyl phthalate	0.195	0.188	0.187	0.221	0.195	0.191	0.190	0.191	0.216	0.217	0.199	5.7
Fluorene	0.236	0.221	0.225	0.227	0.224	0.226	0.220	0.220	0.219	0.222	0.224	2.1

Table 4. Ten Replicate Determinations of 0.2 ppm Samples of Each of 84 Analytes (continued)

	Replicate number											
	1	**2**	**4**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**Average**	**%RSD**
4-Chlorophenyl-phenylether	0.235	0.224	0.228	0.230	0.228	0.234	0.222	0.229	0.228	0.226	0.228	1.8
4-Nitroaniline	1.374	1.353	1.347	1.346	1.343	1.338	1.332	1.333	1.331	1.335	1.343	0.9
N-Nitrosodiphenylamine	0.238	0.217	0.224	0.227	0.225	0.222	0.226	0.224	0.226	0.217	0.224	2.6
Azobenzene	0.225	0.199	0.203	0.204	0.208	0.208	0.208	0.207	0.201	0.193	0.205	4.0
2,4,6-Tribromophenol (surr5)	0.100	0.075	0.066	0.075	0.075	0.075	0.076	0.067	0.062	0.074	0.074	12.7
4-Bromophenylphenyl ether	0.228	0.215	0.213	0.216	0.219	0.220	0.219	0.221	0.220	0.209	0.218	2.4
Hexachlorobenzene	0.234	0.220	0.212	0.218	0.224	0.219	0.221	0.220	0.222	0.227	0.222	2.4
Phenanthrene	0.209	0.213	0.213	0.214	0.206	0.211	0.215	0.209	0.212	0.211	0.211	1.3
Anthracene	0.204	0.203	0.208	0.205	0.202	0.203	0.207	0.202	0.206	0.201	0.204	1.2
Di-n-butylphthalate	0.210	0.172	0.173	0.171	0.170	0.168	0.202	0.199	0.199	0.196	0.186	8.0
Fluoranthene	0.233	0.223	0.232	0.233	0.236	0.234	0.232	0.230	0.229	0.229	0.231	1.5
Pyrene	0.224	0.200	0.208	0.206	0.203	0.215	0.218	0.207	0.213	0.199	0.209	3.7
d14-Terphenyl (surr6)	0.209	0.199	0.208	0.203	0.204	0.212	0.213	0.204	0.213	0.201	0.207	2.3
Butylbenzylphthalate	0.162	0.141	0.135	0.131	0.121	0.129	0.133	0.128	0.124	0.118	0.132	10.2
3,3'-Dichlorobenzidine	0.206	0.193	0.175	0.181	0.168	0.162	0.146	0.174	0.155	0.172	0.173	9.5
Benzo(a)anthracene	0.204	0.196	0.195	0.194	0.191	0.193	0.191	0.194	0.191	0.195	0.194	1.9
Chrysene	0.209	0.205	0.205	0.204	0.206	0.202	0.201	0.202	0.200	0.204	0.204	1.1
Di-n-octyl phthalate	0.120	0.103	0.097	0.091	0.086	0.093	0.081	0.085	0.075	0.078	0.091	16.3
Benzo(b)fluoranthene	0.114	0.114	0.113	0.116	0.113	0.108	0.112	0.108	0.105	0.110	0.111	3.0
Benzo(k)fluoranthene	0.102	0.122	0.102	0.107	0.121	0.102	0.120	0.098	0.112	0.101	0.108	8.6
Benzo(a)pyrene	0.189	0.179	0.172	0.173	0.173	0.170	0.165	0.170	0.167	0.171	0.173	3.7
Indeno(1,2,3-cd)pyrene	0.173	0.169	0.148	0.155	0.149	0.150	0.132	0.152	0.160	0.144	0.153	7.9
Dibenzo(a,h)anthracene	0.290	0.288	0.268	0.275	0.272	0.268	0.261	0.271	0.285	0.268	0.274	3.5
Benzo(g,h,i)perylene	0.176	0.176	0.155	0.169	0.166	0.166	0.152	0.162	0.175	0.162	0.166	4.9

Tune Comparisons

Using Etune provides an increase in signal area counts by more than a factor of two over Atune, offering the potential of reaching lower detection limits (Table 5). The RSD values for the Etune results are generally equivalent or lower.

Table 5. Comparison of Raw Peak Areas at 0.2 ppm for Atune and Etune

	Etune area	Atune area	Ratio Etune/ Atune area	Etune %RSD	Atune %RSD
N-Nitrosodimethylamine	25668	10137	2.53	3%	4%
2-Fluorophenol (surr1)	55575	19289	2.88	1%	2%
Phenol-d5 (surr2)	64597	23493	2.75	1%	1%
Phenol	76070	27647	2.75	1%	2%
Aniline	61226	23781	2.57	2%	2%
bis(2-Chloroethyl)ether	57181	21254	2.69	1%	2%
2-Chlorophenol	63153	21425	2.95	2%	1%
1,3-Dichlorobenzene	87471	30228	2.89	2%	1%
1,4-Dichlorobenzene	90864	31720	2.86	2%	2%
Benzyl Alcohol	26470	11822	2.24	2%	2%
1,2-Dichlorobenzene	89649	31336	2.86	2%	2%
2-Methylphenol	48564	17366	2.80	2%	2%
bis(2-Chloroisopropyl)ether	45851	16710	2.74	2%	2%
4-Methylphenol	49057	17475	2.81	2%	2%
N-Nitroso-di-propylamine	17586	7795	2.26	3%	3%
Hexachloroethane	19941	8221	2.43	2%	2%
Nitrobenzene--d5 (surr3)	22593	9857	2.29	3%	5%
Nitrobenzene	26777	11970	2.24	3%	5%
Isophorone	61483	26257	2.34	3%	2%
2-Nitrophenol	9996	3052	3.28	9%	5%
2,4-Dimethylphenol	37773	14288	2.64	2%	3%
bis(2-Chloroethoxy)methane	61972	23370	2.65	2%	2%
2,4-Dichlorophenol	42091	13855	3.04	3%	2%
1,2,4-Trichlorobenzene	79986	27294	2.93	1%	1%
Naphthalene	221039	78477	2.82	2%	2%
4-Chloroaniline	60551	22027	2.75	2%	2%
Hexachlorobutadiene	41111	15600	2.64	1%	1%
4-Chloro-3-methylphenol	31291	11433	2.74	2%	3%
2-Methylnaphthalene	112984	40027	2.82	1%	2%
Hexachlorocyclopentadiene	9749	3665	2.66	6%	3%
2,4,6-Trichlorophenol	13975	4384	3.19	4%	6%
2,4,5-Trichlorophenol	18233	5897	3.09	5%	10%
2-Fluorobiphenyl (surr4)	166257	57778	2.88	1%	1%
2-Chloronaphthalene	144667	49802	2.90	1%	1%
2-Nitroaniline	7832	2728	2.87	4%	6%

Table 5. Comparison of Raw Peak Areas at 0.2 ppm for Atune and Etune (continued)

	Etune area	Atune area	Ratio Etune/Atune area	Etune %RSD	Atune %RSD
Dimethyl phthalate	113728	41251	2.76	3%	2%
Acenaphthylene	155179	57453	2.70	3%	3%
3-Nitroaniline	7467	2762	2.70	4%	7%
2,6-Dinitrotoluene	349976	136026	2.57	2%	1%
Acenaphthene	139129	48627	2.86	2%	1%
Dibenzofuran	203450	70580	2.88	2%	2%
2,4-Dinitrotoluene	7002	2421	2.89	6%	7%
Diethyl phthalate	76983	30769	2.50	3%	3%
Fluorene	142357	50280	2.83	2%	2%
4-Chlorophenyl-phenylether	87024	29242	2.98	2%	2%
4-Nitroaniline	7294	2703	2.70	4%	5%
N-Nitrosodiphenylamine	83057	29465	2.82	3%	3%
Azobenzene	33767	12258	2.75	3%	3%
2,4,6-Tribromophenol (surr5)	8112	2446	3.32	9%	9%
4-Bromophenylphenyl ether	46174	16368	2.82	2%	2%
Hexachlorobenzene	66655	23317	2.86	2%	2%
Phenanthrene	217071	75086	2.89	2%	2%
Anthracene	153651	56359	2.73	3%	3%
Di-n-butylphthalate	47057	22083	2.13	4%	4%
Fluoranthene	156372	58980	2.65	3%	2%
Pyrene	183429	66699	2.75	5%	2%
d14-Terphenyl (surr6)	124115	42921	2.89	3%	3%
Butylbenzylphthalate	5804	3208	1.81	4%	4%
3,3'-Dichlorobenzidine	7062	3683	1.92	6%	7%
Benzo(a)anthracene	82722	32431	2.55	6%	5%
Chrysene	190329	50968	3.73	4%	2%
bis(2ethylhexyl)phthalate	8024	4943	1.62	6%	4%
Di-n-octyl phthalate	9967	6055	1.65	2%	5%
Benzo(b)fluoranthene	28907	11587	2.49	5%	19%
Benzo(k)fluoranthene	85712	23457	3.65	4%	5%
Indeno(1,2,3-cd)pyrene	28327	11083	2.56	5%	9%
Dibenzo(a,h)anthracene	34104	12335	2.76	2%	6%
Benzo(g,h,i)perylene	73434	26528	2.77	2%	5%
		Average	**2.71**	**3.0%**	**3.5%**

Conclusion

The system shows good performance for all compounds specified by Method 8270 with regards to sensitivity and linearity. The calibration range used is well below what has been historically used by USEPA laboratories. The MassHunter data system brings added value and flexibility to routine analysis while providing visual indicators to supplement the numerical values typically used when indicating the pass/fail criteria defined by Method 8270. Using the extractor lens and Etune tuning procedure offers superior performance and reliability.

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