

EPA 8270E with Pulsed Split Injection and Retention Time Locking on an 8890 GC with a 5977 Series MSD

Author

Rachael Ciotti
Agilent Technologies, Inc

Abstract

United States Environmental Protection Agency (US EPA) Method 8270 provides conditions for analyzing more than 200 semivolatile organic compounds (SVOCs) by gas chromatography/mass spectrometry (GC/MS). This Application Note demonstrates system optimization, calibration, and method performance for the recently revised EPA 8270E on an Agilent 8890 GC system coupled with an Agilent 5977 Series single quadrupole mass spectrometer. It uses a pulsed split injection and a 9 mm extractor lens to enable rapid sample transfer and a wide dynamic range. Agilent's unique retention time locking (RTL) feature was used for ease-of-identification following maintenance. Finally, a DFTPP tune evaluation in accordance with updated tune criteria in EPA Method 8270E is also discussed.

Introduction

The analysis of SVOCs by GC/MS is challenging due to the array of target analytes, including bases, neutrals, and acids that span broad molecular weight and boiling point ranges. EPA Method 8270 provides guidelines for conditions and quality control checks to facilitate successful analysis of SVOCs.¹ System cleanliness and proper column installation are essential to avoid irregular peak shape and enable sufficient response for notoriously problematic compounds, such as those with phenol- and nitro-functional groups. Detector conditions must be optimized so that saturation is not an issue for higher molecular weight polyaromatic hydrocarbons (PAHs) and phthalates. A desirable system configuration allows a wide linear dynamic range for all analytes by introducing just enough sample to meet method detection limits, while avoiding excessive maintenance. Calibration over a wide dynamic range also facilitates better lab productivity and fewer sample reworks.

Traditionally, achieving low method detection limits for EPA 8270E warranted the use of splitless injections.² However, modern mass spectrometers are much more sensitive and capable of reaching lower detection limits with increasingly smaller injection sizes, enabling the use of split injections. Split injections promote faster sample transfer, shortening the time that sensitive and thermally labile compounds interact within the GC inlet or other potentially active sites. They also reduce deposition of nonvolatile matrix material at

the head of the analytical column. Pressure pulsing, which increases the GC inlet pressure just before and during injection, compresses sample vapor volume and reduces residence time in the inlet, further reducing the probability of analyte decomposition. After the specified pulse time, the inlet pressure returns to the setpoint needed to maintain the chosen flow program. The 8890 GC is equipped with highly precise pneumatic modules that enable reproducible pulsed split injections and the implementation of RTL, eliminating the need to adjust retention times after column maintenance.

This Application Note expands on previous SVOC work using a split injection.³ It includes a detailed investigation of system suitability, method optimization, and performance using the 8890 series GC system, evaluated by quality control parameters specified in the recently revised EPA Method 8270E. Strategies for ensuring a wide dynamic range and excellent reproducibility, even after column maintenance, are also discussed.

Experimental

Reagents and standards

A semivolatiles GC/MS tuning standard, containing a nominal concentration of 1,000 µg/mL each of decafluorotriphenylphosphine (DFTPP), benzidine, pentachlorophenol, and 4,4'-dichlorodiphenyltrichloroethane (4,4'-DDT) (Agilent p/n GCM-150), was diluted to a concentration of 25 ng/µL in dichloromethane.

A 1,000 µg/mL stock standard containing 76 commonly analyzed SVOCs in dichloromethane, purchased from Restek (Bellefonte, PA), was used to prepare a 10 µg/mL working level standard in dichloromethane. A 2,000 µg/mL semivolatiles internal standard stock solution, containing six deuterated analytes in dichloromethane, was also acquired from Restek. Initial calibration curve standards were prepared by dilution of the stock and working standards in dichloromethane and contained 4 µg/mL of the semivolatiles internal standard. Thirteen calibration levels were prepared at the following concentrations: 0.2, 0.4, 0.5, 0.8, 1, 2, 4, 10, 25, 50, 75, 100, and 160 µg/mL. Table 1 shows a numbered list of target analytes in retention time order; the internal standards are listed at the end. The 3- and 4-methyl phenol isomers cannot be separated for quantitation; therefore, they are reported as a combined result.

Instruments

Table 2 and Table 3 summarize the system configuration and method conditions. The Agilent 8890 GC was configured with a 30 × 0.25 m DB-UI 8270 column with a film thickness of 0.25 µm to facilitate faster run times. The column was connected to a 5977 single quadrupole mass spectrometer outfitted with an extractor EI source containing a 9 mm aperture extraction lens. The analytical run time was 21.6 minutes. Agilent MassHunter Workstation software was used for acquisition and data analysis.

Table 1. Target analytes and internal standards.

No.	Compound	No.	Compound	No.	Compound	No.	Compound
1	N-Nitrosodimethylamine	22	1,2,4-Trichlorobenzene	43	4-Nitrophenol	64	Butylbenzylphthalate
2	Pyridine	23	Naphthalene	44	2,4-Dinitrotoluene	65	Bis(2-ethylhexyl)adipate
3	Phenol	24	4-Chloroaniline	45	Dibenzofuran	66	Benzo[a]anthracene
4	Aniline	25	Hexachlorobutadiene	46	2,3,5,6-Tetrachlorophenol	67	Chrysene
5	bis(2-Chloroethyl) ether	26	4-Chloro-3-methylphenol	47	2,3,4,6-Tetrachlorophenol	68	Bis(2-ethylhexyl) phthalate
6	2-Chlorophenol	27	2-Methylnaphthalene	48	Diethyl phthalate	69	Di- <i>n</i> -octyl phthalate
7	1,3-Dichlorobenzene	28	1-Methylnaphthalene	49	Fluorene	70	Benzo[b]fluoranthene
8	1,4-Dichlorobenzene	29	Hexachlorocyclopentadiene	50	4-Chlorophenyl-phenyl ether	71	Benzo[k]fluoranthene
9	Benzyl alcohol	30	2,4,6-Trichlorophenol	51	4-Nitroaniline	72	Benzo[a]pyrene
10	1,2-Dichlorobenzene	31	2,4,5-Trichlorophenol	52	4,6-Dinitro-2-methylphenol	73	Indeno[1,2,3- <i>cd</i>]pyrene
11	2-Methylphenol	32	2-Chloronaphthalene	53	Diphenylamine	74	Dibenz[a,h]anthracene
12	2,2'-Oxybis(1-chloropropane)	33	2-Nitroaniline	54	Azobenzene	75	Benzo[ghi]perylene
13	N-Nitrosodi- <i>n</i> -propylamine	34	1,4-Dinitrobenzene	55	4-Bromophenyl phenyl ether	76	1,4-Dichlorobenzene- <i>d</i> ₄ (IS)
14	3/4-Methylphenol	35	Dimethyl phthalate	56	Hexachlorobenzene	77	Naphthalene- <i>d</i> ₈ (IS)
15	Hexachloroethane	36	1,3-Dinitrobenzene	57	Pentachlorophenol	78	Acenaphthene- <i>d</i> ₁₀ (IS)
16	Nitrobenzene	37	2,6-Dinitrotoluene	58	Phenanthrene	79	Phenanthrene- <i>d</i> ₁₀ (IS)
17	Isophorone	38	1,2-Dinitrobenzene	59	Anthracene	80	Chrysene- <i>d</i> ₁₂ (IS)
18	2-Nitrophenol	39	Acenaphthylene	60	Carbazole	81	Perylene- <i>d</i> ₁₂ (IS)
19	2,4-Dimethylphenol	40	3-Nitroaniline	61	Di- <i>n</i> -butylphthalate		
20	bis(2-Chloroethoxy) methane	41	Acenaphthene	62	Fluoranthene		
21	2,4-Dichlorophenol	42	2,4-Dinitrophenol	63	Pyrene		

Table 2. System configuration and consumables.

Parameter	Value
Autosampler	
	Agilent 7693 automatic liquid sampler with tray
Syringe	Agilent Blue Line 10 µL tapered syringe with PTFE tipped plunger (p/n G4513-80203)
Vials	Agilent A-Line certified 2 mL amber screw top vials (p/n 5182-0716)
Vial Inserts	Agilent vial insert, 250 µL, deactivated glass with polymer feet (p/n 5181-8872)
Vial Screw Caps	Agilent screw cap, blue, certified, PTFE/silicone/PTFE septa (p/n 5182-0723)
Gas Chromatograph	
	Agilent 8890A GC with split/splitless inlet
Column	Agilent DB-UI 8270D, 30 m x 0.25 mm, 0.25 µm (p/n 122-9732)
Liner	Agilent Ultra Inert, split liner with low pressure drop and glass wool (p/n 5190-2295)
Septum	Agilent Advanced Green, nonstick 11 mm septum (p/n 5183-4759)
Mass Spectrometer	
	Agilent 5977A MSD with extractor ion source
Extraction Lens	9 mm (p/n G3870-20449)

Results and discussion

Tuning and system performance verification

Before injecting the system performance verification sample, the 5977 MS was tuned with perfluorotributylamine (PFTBA) calibrant using the autotune (Atune) tuning algorithm. When the tuning algorithm was completed, a 1 μL injection of the semivolatiles tuning solution, containing 25 ng/ μL each of DFTPP, pentachlorophenol, benzidine, and 4,4'-DDT, was injected using the previously mentioned method parameters. Figure 1 shows the total ion chromatogram (TIC) with annotated system suitability results.

According to EPA Method 8270E, the mass spectrometer must be tuned so that DFTPP ion abundance criteria match those shown in Table 4. As well as updating the ion abundance criteria to match that specified in EPA Method 525.3, EPA Method 8270E recently decreased the DFTPP tune check frequency to one time before initial calibration.

Table 3. Instrumental conditions.

Agilent 8890 Gas Chromatograph Parameters	
Injection Volume	1 μL
Inlet	280 °C, pulsed split mode, 4:1 Injection pulse pressure 30 psi until 0.6 minutes
Carrier Gas	Helium, constant flow mode at 1.2 mL/min
Oven	40 °C hold 0.5 minutes 10 °C/min to 100 °C, hold 0 minutes 25 °C/min to 260 °C, hold 0 minutes 5 °C/min to 280 °C, hold 0 minutes 15 °C/min to 320 °C, hold 2 minutes
Transfer Line Temperature	320 °C
Agilent 5977 Mass Spectrometer Parameters	
Ion Source Temperature	300 °C
Quadrupole Temperature	150 °C
Scan Mode	El full scan mode, m/z 35 to 500
EMV Mode	Gain factor
Gain Factor	0.4
Solvent Delay	2.75 minutes

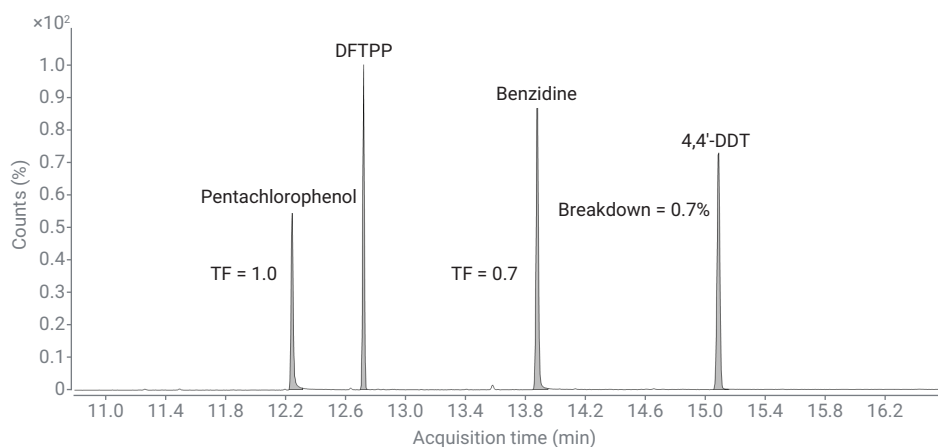


Figure 1. Total ion chromatogram for 25 ng/ μL semivolatiles tune check solution.

Table 4. US EPA 8270E DFTPP ion abundance criteria.

Mass (m/z)	Ion Abundance Criteria
68	<2% of m/z 69
69	Present
70	<2% of m/z 69
197	<2% of m/z 198
198	Base peak of present
199	5 to 9% of m/z 198
365	>1% of base peak
441	<150% of m/z 443
442	Base peak or present
443	15 to 24% of m/z 442

In this study, the Tune Evaluation program within Agilent MassHunter Environmental Quantitative Analysis software was used to automatically evaluate system performance. Updated ion abundance criteria were entered and stored in the method. All DFTPP ion abundance criteria were well within the specified targets, as shown in Figure 2.

The 4,4'-DDT component is a thermally labile chlorinated pesticide commonly used as a probe for system inertness. When exposed to active sites in a high-temperature GC inlet, 4,4'-DDT readily degrades into 4,4'-dichlorodiphenyldichloroethylene (4,4'-DDE) and 4,4'-dichlorodiphenyldichloroethane (4,4'-DDD). According to EPA Method 8270E, degradation of 4,4'-DDT to 4,4'-DDE and 4,4'-DDD should not exceed 20%, as determined by Equation 1. In this study, DDT breakdown was measured at 0.7%.

Pentachlorophenol and benzidine are also used as probes for system activity because they are subject to tailing in the presence of nonvolatile build-up within the chromatographic flowpath. EPA Method 8270E specifies pentachlorophenol and benzidine tailing factors (TF) should not exceed a value of 2 when calculated at 10% height. The Tune Evaluation program calculated peak tailing factors for pentachlorophenol and benzidine at 1.0 and 0.7, respectively.

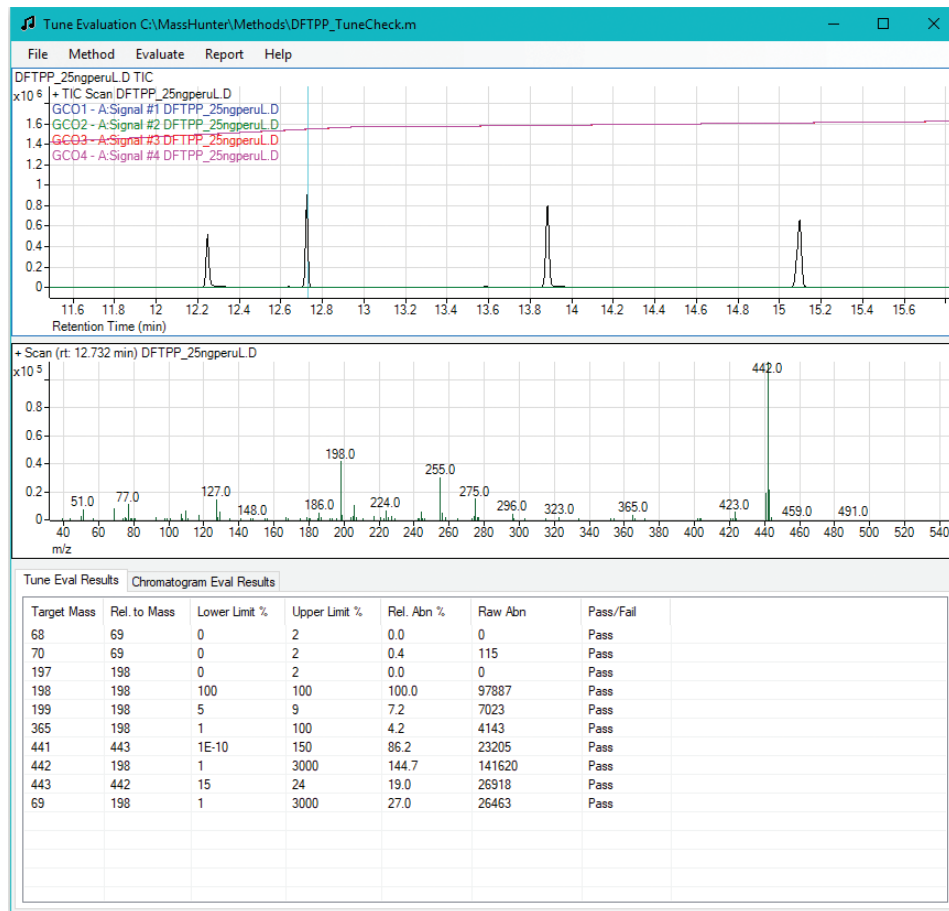


Figure 2. DFTPP tune evaluation results.

$$\% \text{ DDT breakdown} = \frac{(\text{Peak area}_{\text{DDE}} + \text{Peak area}_{\text{DDD}})}{(\text{Peak area}_{\text{DDE}} + \text{Peak area}_{\text{DDD}} + \text{Peak area}_{\text{DDT}})} \times 100$$

Equation 1. DDT breakdown calculation.

System optimization

Before initial calibration, the system was optimized by determining the gain setting that allowed the highest response within the linear detector range for the highest responding peak. This gives the user the greatest working range possible for their system and ensures compound response stability over time. A procedural overview of optimizing detector gain for GC/MS has been published.⁴ The ideal gain factor can be calculated using Equation 2. Previous work indicates that the gain factor adjustment for EPA Method 8270 should be made so that the peak height of the tallest peak within the base peak chromatogram (BPC) ranges between 3 to 5×10^6 counts for a single quadrupole mass spectrometer.³ In this study, detector gain was optimized through acquisition of the highest-level calibration standard ($160 \mu\text{g/mL}$) using a preliminary gain factor of 1.0 . Alternatively, to avoid the potential for erroneous peak height characterization resulting from inadvertent detector saturation, system optimization could be made using a lower initial gain factor and moving upwards. The resultant TIC was loaded in MassHunter Qualitative Analysis software, and from that the BPC was extracted and integrated. The height of the tallest peak (di-*n*-butylphthalate at 13.043 minutes) was approximately 7.8×10^6 counts, as shown in Figure 3. Targeting the lower limit of the suggested signal range resulted in a new calculated gain factor of approximately 0.4 . The $160 \mu\text{g/mL}$ calibration standard was re-acquired with the new gain factor, and the resulting BPC yielded a peak height within the target range of approximately 4.8×10^6 counts.

$$\frac{\text{Present Peak Height}}{\text{Present Gain Factor}} = \frac{\text{Target Peak Height}}{\text{New Gain Factor}}$$
$$\frac{7.8 \times 10^6 \text{ counts}}{1.0} = \frac{3 \times 10^6 \text{ counts}}{\text{New Gain Factor}}$$

$$\text{New Gain Factor} = \sim 0.4$$

Equation 2. Calculating optimum gain factor.

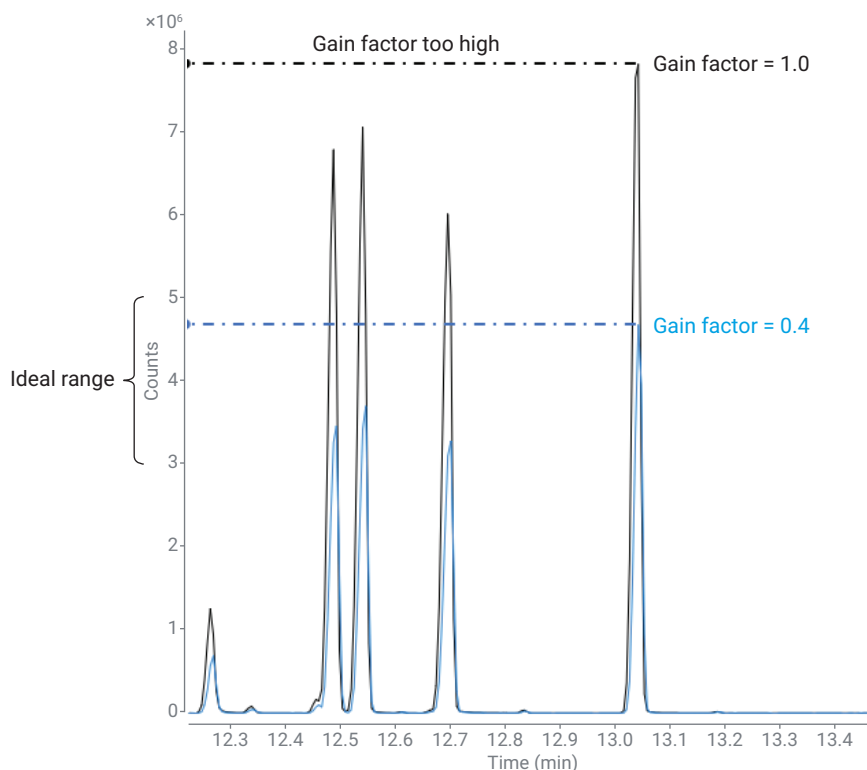


Figure 3. Base peak chromatographic overlay of $160 \mu\text{g/mL}$ standard collected at gain factor 1.0 (black trace) and 0.4 (blue trace).

Initial calibration

The initial calibration consisted of 13 levels spanning the concentration range of 0.2 to 160 µg/mL and was run on the optimized system. Figure 4 depicts the separation of target analytes and internal standards over the 22-minute run.

Chromatographic quality was assessed by evaluating the separation between several isomer pairs. EPA Method 8270E considers isomers resolved if the peaks are least 50% resolved in a midlevel standard. In MassHunter MS Quantitative Analysis, peak resolution outlier limits were specified in the method at 50% using the default resolution calculation shown in the equation in Figure 5. The separation of several isomer pairs is shown in Figure 6. Resolution between benzo(b)fluoranthene and benzo(k)fluoranthene, a key structural isomer pair, was 90.0% in the midlevel standard, and ranged between 80 to 90% over the entire calibrated range. Resolution for isomer pairs phenanthrene and anthracene, and benz[a]anthracene and chrysene, were 100 and 97.8%, respectively.

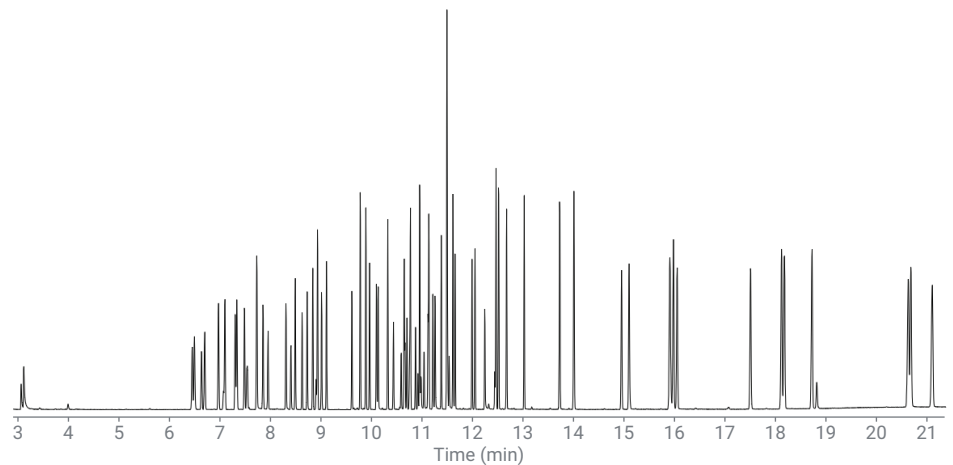


Figure 4. Total ion chromatogram of a 25 µg/mL SVOC calibration standard.

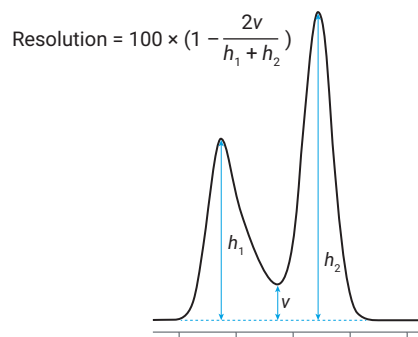


Figure 5. Agilent MassHunter default resolution calculation.

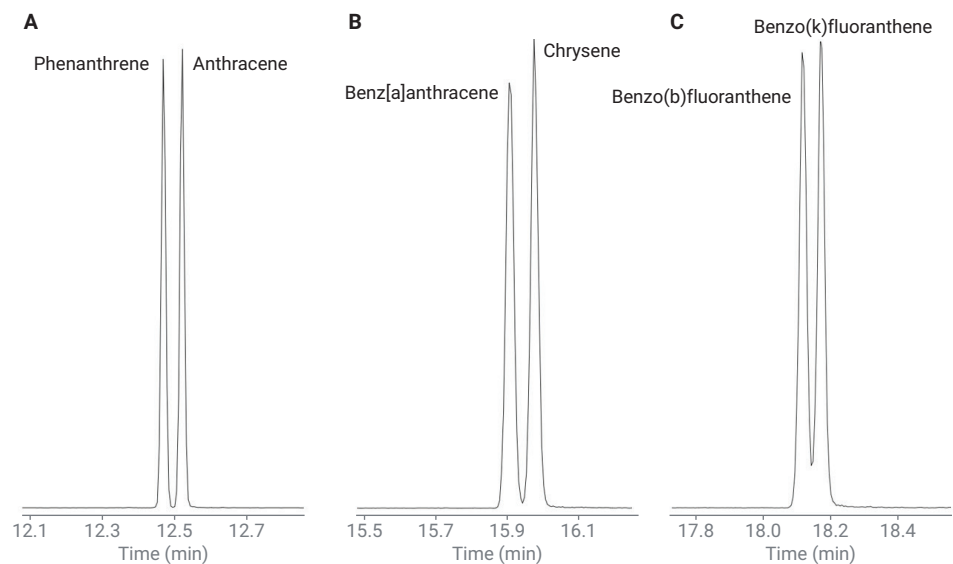


Figure 6. Midlevel standard (4 µg/mL) extracted ion chromatogram for isomer pairs: (A) phenanthrene and anthracene, m/z 178; (B) benz[a]anthracene and chrysene, m/z 228; (C) benzo(b)- and benzo(k)fluoranthene, m/z 252.

Although SVOC calibration can be challenging, EPA Method 8270E allows flexibility in calibration technique to satisfy individual laboratory projects. The preferable calibration model compares response and concentration of each analyte to that of its internal standard to determine a relative response factor (RRF). For each analyte, the average response factor across the calibrated range should be calculated; the relative standard deviation (RSD) must be $\leq 20\%$. However, some SVOCs are prone to erratic chromatographic behavior and may have response factors that vary as a function of concentration. To better characterize these compounds, calibration can be made through least squares regression. Linear regression requires a minimum of five points,

while nonlinear regression requires at least six points to properly characterize the calibration curve. Regression acceptance criteria specifies that the coefficient of determination, R^2 , must be ≥ 0.99 . Each calibration level must be recalculated using the calibration curve. The calculated concentration of the lowest standard must be within $\pm 50\%$ of its true value, and all other levels must be within $\pm 30\%$ of the true value. The use of weighting factors to better fit the curve at lower calibration levels is also acceptable.

In this study, a dynamic range of 0.2 to 160 $\mu\text{g}/\text{mL}$ was achieved for over 90% of the analytes. For six analytes, points at the low end of the calibration curve were dropped to maintain compliance with the

50% accuracy requirement for the lowest data point. Nearly 95% of the analytes were calibrated using RRFs, as shown in Figure 7, with the average RF RSD for these 71 compounds at 6.4%. There were four exceptions that required weighted least squares regression: two analytes (4-nitrophenol and pentachlorophenol) were calibrated through linear regression, and two analytes (2,4-dinitrophenol and 4,6-dinitro-2-methylphenol) required quadratic fitting. Each of the calibration curves used $1/x$ weighting factors and resulted in R^2 values of >0.997 . Detailed information regarding individual compound RRFs, respective %RSDs, and dynamic range can be found in the Appendix.

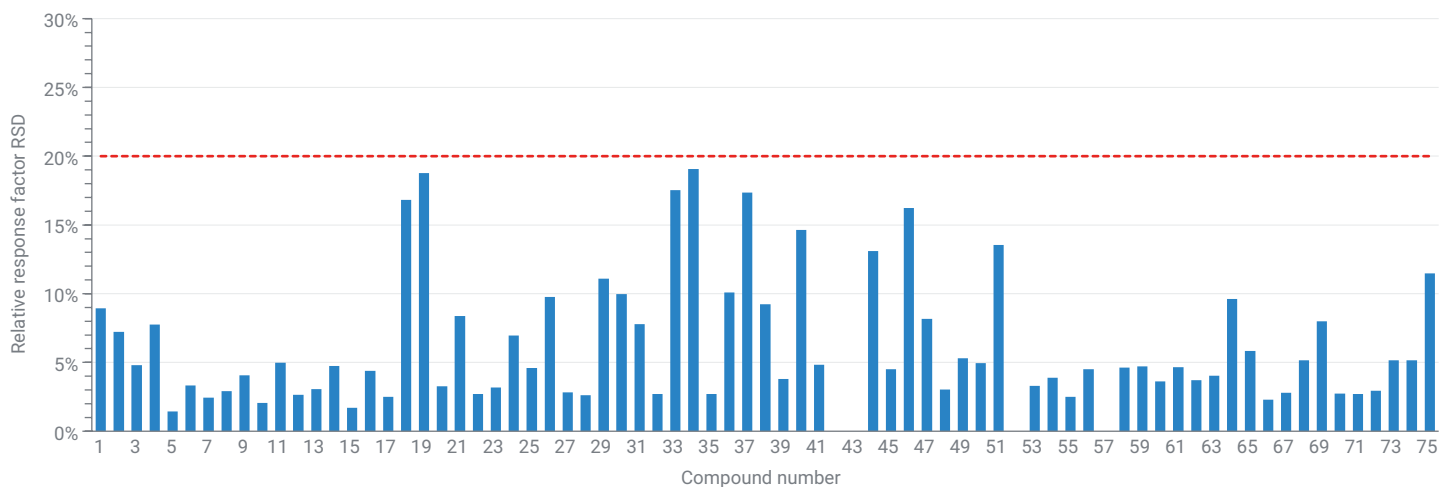
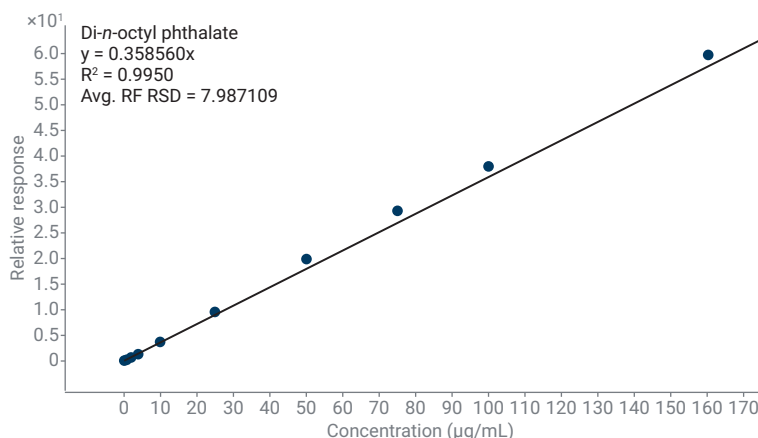


Figure 7. RSD for each calibrated compound's average RRF over its calibrated range. The dotted red line indicates the EPA Method 8270E limit for acceptable RRF calibration.

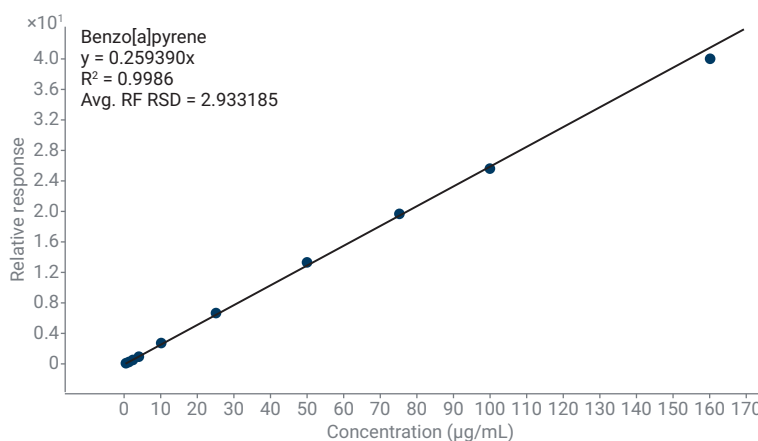
High molecular weight phthalates and PAHs⁵ can be difficult to vaporize, and readily adhere to surfaces along the flowpath. Minimization of surface areas and the use of high temperatures is critical in ensuring proper peak shape and response. A pulsed split injection in tandem with the 9 mm extraction lens heated to 300 °C resulted in an excellent average accuracy of 100.0% over the entire calibrated range for two such analytes, di-*n*-octyl phthalate and benzo[a]pyrene, as shown in Figures 8 and 9.

Method repeatability was assessed by injecting 10 replicates of a 0.8 µg/mL calibration standard and examining the RRF for each analyte. Figure 10 shows that excellent response factor precision was achieved, with the overall RSD for 75 analytes determined at 3.5%. The individual average response factors for each replicate injection for each analyte can be found in the Appendix Table 5.



Conc. (µg/mL)	Accuracy (%)
0.2	89.0
0.4	87.3
0.5	91.1
0.8	93.2
1	97.6
2	98.0
4	100.3
10	105
25	107.7
50	111.1
75	108.9
100	106.3
160	104.3

Figure 8. Di-*n*-octyl phthalate calibration and accuracy.



Conc. (µg/mL)	Accuracy (%)
0.2	99.6
0.4	97.1
0.5	96.1
0.8	96.9
1	99.5
2	100.4
4	102.9
10	103.9
25	104.6
50	102.7
75	101.4
100	98.6
160	96.3

Figure 9. Benzo[a]pyrene calibration and accuracy.

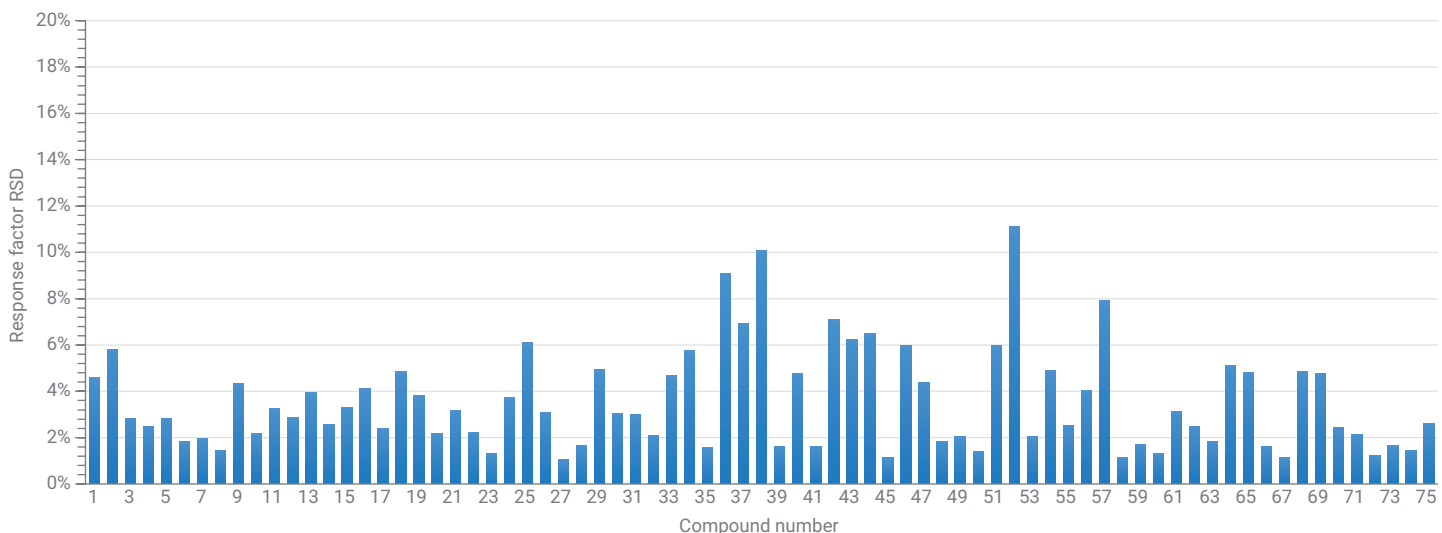


Figure 10. RSD for each calibrated compound's response factor over 10 replicate injections of a 0.8 µg/mL standard.

Retention time locking

The Agilent RTL feature provides long-term repeatability on a given instrument and eliminates the need to adjust analyte retention times after column maintenance.⁶ It can maintain the same retention times after moving the method to a different GC, which facilitates easier method transfer and simplifies interlaboratory comparisons. RTL correctly matches and locks retention times for a specified compound by studying the relationship between column flow and the retention time of a given analyte during a series of reference runs. It calibrates the system using the results and stores the relationship within the method file. The array of target compounds in a typical laboratory project coupled with frequent injections of heavy-matrix sample types makes EPA

Method 8270E an ideal candidate for RTL. This is true because the hassle of retention time re-alignment after column maintenance can be avoided.

In this study, the 10 µg/mL calibration standard was used to RTL the system to the internal compound acenaphthene using m/z 164. RTL calibration was started through MassHunter GC/MS Acquisition, which automatically scheduled five runs at the method setpoint of 1.2 mL/min constant flow, and $\pm 10\%$ and $\pm 20\%$ flow values, respectively. Following a cleanout run, the 10 µg/mL standard was collected at each of the five flow setpoints, and a calibration curve of the acenaphthene- d_{10} retention times at each setpoint was generated, as shown in Figure 11. The coefficient of determination for the RTL calibration run was 0.999,

indicating excellent precision in the performance of the sixth generation 8890 pneumatics module.

After the method was locked, maintenance was performed by trimming approximately 0.5 m from the head of the analytical column. The magnitude of retention shift following maintenance was then investigated using the original method setpoint of 1.2 mL/min constant flow. The average post trim retention shift for the 75 calibrated compounds and six internal standards was 0.097 minutes earlier than the original retention times. Relocking was then started using MassHunter GC/MS Acquisition. After comparing the post trim retention time for acenaphthene- d_{10} to the stored RTL calibration curve, the software automatically determined and programmed the new flow rate to

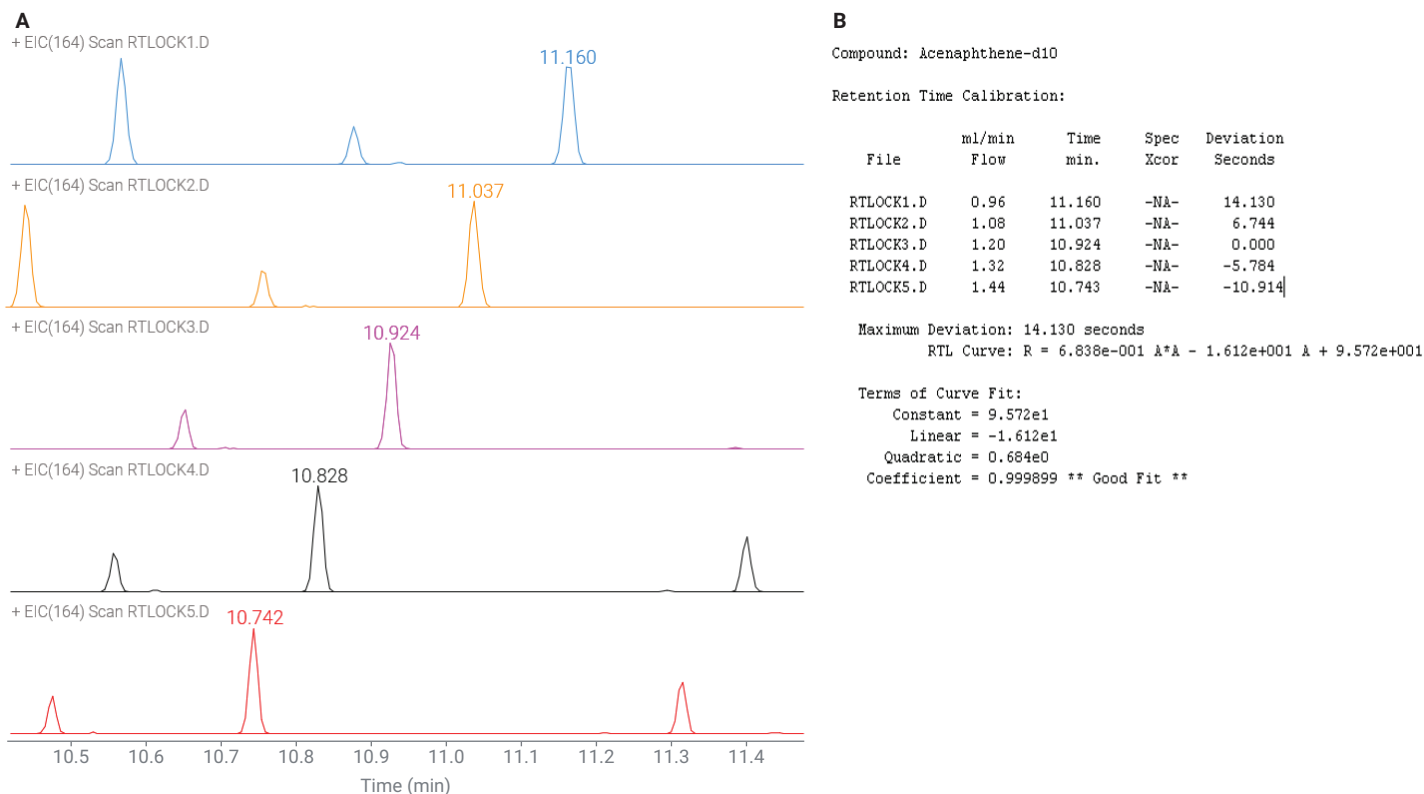


Figure 11. (A) Extracted ion chromatograms for acenaphthene- d_{10} , m/z 164, and (B) calibration results for RTL runs collected at five flow setpoints. Injections of a 0.8 µg/mL standard.

1.108 mL/min to match the original retention times. The efficacy of the relocked method was tested by re-injecting the 10 ppm standard, and the relocked retention times were compared to the original retention times. The overall average delta was 0.003 minutes, or only 0.17 seconds difference from the original compound retention time before column maintenance. Figure 12 demonstrates the change in retention for selected analytes around the 18 minutes region, and illustrates the effective use of RTL to shift the peak back into the identification window. This facilitates more accurate analyte identification and eliminates the need to adjust retention windows. Individual retention times for the entire list of analytes, before and after relocking, are included in the Appendix.

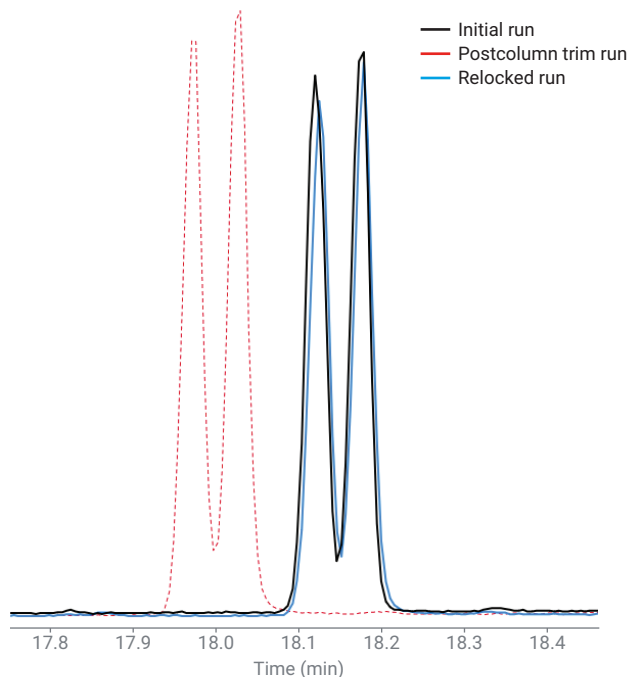


Figure 12. Chromatographic overlay of: initial calibration run (black trace), after clipping 0.5 m from the front end of the column illustrating shift in retention (red trace), and after relocking the method to maintain retention time consistency (blue trace).

Conclusion

The Agilent 8890 GC with an Agilent 5977 MSD system using a pulsed split injection, 9 mm extractor lens, and gain-optimized detector enables excellent response factor precision over a wide dynamic range for commonly analyzed SVOCs. In this study, the initial calibration curve met all key quality control parameters specified by US EPA Method 8270E, and the RSD of all response factors was extremely low. Finally, the implementation of RTL methods on the 8890 GC facilitates retention time repeatability after column maintenance, reducing data processing time and downtime.

References

1. Semivolatile Organic Compounds by Gas Chromatography/Mass Spectrometry (GC/MS); Method 8270E; *United States Environmental Protection Agency*, Revision 4, June **2018**.
2. EPA Method 8270 for SVOC Analysis on the 5977A Series GC/MSD, *Agilent Technologies*, publication number 5991-2153EN, **2013**.
3. EPA 8270 Re-optimized for Widest Calibration Range on the 5977 Inert Plus GC/MSD, *Agilent Technologies*, publication number 5994-0350EN, **2018**.
4. A Quick Start to Optimizing Detector Gain for GC/MSD, *Agilent Technologies*, publication number 5991-2105EN, **2013**.
5. Optimized GC/MS Analysis for PAHs in Challenging Matrices, *Agilent Technologies*, publication number 5994-0499EN, **2019**.
6. Retention Time Locking with the MSD Productivity ChemStation, *Agilent Technologies*, publication number 5989-8574EN, **2008**.

Appendix

Table 5. Calibration data for 75 compounds determined by EPA method 8270E.

No.	Compound	RT (min)	Response Factor at Concentration (µg/mL)													Avg RF	% RSD
			0.2	0.4	0.5	0.8	1	2	4	10	25	50	75	100	160		
1	N-Nitrosodimethylamine	3.062	0.565	0.555	0.544	0.495	0.504	0.563	0.571	0.574	0.592	0.623	0.644	0.650	0.654	0.580	8.9
2	Pyridine	3.121		0.919	0.945	0.939	0.945	0.971	0.991	0.936	1.038	1.058	1.087	1.119	1.101	1.004	7.2
3	Phenol	6.453	1.337	1.320	1.295	1.317	1.355	1.347	1.401	1.413	1.426	1.440	1.459	1.485	1.491	1.391	4.8
4	Aniline	6.496	1.497	1.424	1.569	1.581	1.635	1.686	1.721	1.777	1.753	1.785	1.813	1.822	1.807	1.682	7.8
5	bis(2-Chloroethyl) ether	6.640	1.109	1.136	1.100	1.094	1.133	1.120	1.120	1.134	1.131	1.130	1.146	1.147	1.131	1.125	1.4
6	2-Chlorophenol	6.704	1.207	1.246	1.253	1.254	1.285	1.264	1.312	1.332	1.324	1.329	1.337	1.338	1.316	1.292	3.3
7	1,3-Dichlorobenzene	6.977	1.436	1.434	1.384	1.431	1.476	1.463	1.476	1.507	1.490	1.489	1.505	1.481	1.437	1.462	2.4
8	1,4-Dichlorobenzene	7.100	1.553	1.396	1.440	1.445	1.469	1.472	1.496	1.544	1.504	1.501	1.506	1.491	1.450	1.482	2.9
9	Benzyl alcohol	7.309	0.737	0.754	0.757	0.723	0.744	0.753	0.795	0.788	0.793	0.799	0.810	0.818	0.807	0.775	4.1
10	1,2-Dichlorobenzene	7.341	1.385	1.421	1.444	1.375	1.388	1.400	1.430	1.435	1.420	1.404	1.421	1.395	1.337	1.404	2.1
11	2-Methylphenol	7.490	0.927	0.983	0.998	1.009	1.044	1.044	1.075	1.102	1.088	1.083	1.082	1.093	1.066	1.046	5.0
12	2,2'-Oxybis(1-chloropropane)	7.549	1.110	1.029	1.088	1.009	1.072	1.053	1.069	1.067	1.045	1.035	1.039	1.042	1.023	1.052	2.7
13	N-Nitrosodi-n-propylamine	7.731	0.607	0.673	0.660	0.690	0.684	0.664	0.674	0.685	0.670	0.669	0.676	0.676	0.677	0.670	3.1
14	3/4-Methylphenol	7.737	1.016	1.013	0.985	1.061	1.038	1.088	1.119	1.120	1.118	1.123	1.122	1.127	1.112	1.080	4.7
15	Hexachloroethane	7.860	0.550	0.523	0.543	0.540	0.547	0.549	0.556	0.556	0.552	0.553	0.552	0.554	0.537	0.547	1.7
16	Nitrobenzene	7.961	0.296	0.269	0.275	0.275	0.289	0.284	0.294	0.292	0.302	0.302	0.303	0.307	0.307	0.292	4.4
17	Isophorone	8.314	0.531	0.505	0.527	0.529	0.531	0.537	0.543	0.543	0.551	0.546	0.550	0.553	0.549	0.538	2.5
18	2-Nitrophenol	8.410	0.120	0.121	0.126	0.125	0.136	0.146	0.154	0.160	0.174	0.178	0.180	0.186	0.186	0.153	16.8
19	2,4-Dimethylphenol	8.496		0.181	0.185	0.231	0.238	0.251	0.277	0.291	0.310	0.312	0.312	0.317	0.315	0.268	18.8
20	bis(2-Chloroethoxy) methane	8.635	0.354	0.343	0.345	0.344	0.361	0.361	0.372	0.362	0.369	0.373	0.370	0.377	0.371	0.362	3.3
21	2,4-Dichlorophenol	8.737	0.259	0.239	0.234	0.250	0.253	0.278	0.284	0.288	0.295	0.295	0.290	0.295	0.292	0.273	8.4
22	1,2,4-Trichlorobenzene	8.849	0.311	0.304	0.315	0.312	0.322	0.331	0.332	0.327	0.327	0.326	0.321	0.324	0.314	0.320	2.7
23	Naphthalene	8.940	0.973	0.924	0.962	0.952	0.981	0.984	1.010	0.997	1.002	0.979	0.957	0.952	0.901	0.967	3.2
24	4-Chloroaniline	9.020	0.352	0.349	0.338	0.372	0.386	0.389	0.406	0.405	0.415	0.412	0.407	0.415	0.405	0.389	7.0
25	Hexachlorobutadiene	9.116	0.187	0.161	0.183	0.171	0.187	0.188	0.191	0.188	0.190	0.187	0.184	0.184	0.178	0.183	4.6
26	4-Chloro-3-methylphenol	9.619	0.210	0.229	0.202	0.231	0.231	0.248	0.255	0.259	0.264	0.267	0.267	0.274	0.274	0.247	9.8
27	2-Methylnaphthalene	9.785	0.665	0.629	0.623	0.650	0.649	0.663	0.670	0.673	0.674	0.662	0.650	0.652	0.620	0.652	2.8
28	1-Methylnaphthalene	9.897	0.628	0.599	0.593	0.612	0.606	0.619	0.629	0.623	0.623	0.616	0.602	0.605	0.573	0.610	2.6
29	Hexachlorocyclopentadiene	9.972	0.358	0.379	0.415	0.383	0.423	0.424	0.471	0.486	0.491	0.493	0.499	0.480	0.471	0.444	11.1
30	2,4,6-Trichlorophenol	10.106	0.313	0.311	0.300	0.341	0.352	0.356	0.378	0.398	0.391	0.395	0.393	0.393	0.389	0.362	10.0
31	2,4,5-Trichlorophenol	10.143	0.329	0.347	0.362	0.372	0.380	0.393	0.411	0.413	0.413	0.420	0.425	0.408	0.411	0.391	7.8
32	2-Chloronaphthalene	10.331	1.183	1.152	1.201	1.192	1.194	1.205	1.225	1.245	1.199	1.199	1.176	1.156	1.121	1.188	2.7
33	2-Nitroaniline	10.443	0.254	0.242	0.293	0.295	0.305	0.325	0.345	0.375	0.382	0.395	0.404	0.404	0.417	0.341	17.5
34	1,4-Dinitrobenzene	10.593	0.096	0.103	0.099	0.104	0.107	0.110	0.124	0.136	0.140	0.146	0.155	0.156	0.161	0.126	19.1
35	Dimethyl phthalate	10.652	1.337	1.260	1.234	1.308	1.301	1.337	1.341	1.355	1.290	1.291	1.324	1.301	1.271	1.304	2.7
36	1,3-Dinitrobenzene	10.668	0.081	0.072	0.076	0.086	0.078	0.089	0.084	0.094	0.086	0.093	0.098	0.097	0.099	0.087	10.1
37	2,6-Dinitrotoluene	10.710	0.206	0.194	0.208	0.222	0.222	0.250	0.273	0.298	0.294	0.297	0.307	0.309	0.315	0.261	17.4
38	1,2-Dinitrobenzene	10.753	0.117	0.109	0.110	0.123	0.127	0.127	0.137	0.138	0.138	0.139	0.144	0.140	0.140	0.130	9.2
39	Acenaphthylene	10.780	1.946	1.841	1.834	1.853	1.871	1.893	1.937	1.947	1.896	1.867	1.839	1.771	1.694	1.861	3.8
40	3-Nitroaniline	10.876	0.223	0.246	0.234	0.262	0.252	0.282	0.304	0.320	0.312	0.327	0.338	0.340	0.336	0.290	14.6
41	Acenaphthene	10.962	1.106	1.033	1.103	1.060	1.088	1.102	1.144	1.178	1.155	1.150	1.081	1.029	1.006	1.095	4.8
42	2,4-Dinitrophenol	10.989	Quadratic regression, weighted 1/x													R ² 0.9977	
43	4-Nitrophenol	11.047	Linear regression, weighted 1/x													R ² 0.9984	

Table 5. Calibration data for 75 compounds determined by EPA method 8270E (continued).

No.	Compound	RT (min)	Response Factor at Concentration (µg/mL)													Avg RF	% RSD
			0.2	0.4	0.5	0.8	1	2	4	10	25	50	75	100	160		
44	2,4-Dinitrotoluene	11.122	0.209	0.212	0.208	0.229	0.221	0.258	0.266	0.276	0.277	0.289	0.293	0.286	0.282	0.254	13.1
45	Dibenzofuran	11.144	1.712	1.593	1.642	1.632	1.682	1.687	1.715	1.762	1.671	1.648	1.624	1.560	1.474	1.646	4.5
46	2,3,5,6-Tetrachlorophenol	11.224	0.208	0.232	0.230	0.251	0.256	0.288	0.305	0.322	0.323	0.329	0.335	0.334	0.338	0.288	16.2
47	2,3,4,6-Tetrachlorophenol	11.267	0.273	0.275	0.289	0.287	0.282	0.325	0.319	0.337	0.325	0.331	0.333	0.335	0.333	0.311	8.2
48	Diethyl phthalate	11.384	1.319	1.227	1.242	1.289	1.275	1.309	1.332	1.316	1.298	1.297	1.272	1.227	1.218	1.279	3.0
49	Fluorene	11.497	1.384	1.275	1.245	1.280	1.326	1.328	1.346	1.363	1.290	1.263	1.241	1.195	1.143	1.283	5.3
50	4-Chlorophenyl-phenyl ether	11.502	0.628	0.616	0.611	0.592	0.642	0.654	0.646	0.658	0.627	0.616	0.599	0.575	0.556	0.617	4.9
51	4-Nitroaniline	11.507	0.220	0.227	0.255	0.264	0.274	0.300	0.321	0.330	0.333	0.284	0.306	0.315	0.334	0.289	13.5
52	4,6-Dinitro-2-methylphenol	11.544	Quadratic regression, weighted 1/x													R ² 0.9984	
53	Diphenylamine	11.620	0.621	0.593	0.593	0.606	0.636	0.611	0.638	0.637	0.621	0.622	0.619	0.610	0.568	0.613	3.3
54	Azobenzene	11.662	0.171	0.169	0.178	0.175	0.192	0.187	0.185	0.187	0.185	0.186	0.189	0.187	0.183	0.183	3.9
55	4-Bromophenyl phenyl ether	11.999	0.240	0.225	0.226	0.230	0.224	0.230	0.237	0.240	0.235	0.232	0.234	0.236	0.224	0.232	2.5
56	Hexachlorobenzene	12.058	0.256	0.245	0.264	0.266	0.292	0.276	0.285	0.278	0.277	0.276	0.275	0.277	0.267	0.272	4.5
57	Pentachlorophenol	12.251	Linear regression, weighted 1/x													R ² 0.9991	
58	Phenanthrene	12.470	1.107	1.053	1.068	1.075	1.081	1.090	1.106	1.095	1.095	1.060	1.030	0.992	0.938	1.061	4.6
59	Anthracene	12.524	1.105	1.015	1.079	1.079	1.103	1.103	1.134	1.129	1.117	1.085	1.052	1.030	0.956	1.076	4.7
60	Carbazole	12.679	0.940	0.924	0.938	0.944	0.988	0.996	1.007	1.025	0.980	0.939	0.936	0.943	0.917	0.960	3.6
61	Di- <i>n</i> -butylphthalate	13.032	1.208	1.118	1.139	1.146	1.149	1.196	1.230	1.242	1.274	1.255	1.241	1.212	1.109	1.194	4.6
62	Fluoranthene	13.732	1.135	1.082	1.105	1.101	1.151	1.148	1.187	1.211	1.201	1.186	1.184	1.159	1.100	1.150	3.7
63	Pyrene	14.011	1.297	1.259	1.263	1.324	1.310	1.328	1.315	1.333	1.334	1.297	1.258	1.213	1.160	1.284	4.0
64	Butylbenzylphthalate	14.957	0.492	0.485	0.476	0.496	0.510	0.537	0.554	0.579	0.592	0.608	0.611	0.604	0.606	0.550	9.6
65	<i>bis</i> (2-Ethylhexyl)adipate	15.107	0.526	0.486	0.486	0.500	0.511	0.527	0.528	0.545	0.554	0.580	0.570	0.559	0.557	0.533	5.8
66	Benzo[<i>a</i>]anthracene	15.909	1.274	1.186	1.192	1.192	1.206	1.204	1.213	1.228	1.235	1.243	1.211	1.185	1.176	1.211	2.3
67	Chrysene	15.979	1.182	1.147	1.143	1.200	1.177	1.223	1.215	1.238	1.221	1.211	1.179	1.134	1.176	1.188	2.8
68	<i>bis</i> (2-Ethylhexyl) phthalate	16.054	0.810	0.785	0.780	0.809	0.841	0.839	0.837	0.877	0.897	0.917	0.896	0.873	0.858	0.848	5.2
69	Di- <i>n</i> -octyl phthalate	17.509	1.276	1.252	1.307	1.337	1.400	1.406	1.439	1.506	1.545	1.593	1.562	1.525	1.496	1.434	8.0
70	Benzo[<i>b</i>]fluoranthene	18.118	1.022	0.990	1.011	1.041	1.039	1.049	1.076	1.078	1.076	1.071	1.073	1.027	1.028	1.045	2.7
71	Benzo[<i>k</i>]fluoranthene	18.177	1.113	1.081	1.040	1.081	1.076	1.100	1.101	1.100	1.107	1.079	1.075	1.027	1.028	1.078	2.7
72	Benzo[<i>a</i>]pyrene	18.717	1.034	1.008	0.997	1.005	1.032	1.042	1.068	1.078	1.085	1.065	1.052	1.024	1.000	1.038	2.9
73	Indeno[1,2,3- <i>cd</i>]pyrene	20.627	0.995	0.973	0.973	0.982	0.999	1.038	1.058	1.074	1.078	1.028	0.984	0.944	0.901	1.002	5.2
74	Dibenz[<i>a,h</i>]anthracene	20.680	1.006	0.983	1.029	1.047	1.042	1.065	1.112	1.113	1.097	1.076	1.048	0.993	0.930	1.042	5.1
75	Benzo[<i>ghi</i>]perylene	21.103	1.064	1.049	1.049	1.063	1.089	1.101	1.130	1.117	1.098	1.002	0.920	0.832	0.747	1.020	11.5

Table 6. Response factors for 10 replicate determinations of 0.8 µg/mL sample of 75 analytes.

Compound	Replicate number										Statistics	
	1	2	3	4	5	6	7	8	9	10	Avg.	%RSD
N-Nitrosodimethylamine	0.444	0.405	0.405	0.415	0.400	0.406	0.396	0.369	0.393	0.408	0.404	4.6
Pyridine	0.707	0.727	0.766	0.714	0.764	0.777	0.707	0.687	0.659	0.663	0.717	5.8
Phenol	1.160	1.106	1.117	1.106	1.144	1.116	1.090	1.049	1.080	1.099	1.107	2.8
Aniline	1.387	1.409	1.419	1.408	1.439	1.347	1.406	1.382	1.397	1.322	1.392	2.5
bis(2-Chloroethyl) ether	1.036	0.953	1.020	1.020	1.052	0.982	1.004	0.987	0.992	1.005	1.005	2.8
2-Chlorophenol	1.113	1.073	1.120	1.117	1.115	1.123	1.115	1.064	1.098	1.096	1.103	1.8
1,3-Dichlorobenzene	1.435	1.392	1.465	1.391	1.459	1.431	1.430	1.396	1.393	1.413	1.420	2.0
1,4-Dichlorobenzene	1.468	1.475	1.457	1.467	1.481	1.497	1.512	1.436	1.470	1.490	1.475	1.4
Benzyl alcohol	0.625	0.630	0.624	0.637	0.633	0.645	0.625	0.606	0.554	0.593	0.617	4.3
1,2-Dichlorobenzene	1.411	1.342	1.399	1.384	1.451	1.411	1.357	1.382	1.378	1.384	1.390	2.2
2-Methylphenol	0.903	0.827	0.897	0.878	0.897	0.861	0.841	0.845	0.834	0.861	0.864	3.2
2,2'-Oxybis(1-chloropropane)	0.888	0.847	0.858	0.836	0.903	0.859	0.857	0.884	0.823	0.853	0.861	2.9
N-Nitrosodi-n-propylamine	0.571	0.509	0.511	0.539	0.536	0.539	0.518	0.508	0.503	0.522	0.526	3.9
3/4-Methylphenol	0.934	0.870	0.918	0.887	0.901	0.902	0.862	0.900	0.868	0.883	0.892	2.6
Hexachloroethane	0.492	0.501	0.505	0.497	0.537	0.509	0.476	0.510	0.484	0.496	0.501	3.3
Nitrobenzene	0.246	0.230	0.226	0.229	0.225	0.227	0.213	0.217	0.231	0.218	0.226	4.1
Isophorone	0.431	0.443	0.428	0.419	0.431	0.422	0.415	0.411	0.411	0.424	0.423	2.4
2-Nitrophenol	0.108	0.109	0.107	0.101	0.105	0.105	0.094	0.102	0.099	0.097	0.103	4.9
2,4-Dimethylphenol	0.181	0.178	0.180	0.188	0.184	0.177	0.174	0.167	0.167	0.175	0.177	3.8
bis(2-Chloroethoxy) methane	0.310	0.313	0.311	0.298	0.309	0.312	0.293	0.303	0.303	0.304	0.305	2.2
2,4-Dichlorophenol	0.249	0.226	0.240	0.225	0.236	0.232	0.227	0.238	0.236	0.233	0.234	3.2
1,2,4-Trichlorobenzene	0.339	0.339	0.336	0.328	0.343	0.332	0.333	0.322	0.341	0.347	0.336	2.2
Naphthalene	0.967	0.962	0.941	0.967	0.962	0.954	0.937	0.936	0.966	0.949	0.954	1.3
4-Chloroaniline	0.341	0.347	0.339	0.322	0.337	0.319	0.319	0.325	0.312	0.343	0.330	3.7
Hexachlorobutadiene	0.171	0.200	0.195	0.199	0.202	0.200	0.193	0.175	0.198	0.207	0.194	6.1
4-Chloro-3-methylphenol	0.193	0.195	0.186	0.191	0.182	0.179	0.185	0.186	0.178	0.182	0.186	3.1
2-Methylnaphthalene	0.637	0.626	0.629	0.627	0.619	0.617	0.618	0.621	0.630	0.631	0.625	1.0
1-Methylnaphthalene	0.572	0.595	0.579	0.585	0.587	0.565	0.576	0.591	0.595	0.582	0.583	1.7
Hexachlorocyclopentadiene	0.399	0.378	0.394	0.393	0.365	0.397	0.393	0.343	0.394	0.364	0.382	4.9
2,4,6-Trichlorophenol	0.300	0.293	0.295	0.282	0.282	0.297	0.278	0.286	0.277	0.277	0.287	3.0
2,4,5-Trichlorophenol	0.337	0.321	0.339	0.336	0.334	0.325	0.327	0.310	0.322	0.315	0.327	3.0
2-Chloronaphthalene	1.182	1.161	1.205	1.165	1.193	1.179	1.133	1.169	1.159	1.126	1.167	2.1
2-Nitroaniline	0.231	0.235	0.220	0.224	0.222	0.218	0.213	0.225	0.200	0.209	0.220	4.7
1,4-Dinitrobenzene	0.095	0.089	0.088	0.090	0.094	0.089	0.082	0.087	0.078	0.085	0.088	5.8
Dimethyl phthalate	1.261	1.252	1.247	1.202	1.223	1.224	1.214	1.248	1.242	1.252	1.237	1.6
1,3-Dinitrobenzene	0.114	0.106	0.118	0.117	0.105	0.093	0.097	0.111	0.093	0.099	0.105	9.1
2,6-Dinitrotoluene	0.212	0.183	0.195	0.177	0.186	0.183	0.167	0.174	0.177	0.177	0.183	6.9
1,2-Dinitrobenzene	0.074	0.078	0.085	0.073	0.082	0.072	0.075	0.076	0.060	0.064	0.074	10.1
Acenaphthylene	1.726	1.712	1.746	1.677	1.747	1.718	1.688	1.716	1.763	1.690	1.718	1.6
3-Nitroaniline	0.205	0.186	0.201	0.196	0.188	0.206	0.191	0.185	0.197	0.178	0.193	4.8
Acenaphthene	1.048	1.036	1.068	1.038	1.072	1.085	1.070	1.077	1.055	1.048	1.059	1.6
2,4-Dinitrophenol	0.036	0.032	0.032	0.037	0.035	0.030	0.036	0.031	0.033	0.033	0.033	7.1
4-Nitrophenol	0.115	0.099	0.112	0.103	0.102	0.102	0.100	0.103	0.106	0.092	0.103	6.3
2,4-Dinitrotoluene	0.237	0.211	0.211	0.193	0.211	0.195	0.192	0.203	0.206	0.195	0.205	6.5
Dibenzofuran	1.692	1.684	1.711	1.661	1.711	1.721	1.686	1.703	1.691	1.665	1.692	1.2

Table 6. Response factors for 10 replicate determinations of 0.8 µg/mL sample of 75 analytes (continued).

Compound	Replicate number										Statistics	
	1	2	3	4	5	6	7	8	9	10	Avg.	%RSD
2,3,5,6-Tetrachlorophenol	0.243	0.230	0.205	0.213	0.213	0.231	0.208	0.204	0.213	0.210	0.217	6.0
2,3,4,6-Tetrachlorophenol	0.273	0.263	0.257	0.241	0.263	0.235	0.252	0.255	0.253	0.245	0.254	4.4
Diethyl phthalate	1.172	1.177	1.147	1.134	1.161	1.162	1.124	1.126	1.173	1.128	1.150	1.8
Fluorene	1.254	1.269	1.322	1.241	1.256	1.260	1.224	1.250	1.269	1.246	1.259	2.0
4-Chlorophenyl-phenyl ether	0.668	0.657	0.645	0.658	0.647	0.661	0.642	0.651	0.641	0.660	0.653	1.4
4-Nitroaniline	0.231	0.208	0.216	0.215	0.226	0.213	0.204	0.217	0.202	0.186	0.212	6.0
4,6-Dinitro-2-methylphenol	0.038	0.041	0.040	0.040	0.034	0.041	0.046	0.036	0.032	0.033	0.038	11.1
Diphenylamine	0.575	0.559	0.570	0.553	0.552	0.557	0.549	0.545	0.544	0.539	0.554	2.0
Azobenzene	0.165	0.174	0.165	0.155	0.162	0.174	0.162	0.169	0.151	0.154	0.163	4.9
4-Bromophenyl phenyl ether	0.230	0.236	0.221	0.220	0.230	0.220	0.229	0.235	0.227	0.231	0.228	2.5
Hexachlorobenzene	0.276	0.305	0.306	0.291	0.293	0.304	0.311	0.305	0.292	0.279	0.296	4.0
Pentachlorophenol	0.084	0.086	0.084	0.079	0.070	0.083	0.076	0.084	0.086	0.069	0.080	7.9
Phenanthrene	1.044	1.072	1.075	1.065	1.055	1.068	1.069	1.049	1.044	1.069	1.061	1.1
Anthracene	1.012	1.021	1.014	1.014	0.975	1.016	1.011	0.983	0.981	1.013	1.004	1.7
Carbazole	0.868	0.871	0.842	0.857	0.858	0.859	0.851	0.842	0.859	0.837	0.854	1.3
Di- <i>n</i> -butylphthalate	0.931	0.924	0.867	0.884	0.870	0.889	0.882	0.856	0.855	0.852	0.881	3.1
Fluoranthene	1.048	1.084	1.018	1.042	1.056	1.034	1.042	1.051	0.998	1.003	1.038	2.5
Pyrene	1.264	1.228	1.291	1.262	1.243	1.282	1.269	1.291	1.291	1.240	1.266	1.8
Butylbenzylphthalate	0.354	0.328	0.333	0.311	0.326	0.313	0.303	0.307	0.303	0.312	0.319	5.1
<i>bis</i> (2-Ethylhexyl)adipate	0.302	0.284	0.275	0.278	0.274	0.266	0.281	0.262	0.254	0.269	0.275	4.8
Benzo[<i>a</i>]anthracene	1.068	1.050	1.064	1.056	1.062	1.047	1.023	1.074	1.027	1.040	1.051	1.6
Chrysene	1.242	1.216	1.209	1.216	1.225	1.208	1.189	1.212	1.200	1.211	1.213	1.2
<i>bis</i> (2-Ethylhexyl) phthalate	0.517	0.518	0.493	0.502	0.474	0.458	0.468	0.480	0.462	0.455	0.483	4.9
Di- <i>n</i> -octyl phthalate	0.743	0.708	0.659	0.668	0.659	0.649	0.642	0.664	0.664	0.639	0.669	4.8
Benzo[<i>b</i>]fluoranthene	0.982	0.968	0.934	0.970	0.924	0.975	0.955	0.929	0.932	0.984	0.955	2.5
Benzo[<i>k</i>]fluoranthene	1.023	1.017	1.067	1.086	1.052	1.053	1.044	1.035	1.053	1.015	1.044	2.2
Benzo[<i>a</i>]pyrene	0.895	0.897	0.885	0.893	0.903	0.883	0.875	0.888	0.902	0.911	0.893	1.2
Indeno[1,2,3- <i>cd</i>]pyrene	0.842	0.845	0.827	0.839	0.817	0.834	0.866	0.840	0.857	0.842	0.841	1.7
Dibenz[<i>a,h</i>]anthracene	0.918	0.926	0.940	0.921	0.936	0.922	0.921	0.944	0.957	0.950	0.934	1.5
Benzo[<i>ghi</i>]perylene	0.979	1.041	1.052	1.031	1.046	1.065	1.003	1.005	1.044	1.016	1.028	2.6

Table 7. RTL data for 75 analytes before and after trimming 0.5 m from the analytical column.

No.	Compound	Initial RT (min)	Post trim RT (min)	Relocked RT (min)
1	N-Nitrosodimethylamine	3.062	2.960	3.056
2	Pyridine	3.121	3.019	3.115
3	Phenol	6.453	6.341	6.458
4	Aniline	6.496	6.378	6.501
5	bis(2-Chloroethyl) ether	6.64	6.522	6.640
6	2-Chlorophenol	6.704	6.587	6.704
7	1,3-Dichlorobenzene	6.977	6.865	6.977
8	1,4-Dichlorobenzene	7.1	6.999	7.105
9	Benzyl alcohol	7.309	7.207	7.309
10	1,2-Dichlorobenzene	7.341	7.239	7.341
11	2-Methylphenol	7.49	7.394	7.496
12	2,2'-Oxybis(1-chloropropane)	7.549	7.442	7.549
13	N-Nitrosodi-n-propylamine	7.731	7.640	7.737
14	3/4-Methylphenol	7.737	7.646	7.737
15	Hexachloroethane	7.86	7.763	7.865
16	Nitrobenzene	7.961	7.865	7.961
17	Isophorone	8.314	8.223	8.314
18	2-Nitrophenol	8.41	8.325	8.416
19	2,4-Dimethylphenol	8.496	8.416	8.501
20	bis(2-Chloroethoxy) methane	8.635	8.550	8.635
21	2,4-Dichlorophenol	8.737	8.651	8.737
22	1,2,4-Trichlorobenzene	8.849	8.764	8.849
23	Naphthalene	8.94	8.855	8.945
24	4-Chloroaniline	9.02	8.940	9.026
25	Hexachlorobutadiene	9.116	9.036	9.122
26	4-Chloro-3-methylphenol	9.619	9.545	9.625
27	2-Methylnaphthalene	9.785	9.705	9.790
28	1-Methylnaphthalene	9.897	9.817	9.903
29	Hexachlorocyclopentadiene	9.972	9.892	9.978
30	2,4,6-Trichlorophenol	10.106	10.026	10.111
31	2,4,5-Trichlorophenol	10.143	10.063	10.143
32	2-Chloronaphthalene	10.331	10.251	10.336
33	2-Nitroaniline	10.443	10.363	10.443
34	1,4-Dinitrobenzene	10.593	10.513	10.598
35	Dimethyl phthalate	10.652	10.571	10.652
36	1,3-Dinitrobenzene	10.668	10.593	10.673
37	2,6-Dinitrotoluene	10.71	10.630	10.710
38	1,2-Dinitrobenzene	10.753	10.678	10.759
39	Acenaphthylene	10.78	10.694	10.780
40	3-Nitroaniline	10.876	10.796	10.882
41	Acenaphthene	10.962	10.882	10.967
42	2,4-Dinitrophenol	10.989	10.908	10.989
43	4-Nitrophenol	11.047	10.967	11.047
44	2,4-Dinitrotoluene	11.122	11.047	11.128
45	Dibenzofuran	11.144	11.064	11.144
46	2,3,5,6-Tetrachlorophenol	11.224	11.144	11.229
47	2,3,4,6-Tetrachlorophenol	11.267	11.187	11.272
48	Diethyl phthalate	11.384	11.310	11.390
49	Fluorene	11.497	11.417	11.502
50	4-Chlorophenyl-phenyl ether	11.502	11.422	11.502
51	4-Nitroaniline	11.507	11.427	11.507
52	4,6-Dinitro-2-methylphenol	11.544	11.459	11.545
53	Diphenylamine	11.62	11.540	11.620
54	Azobenzene	11.662	11.582	11.662
55	4-Bromophenyl phenyl ether	11.999	11.919	11.999
56	Hexachlorobenzene	12.058	11.973	12.058
57	Pentachlorophenol	12.251	12.171	12.256
58	Phenanthrene	12.47	12.390	12.475
59	Anthracene	12.524	12.438	12.524
60	Carbazole	12.679	12.599	12.684
61	Di-n-butylphthalate	13.032	12.952	13.032
62	Fluoranthene	13.732	13.631	13.732
63	Pyrene	14.011	13.909	14.016
64	Butylbenzylphthalate	14.957	14.834	14.957
65	bis(2-Ethylhexyl)adipate	15.107	14.984	15.102
66	Benzo[a]anthracene	15.909	15.770	15.915
67	Chrysene	15.979	15.835	15.984
68	bis(2-Ethylhexyl) phthalate	16.054	15.915	16.054
69	Di-n-octyl phthalate	17.509	17.359	17.509
70	Benzo[b]fluoranthene	18.118	17.974	18.124
71	Benzo[k]fluoranthene	18.177	18.028	18.177
72	Benzo[a]pyrene	18.717	18.578	18.723
73	Indeno[1,2,3-cd]pyrene	20.627	20.467	20.638
74	Dibenz[a,h]anthracene	20.68	20.520	20.686
75	Benzo[ghi]perylene	21.103	20.927	21.114
76	1,4-Dichlorobenzene-d ₄ (ISTD)	7.073	6.966	7.079
77	Naphthalene-d ₈ (ISTD)	8.913	8.828	8.919
78	Acenaphthene-d ₁₀ (ISTD)	10.924	10.844	10.930
79	Phenanthrene-d ₁₀ (ISTD)	12.449	12.363	12.449
80	Chrysene-d ₁₂ (ISTD)	15.931	15.786	15.931
81	Perylene-d ₁₂ (ISTD)	18.819	18.680	18.824

www.agilent.com/chem

DE.4455439815

This information is subject to change without notice.