

Gas Chromatograph (GC) Evaluation Study

Field Deployment Evaluation Report

Prepared by
EC/R Incorporated and RTI International
Under Contract EP-D-12-043, Work Assignment 4-01

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February 28, 2017

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1.0 Introduction

1.1 Background

On February 12, 1993, the U.S. Environmental Protection Agency (EPA) revised ambient air quality surveillance regulations in Title 40 Part 58 of the Code of Federal Regulations (40 CFR Part 58) to include provisions for enhanced monitoring of ozone (O₃), oxides of nitrogen (NO_x), volatile organic compounds (VOCs), and selected carbonyl compounds, as well as monitoring of meteorological parameters. On October 1, 2015, EPA made significant changes to the PAMS monitoring requirements and applicability (40 CFR part 58 Appendix D, section 5.0). The new requirements will result in a network of approximately 40 required sites (“Core Precursor” sites). The requirements also call for enhanced monitoring for ozone and ozone precursors as part of state and local monitoring agency directed Enhanced Monitoring Plans (EMP sites).

Under the original PAMS requirements, monitoring agencies were given options to measure VOCs using either an automated gas chromatograph (auto-GC) or collect samples in the field and analyze them in a laboratory (i.e., canister sampling). At the time the PAMS program was implemented, field rugged auto-GCs were not available and, as such, many monitoring agencies relied on conventional laboratory GCs equipped with automatic samplers. Since that time, new auto-GCs have been developed that can provide near real-time data and are designed for use in monitoring stations. As such, the revisions to the PAMS requirements made in October 2015 require hourly VOC measurements (most likely via auto-GC), with only limited options to measure VOCs via canister sampling.

The PAMS program has been in operation for more than 15 years, and much of the equipment used at PAMS sites is old and in need of replacement. Before recapitalizing the network, the EPA wants to evaluate the current state and availability of auto-GCs. The purpose of this report is to illustrate activities performed during the work assignment (WA) to collect information on the existing commercially available auto-GCs in order to determine their suitability for use in the PAMS (and possibly other monitoring) programs.

The Office of Air Quality Planning and Standards (OAQPS) of EPA located in Research Triangle Park (RTP), NC assigned EC/R Incorporated the responsibility of completing all tasks under EPA Contract Number 68-D-12-043, WA 2-01, WA 3-03, and WA 4-01. EC/R engaged its subcontractor, RTI International, to provide support in completing the tasks described in the Automated GC Evaluation WA. These tasks consisted of conducting a literature search of auto-GC vendors, developing a test plan and quality assurance project plan (QAPP) for the laboratory and field deployment evaluation phases, conducting a laboratory evaluation, and conducting a field deployment evaluation.

1.2 Test Plan and QAPP Development

Prior to conducting the Laboratory Evaluation Phase, the project team developed a test plan and QAPP that were approved by the EPA technical team. The test plan presented an approach for assessing the suitability of selected auto-GC units for the automated collection, analysis, and reporting of PAMS target compounds in both a controlled laboratory setting and field deployable environment. This plan described the activities to be conducted during the laboratory evaluation phase, as well as the subsequent field deployment phase. During both phases, the overall objective was to challenge the candidate auto-GC units with a breadth of technical and environmental conditions in a manner sufficiently rigorous to reveal performance and capability differences among the units. Evaluation criteria were developed to assess capabilities in sample collection and analysis, data management (reduction, storage, and transfer), stability during unattended operation, and robust field-deployment environmental conditions.

The second document developed for the work was the QAPP, which was prepared based on EPA guidelines for collecting environmental data set out in the document "*EPA Requirements for Quality Assurance Project Plans (QA/R-5)*." The project team worked with the EPA work assignment manager (WAM) and EPA QA Officer to

develop data parameters to support the qualitative and quantitative design of a data collection for the laboratory and field deployment evaluation phases.

The project team revised the test plan and QAPP in advance of the field deployment phase to incorporate changes to the evaluation plan directed by the WAM.

1.3 Laboratory Evaluation Phase

The project team first generated a comprehensive list of potential candidate vendors for the laboratory evaluation, both domestically and internationally, by reviewing Internet sites, trade publications, and exhibitor lists from recent trade association meetings; searching the Internet; and adding potential candidates identified by the EPA that were not otherwise found in the search. Through these processes, the project team identified and contacted over 40 potential vendors.

A detailed questionnaire was sent to each candidate, followed by direct telephone or email contact to describe the purpose and general design of the study and the criteria for inclusion. Information from the questionnaires was transferred into the spreadsheet, and any missing information was obtained in follow-up conversations. The EPA technical team reviewed the detailed specifications of each vendor's auto-GC unit and reduced the number of candidates to fewer than 10 participants for the laboratory evaluation phase.

The laboratory evaluation phase was conducted at RTI's Air Monitoring Laboratory over the course of a 4-month period. The focal point of the laboratory evaluation phase was to conduct a simultaneous comparison of the vendor-provided auto-GC units. Synthetic atmospheric concentrations of the target compounds were generated through accurate zero-air dilution of certified standard gas mixtures (NIST-traceable, if available) in a deactivated glass manifold to which individual sampling ports were provided for each auto-GC unit.

Prior to the laboratory evaluation, the candidate vendors performed the installation, setup, and calibration of their auto-GC units. During the evaluation, the candidates operated their equipment and provided data for the evaluation. At the conclusion of the laboratory evaluation phase, the project team prepared and submitted data packets to each vendor for validation prior to carrying out the analysis for the evaluation.

Using the validated data, the project team conducted the analysis as set out in the test plan and QAPP and prepared a draft report of the results of the laboratory evaluation. After review by the EPA technical team, the project team prepared the final report of the laboratory evaluation.

1.4 Field Deployment Phase

Based on the results contained in the laboratory evaluation report, the WAM selected three candidate auto-GC systems to be purchased for the field deployment phase. In addition, the WAM allowed three additional vendors to loan their auto-GC systems for evaluation during this phase. The six auto-GC systems were installed in a mobile laboratory, i.e., a trailer owned by the EPA. The field deployment of the auto-GC systems was conducted at the RTI Field Site in Research Triangle Park (RTP), NC.

During the field deployment phase, the project team downloaded the data recorded by each auto-GC system, including data recorded during verification calibration checks, weekly precision checks, and Method Detection Limit (MDL) checks conducted using accurate zero-air dilution of a certified standard gas mixture of 102 VOCs (referred to as the "TCEQ blend"). These data, as well as qualitative observations, were analyzed according to the test plan and QAPP to prepare a draft report of the results. After review by the EPA technical team, the project team prepared this final report of the field deployment evaluation.

2.0 Overview of the Field Deployment Phase

The purpose of the field deployment phase of the GC evaluation study was to evaluate the performance of the candidate auto-GC systems under field conditions. The subsections that follow discuss the schedule of activities and provide additional detail on each stage of the field deployment.

2.1 Schedule of Activities

The field deployment phase was comprised of five key stages: (1) setup of the mobile laboratory, (2) delivery and setup of the candidate vendors' equipment, (3) 30-day test trial of the mobile laboratory and candidate systems, (4) field deployment of the auto-GC systems, and (5) shut-down of the systems and transfer to the EPA's laboratory or removal by the vendors. These stages occurred over a 23-month time span (June 2014 – April 2016). The schedule included an extended shakedown period resulting from issues not related to equipment performance.

Prior to the fourth of these stages, the field deployment, the project team revised the test plan and QAPP as described in Section 1.2 to conform to the revised scope of the auto-GC evaluation project. The draft revised test plan and QAPP were submitted for EPA review on August 13, 2015. Further revisions were submitted on August 18, and the revised test plan and QAPP were approved for the field evaluation phase by the WAM and EPA QA Officer on August 26. The QAPP with the test plan as an appendix was electronically transmitted to each candidate vendor on August 27.

2.2 Mobile Laboratory Setup

The project team worked with the WAM to locate a suitable mobile laboratory to simulate conditions likely to be found at PAMS sites in the field. An EPA-owned, 21-foot Wells Fargo trailer that was not currently in use was identified, and the project team obtained permission to use this trailer.

The WAM towed the trailer to an automotive service provider on June 25, 2014, and, after an inspection of the tires and wheel bearings revealed that no repairs were needed, towed the trailer to the RTI Field Site. On June 26, RTI Facilities staff assessed the electrical capability at the Field Site and subsequently connected an electrical line to the trailer. The project team confirmed that all the electrical outlets in the trailer were operational.

The project team transported the equipment, supplies, and materials from the evaluation laboratory that would be used during the field deployment phase to the trailer. The project team then developed and installed the sampling and calibration system and marked out where the six candidate auto-GC systems would be installed (Figure 1) to transform the trailer into a mobile laboratory. Specifically, the project team installed 1/4-inch stainless steel tubing for sample lines and carrier gas supply lines. These lines were cleaned, then conditioned with zero air from the calibration gas dilution system. The inlet, down tube, and 10-port borosilicate glass manifold (constructed by URG Corporation, Chapel Hill, NC) were assembled as displayed in Figure 1. The calibration gas dilution system (Envionics® Series 2014 Computerized VOC Gas Dilution System and Envionics® Series 7000 Zero Air Generator) was set up with NIST-traceable VOCs standard from Linde Specialty Gases (TCEQ blend). The Entech 42280 Humidity/Temperature USB Datalogger was set up to begin monitoring relative humidity (RH) and temperature in the mobile laboratory.

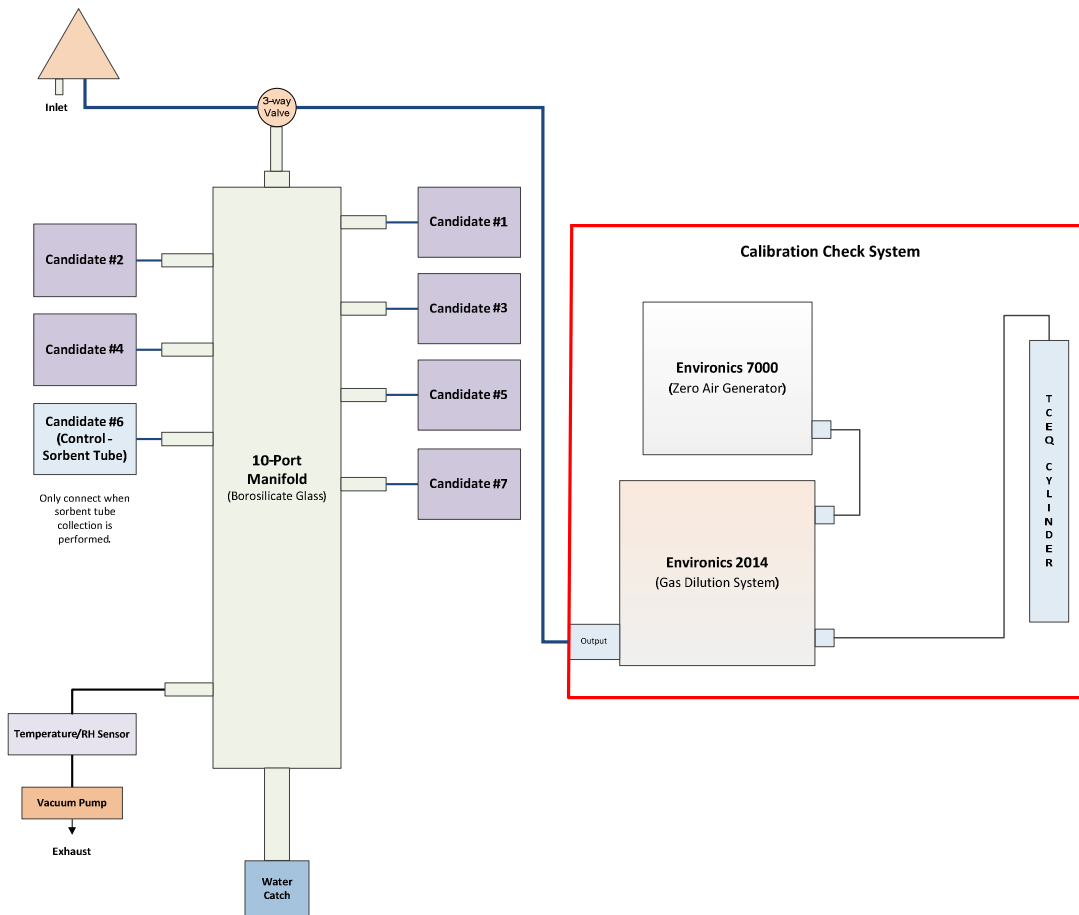


Figure 1. System Overview for Mobile Lab for the Field Deployment Phase

The test plan outlined three tests to be completed before the field evaluation phase could begin. These tests ensured the integrity of the system by (1) confirming there were no leaks, (2) verifying there was adequate flow at each sample port, and (3) verifying that the gas dilution system points were achievable and stable. From November 4 through December 2, 2014, the project team conducted the following tests:

1. Ran zero air to confirm that there were no leaks.
2. Checked the flow rates to all ports to verify adequate flow from the delivery system.
3. Ran test dilutions to confirm that all ports were receiving proper concentrations. Verified the test concentrations by using sorbent tubes under TO-17 Method.

The leak test was conducted by capping the ends to all sampling ports and running 8 L/min zero air flow through the sampling system using the Environics 2014 Gas Dilution System. The flow at the exhaust was measured and all joints were checked for leaks. Due to leaking around the temperature/RH sensor box, the box was replaced and the system was re-checked for leaks. A re-measured flow rate of 7.88 L/min (-1.5 percent difference) was detected at the exhaust port. The next step was to check each sample port using the vacuum pump that would be used for the field study. A shutoff valve was placed in line between the vacuum pump and the temperature/RH box. This valve was used during the field study to maintain a flow rate near 8 L/min and was checked using a BIOS flow meter. Ambient air was pulled through the inlet and the table below shows an average 2.28 percent difference for 10 tests.

Check 1 (Measure flow rate at inlet)

Test	Target Flow Rate (L/min)	Measured Flow Rate (L/min)	Difference (L/min)	% Difference
1	8.03	7.87	-0.16	-1.99
2	8.03	7.86	-0.17	-2.12
3	8.03	7.86	-0.17	-2.12
4	8.03	7.84	-0.19	-2.37
5	8.03	7.84	-0.19	-2.37
6	8.03	7.85	-0.18	-2.24
7	8.03	7.83	-0.20	-2.49
8	8.03	7.85	-0.18	-2.24
9	8.03	7.84	-0.19	-2.37
10	8.03	7.83	-0.20	-2.49
Average	8.03	7.85	-0.18	-2.28

The next step was to measure the flow at each port. All ports were capped except the port in which flow was being measured. The results of this test are displayed in the table below. The project team concluded that the sampling system was not leaking when air was either pushed (Environics 2014 Gas Dilution System) or pulled (vacuum pump) through the sampling and dilution systems.

Check 2 (Measure flow rate at each port with other ports closed)

Port	Target Flow Rate (L/min)	Measured Flow Rate (L/min)	Difference (L/min)	% Difference
1	8.03	7.94	-0.09	-1.1
2	8.03	7.92	-0.11	-1.4
3	8.03	7.96	-0.07	-0.9
4	8.03	7.92	-0.11	-1.4
5	8.03	7.94	-0.09	-1.1
6	8.03	7.92	-0.11	-1.4
7	8.03	7.92	-0.11	-1.4
Exhaust	8.03	7.96	-0.07	-0.9

To verify adequate flow from the delivery system, each vendor was assigned a sampling port on the manifold. The project team requested the sampling flow rate for the front end sampler from each of the six vendors. These flow rates were used to determine the total flow rate needed for the GC systems. The project team used small individual pumps that were attached to each sample port to mimic the flow rate that each instrument would require under the actual testing. The pumps were set to pull slightly in excess of what each vendor indicated the required flow rate would be, and the total system flow was set to mimic testing conditions. (Only five small pumps were available for this test, so five of the six candidate ports were connected for each test. The total flow rate of the five pumps was in excess the total required by the six GC systems, per the vendors.) The open line test confirmed that an excess flow was present in the exhaust line to ensure that adequate sample was available to each candidate instrument during challenge gas testing. The adequate flow rate check was conducted using the vacuum pump running at 8 L/min, which flow rate was confirmed by the BIOS flow meter. Two test runs were conducted, and excess exhaust flows of 3.07 and 3.05 L/min were measured, as shown in the table below. This confirms that at a rate of 8 L/min, each sampling port has sufficient air flow, based on the requests of the vendors for their systems, with an exhaust of nearly 40 percent of the total flow.

Check 3 (Measure flow rate at each port with all ports having a pump set at 1 L/min flow rate)

Test Run	Pump Set Flow Rate (L/min)	Set Flow Rate (L/min)							Measured Flow Rate at Exhaust (L/min)	Total Flow Rate (L/min)	% Difference
		Port 1	Port 2	Port 3	Port 4	Port 5	Port 6 (Control)	Port 7			
1	8.03	1.00	0.88	0.93	0.00	1.00	0.00	1.00	3.07	7.88	-1.87
2	8.03	1.00	0.88	0.93	1.00	1.00	0.00	0.00	3.05	7.86	-2.12

For the confirmation that all ports were receiving proper concentrations, after test point concentrations were assigned, a dilution spreadsheet was used to confirm that all the points could be delivered by the gas dilution system based on the concentration of benzene in the TCEQ gas mixture. The gas dilution system was programmed using the certified concentration of benzene in the TCEQ gas mixture to target the multi-point verification points (0-, 3-, 6-, 9-, and 12-ppb) during the study.

The final step in the mobile laboratory setup involved the sampling of sorbent tubes containing Carbopack B[®] sorbent material. Sorbent tube sampling verified four things:

1. The system produced non-detectable levels of VOCs when zero air was run through the system.
2. The sorbent tubes had the capacity to collect and retain VOC sample which could be detected by a GC-MS.
3. The TO-17 Method used by RTI as a seventh “candidate” was a viable method to confirm target concentrations delivered by the dilution system were consistent over the pre- and post-verification checks. (These results were not meant to be used for candidate comparison.)
4. There was near equal distribution of challenge gas at each of the ports.

Sorbent tube samples were collected at five concentrations to be used during the lab phase testing. Based on results, recovery of target VOCs were determined to be satisfactory, and the bias between ports was calculated to be within 15 percent of each other. The bias is deemed to be an over-estimation since it also includes instrument uncertainty, and individual tubes and flow variabilities, along with other factors. All testing was completed by December 2, 2014, and zero-air was run through the system for the weeks leading up to the vendor setup from January through April 2015.

In November 2014, a DSL line was installed at the mobile laboratory to enable remote access to the auto-GC systems, and lines were run to the designated locations for each system. In December 2014, the WAM provided a dehumidifier for the mobile laboratory to counteract elevated relative humidity levels that had been encountered. Also in December 2014, a maintenance kit for the Environics zero air generator was obtained and the scheduled maintenance was performed.

2.3 Vendor Setup

The six candidate vendors shipped or brought their auto-GC units and supporting equipment to the mobile laboratory between December 2014 and April 2015. During this time, the project team assisted the six vendors in installing, setting up, testing, calibrating, and troubleshooting their auto-GC systems. The project team also received basic training on the operations of the vendors’ auto-GC systems.

The project team ran setup calibration points for the vendors on January 30, March 11, and March 27. These were five-point calibration runs at 0-, 3-, 6-, 9-, and 12-ppb benzene points generated using the calibration gas dilution system and the TCEQ blend. That is, based on the certified concentration of benzene in the TCEQ blend, the dilution system was programmed to dilute the gas with zero air to the specified benzene calibration points. The vendors were provided a spreadsheet showing the target concentrations of benzene and the other target compounds in the TCEQ blend at each of the calibration points, calculated based on the certified concentration of each compound in the TCEQ blend.

2.4 30-Day Test Trial

As noted previously, the WAM determined that it would be advisable to conduct a test of the mobile laboratory systems, the functioning of the auto-GC systems within the laboratory, the VOC standard dilution and delivery system, and the data acquisition procedures to identify and work through any problems prior to beginning the field deployment evaluation. Accordingly, the vendors were informed of the test and given the schedule for the test on April 20. In addition, the project team informed the vendors that the measurement data gathered during this 30-day test would not be included in the evaluation. Thus, the quantitative data from this period are not included in this evaluation, although the qualitative observations on system performance are reported below in Section 6.9.

On April 24, the project team conducted a five-point pre-verification run at the 0-, 3-, 6-, 9-, and 12-ppb benzene calibration points, and the vendors were provided passwords to allow remote access to their systems to complete setup for the 30-day test. The project team worked with the vendors as necessary to ready the systems for the test. On April 29, the vendors' access to their systems was curtailed (i.e., passwords changed), and the 30-day test trial was commenced on April 30.

On May 8, the project team discovered that the mobile laboratory was overheating as the ambient temperature rose at the site. It was determined that the built-in air conditioning system in mobile laboratory could not adequately counteract the heat generated by the auto-GC systems in the face of elevated ambient temperatures and direct sun at the site. A portable air conditioner was added to the mobile laboratory, which successfully brought the temperature down to an acceptable operating range. A five-point verification check was conducted after the temperature was brought under control, and the vendors were permitted access to their systems to determine whether the elevated temperatures had affected retention times or other aspects of operation. The elevated temperatures did not cause permanent damage to any of the auto-GC systems.

The 30-day test was concluded on April 29. During the test period, the project team conducted four precision checks (3-ppb benzene standard) and seven MDL checks (0.5-ppb benzene standard) as planned. Also as planned, a five-point post-verification check was conducted at the conclusion of the test period on June 1, and the vendors were given access to their systems to make any adjustments indicated by the post-verification check. During this test period and at its conclusion, the project team downloaded the data from each system and reviewed the data for completeness. However, as noted, these data are not included in this evaluation.

2.5 Field Deployment

As previously noted, the field deployment included an extended shakedown period resulting from issues not related to equipment performance. The quantitative data gathered during this shakedown period are not included in this evaluation, although the qualitative observations on system performance are reported below in Section 6.9.

During this shakedown period, it was determined that the higher-boiling compounds in the TCEQ blend were being held up in the sample lines so that they were not reaching the auto-GC systems to be measured and reported during the expected time periods. The following were suggested as possible factors leading to this situation:

- Retention times in the sample lines that were too long, caused by line lengths (up to 16 feet) not normally used in field monitoring stations coupled with the 1/4-inch internal diameter of the lines.
- “Cold-trapping” in the sample lines caused by the cool temperatures in the mobile laboratory since the ambient temperatures had cooled off.
- Accumulation of particulate matter in the sample lines over the months of ambient sampling, on which compounds may be adsorbed.

- The use of dry zero air in the dilution system to prepare the gas standards for the verification, precision, and MDL checks and for purging the system. Dry zero air has been shown to make sample lines “sticky” in some applications.

To remedy the situation and put all the vendors on the same footing, the WAM determined that the existing sample lines would be replaced. As a default, the project team would install new 1/8-inch, chromatographic grade, silica-treated stainless steel tubing, with all lines 16 feet long and insulated but not heat-traced. As an alternative, the vendors were permitted to install sample lines of their choice, provided that they were 16 feet long and unheated. The 16-foot minimum length was necessary because, due to the configuration of the mobile laboratory, one of the auto-GC systems required a sample line of that length. Three vendors elected to use the default sample lines, and three provided their own sample lines.

Line heating was not allowed on the new sample lines due to power limitations in the mobile laboratory. The lack of heated lines also prompted the WAM to request a switch from sampling ambient air to sampling air from within the mobile laboratory. In addition, a humidifying system was placed between the gas dilution system and the manifold to maintain the relative humidity of the zero air and gas standards at 30 to 45 percent. This modified mobile laboratory setup was used to complete the field deployment evaluation.

After the new sample lines and humidifying system were installed, three-point calibration standards (0-, 6-, and 12-ppb benzene standards) were run December 15, 17, 29, and 31. The vendors were allowed access to their systems during this period to ready the systems for the remainder of the field deployment evaluation.

The field deployment during which the quantitative data reported in Section 6 of this report were gathered consisted of a 45-day session, with pre- and post-tests, on the following schedule:

Date	Event
1/4/2016	Pre-verification check at 0-, 3-, 6-, 9-, and 12-ppb benzene standards (2 hours at each point). Vendors were subsequently given access to review the verification check data and make corrections to their systems. Vendors provided the revised data, which serve as the starting point for the analysis.
1/8/2016	MDL check at 0.5-ppb benzene standard (15 hours).
1/9/2016	Start 45-day session sampling indoor air of the mobile lab.
1/12/2016	Weekly 3-ppb benzene standard precision check (2 hours).
1/19/2016	Weekly 3-ppb benzene standard precision check (2 hours).
1/26/2016	Weekly 3-ppb benzene standard precision check (2 hours).
2/2/2016	Weekly 3-ppb benzene standard precision check (2 hours).
2/9/2016	Weekly 3-ppb benzene standard precision check (2 hours).
2/16/2016	Weekly 3-ppb benzene standard precision check (2 hours).
2/22/2016	End of 45-day session.
2/23/2016	Post-verification check at 0-, 3-, 6-, 9-, and 12-ppb benzene standards 2 hours at each point). Vendors were subsequently given access to review the verification check data and make corrections to their systems, but the uncorrected data were used in the analysis.
3/1/2016	Setup run at 0-, 0.5-, and 3-ppb benzene standards for the MDL check. Only the data from the 3-ppb benzene standard (2 hours) are included in the analysis.
3/7/2016	MDL check at 0.5-ppb benzene standard (15 hours).

Prior to the start of this 45-day session, the project team developed computer scripts to convert the data output from each auto-GC system into a common format, aligned temporally, to create a database for use in the statistical analyses reported in Section 6 below. This required aligning the various abbreviated names for the target compounds used in the output files with the database’s master list, as well as translating the various file formats into the common format of the database. In addition, the project team worked with the vendors to understand the operating schedule of each system, including the frequency and duration of sample collection and analysis, and how each system assigns timestamps to its output files. Timestamping varied considerably among

the systems, and could represent the beginning or end of the sampling cycle or the analysis cycle, or the hour during which sampling and analysis occurred. Using this information, the project team's computer scripts aligned the data from all the instruments in time to ensure that the data in the combined database reflected the concentrations each system measured during each hour when gas standards were delivered for the verification, precision, and MDL runs. The project team requested and received confirmation from each of the vendors that the processing scripts accurately transcribe the data to the correct time periods.

During the 45-day session, between the second and third precision checks, the TCEQ blend cylinder and was replaced by a fresh cylinder. The concentrations of most compounds in the new cylinder were only marginally different from those in the first cylinder, but for five compounds the concentrations decreased by approximately half. For all compounds, the analyses reported in Section 6 were carried out considering the change in target concentrations during the test period.

Following each verification, precision, and MDL check associated with the 45-day session, the project team downloaded, processed, and entered the corresponding data into the master database. The data during periods of "sampling" the air within the mobile laboratory were not processed.

In general, the vendors were not allowed access to their instruments during the 45-day session. However, after precision checks (beginning with the second precision check on January 19), the vendors were allowed access to their systems if they recorded measurements that were greater than ± 20 percent off from the target concentration of any of the compounds of interest. In these cases, the project team sent the results of the precision check to each such vendor along with the target concentrations for the compounds of interest and the password allowing remote access to that auto-GC system. The vendors were permitted to adjust their systems as they wished, and were instructed to report what actions they took. The vendors were not permitted to alter the data recorded during each precision check; any adjustments only affected the system performance going forward. Additional information on this is presented in Section 6.8 below.

2.6 Removal of the Auto-GC Systems

At the conclusion of the field deployment, the project team shut down the auto-GC systems. The three systems that had been purchased by the EPA for the field deployment evaluation were disassembled as necessary and transported by the project team to the EPA campus in RTP, NC. The EPA purchased one of the auto-GC systems that had been loaned for the field deployment evaluation, and the project team likewise disassembled and transported that system to the EPA campus. The remaining two systems were packed up and removed by the vendors.

When all the auto-GC systems were removed from the mobile laboratory, the project team removed the sampling system, the gas dilution system, the sample lines, and the Internet access equipment from the mobile laboratory, restoring the trailer to as-received condition. The WAM subsequently towed the trailer back to the EPA RTP campus.

3.0 List of Candidate Auto-GC System Vendors

Based on the results of the laboratory evaluation, the WAM selected three candidate auto-GC systems to be purchased for the field deployment phase. In addition, the WAM allowed three additional vendors to loan their auto-GC systems for evaluation during this phase. Table 1 below displays the candidate vendors in alphabetical order, with contact information. For the field deployment phase, these vendors were randomly assigned a Vendor ID (A through F). In this report, these candidate vendors are identified only by their Vendor IDs.

For the field deployment evaluation, the candidate vendors were responsible for:

Shipping the auto-GC unit and all necessary supportive equipment to RTI.
Installing the auto-GC system in the mobile laboratory.

- Training the project team on basic operations of the auto-GC system.
- Calibrating the auto-GC system based on gas standards generated by the project team using the gas dilution system in the mobile laboratory.

Working with the project team in interpreting the auto-GC output and confirming that the team's data processing scripts accurately transcribed the system's data to the correct time periods.

- To the extent desired, reviewing the data after verification, precision, and MDL checks and adjusting the auto-GC system accordingly.

Troubleshooting and repairing units as required.

Table 1. Candidate Auto-GC System Vendors for the Field Deployment Evaluation Phase

Candidate Vendor	Contact Information
Agilent Technologies/ Markes International	Kelly Beard (Agilent; 970-310-0324; kelly.beard@agilent.com) Michael Cox (Agilent; 866-793-4961; michael_g_cox@agilent.com) David Wevill (Markes; 866-483-5684; Dwevill@Markes.com)
Baseline	Brian Bischof (303-823-6661 x6139; brian.bischof@baselineindustries.com) Steve Grantham (303-823-6661 x6134; steve.grantham@baselineindustries.com) Ben Kahn (303-823-6661 x6135; ben.kahn@baselineindustries.com)
CAS/Chromatotech	Christina Cloran (513-542-1200; ccloran@cas-en.com) Seth Cloran (513-542-1200; scloran@cas-en.com) Tomek Marchlewski (513-542-1200; tmarch@cas-en.com)
Perkin Elmer	Bill Goodman (203-402-1960; william.goodman@perkinelmer.com) Lee Marotta (914-954-1779; lee.Marotta@perkinelmer.com) Cory Whipp (225-747-7707; cory.whipp@perkinelmer.com)
Synspec	Thomas Wilbur (603-880-7100); thomasw@jjwilbur.com) John Wilbur (603-880-7100; johnw@jjwilbur.com) Wouter Lautenbach (+11 31 50 5266454; W.Lautenbach@snyspec.nl) Michael Rijpkema (+11 31 50 5266454; M.Rijpkema@snyspec.nl)
Thermo Scientific/ Markes International	Nick Hubbard (919-414-7497; Nicholas.Hubbard@thermofisher.com) Terry Jeffers (Thermo; 904-248-8204, Terry.Jeffers@thermofisher.com) Suresh Seethapathy (Thermo; 301-803-0896; Suresh.seethapathy@thermofisher.com) David Wevill (Markes; 866-483-5684; Dwevill@Markes.com)

A short description of each of the candidate auto-GC systems is presented below. These descriptions do not include the gas generators included in some systems because to do so might compromise anonymity. Gas generators can provide zero air, hydrogen, or nitrogen.

Agilent/Markes System

The bench-top Agilent/Markes system consists of an Agilent 7890B GC with the Markes UNITY 2 Air Server 3 sampling system. The Markes sampling system uses an electrically-cooled trap which quantitatively retains volatiles from acetylene to C₁₄ compounds. Samples are subsequently conveyed to the Agilent GC, where they are split between two chromatographic columns, each equipped with a flame ionization detector (FID). One detector/column is for analytes ranging from C₂-C₅, the other detector/column is for analytes ranging from C₆-C₁₄.

For the purpose of this study the Agilent 7890B Unit used helium as the column carrier gas. The FIDs used hydrogen and zero air as fuel gases and helium as make-up gas. The Markes unit was supplied with nitrogen as a drying and purge gas.

Baseline System

The rack-mounted Baseline Automated PAMS system consists of a CDS 9350 BL Thermal Desorption Sampler Unit, one 9100 FID GC analyzer, and one 9100 photoionization detector (PID) GC analyzer. The sampler unit contains two three-phase sorbent tubes for the collection of VOC from the sample stream, which are alternated to allow for continuous sampling, and a separate focus trap which concentrates the collected gas after desorption from the sorbent tube. The concentrated samples are subsequently directed to the two GCs, where they are analyzed. The FID GC measures the analytes ranging from C₂-C₅, the PID GC measures the heavier analytes.

The Baseline system used hydrogen as the column carrier gas and sample purge gas. The FID used hydrogen and zero air as fuel gases and hydrogen as make-up gas.

CAS/Chromatotec System

The rack-mounted CAS/Chromatotec AirmOzone system consists of an AirmoVOC C₂-C₆, GC/FID for light hydrocarbons and an AirmoVOC C₆-C₁₂, GC/FID for heavy hydrocarbons. The gas sample is split between the two GCs, and the gas samples flowing to each of the two GCs are drawn through traps which extract the target gas components (C₂-C₆ or C₆-C₁₂) from the samples. To enhance adsorption of compounds with lower boiling points, the traps are cooled; the C₂-C₆ trap is set at -10 °C, and the C₆-C₁₂ trap is set at 20 to 25 °C. The concentrated analytes are then desorbed and routed to the two chromatographic columns for measurement.

The CAS/Chromatotec system uses hydrogen as the carrier gas. The FIDs use hydrogen and zero air as fuel gases. Both hydrogen and zero air are supplied by gas generators that are provided with this turn-key system. This system also includes a calibration gas generator, which allows for automatic data validation and sample conditioning.

The CAS/Chromatotec system comes standard with an embedded PC and software. The Vistachrom software allows the determination of concentrations, retention times and peak areas. There is ample storage for the automatic archiving of years of data. This software incorporates several utilities to enable the user to interface with the analyzers, to configure the measurements, and to setup and control threshold alarms. This capability includes features such as manipulating and reprocessing data, performing system checks, exporting data, and remotely monitoring the system.

Perkin Elmer System

The bench-top Perkin Elmer system consists of a Clarus ATX 580 GC and a TurboMatrix Thermal Desorber fitted with an Air Sampler Accessory. The Clarus 580 GC comes equipped with two chromatographic columns, each with an FID. The TurboMatrix is a two-stage, thermal desorption system that uses cold trap (at -30 °C) packed with the correct adsorbents for quantitative trapping of the C₂-C₁₁ components of the US PAMS program. The desorbed sample is split and routed to the two chromatographic columns for measuring the lighter and heavier analytes.

The Perkin Elmer system used helium as the column carrier gas. The FIDs used hydrogen and zero air as fuel gases.

Synspec System

The rack-mounted Synspec GC955-Series system consists of a sampling and preconcentration module and two GC955 units (Model 811 for C₂-C₅ and Model 611 for C₆-C₁₂), each equipped with a FID and a PID. The sample is drawn into a preconcentration tube that is cooled to -5 °C; the concentrated sample is desorbed by heating the preconcentration tube quickly. The concentrated sample is split between the two GC units, where the target compounds are separated chromatographically and measured.

The Synspec system used nitrogen as the column carrier gas. The FIDs used hydrogen and zero air as fuel gases.

Thermo/Markes System

The bench-top Thermo/Markes system consists of a TRACE 1310 GC / ISQ LT mass spectrometer (MS) with the Markes UNITY 2 Air Server 3 sampling system. The Markes sampling system uses an electrically-cooled trap which quantitatively retains volatiles from acetylene to C₁₄ compounds. Samples are subsequently conveyed to the GC where they are separated chromatographically. The separated analytes enter the vacuum chamber of the MS, where they are individually detected and quantified by their almost unique mass fragmentation patterns using an ion source detector.

The Thermo system was set up to use helium as the column carrier gas. The Markes unit was supplied with nitrogen as a drying and purge gas.

4.0 VOCs Measured by Vendors

Target compounds were selected by the EPA technical team from among the 102 VOCs contained in the TCEQ blend. Table 2 lists the chemical compounds evaluated in the field deployment phase. Due to the nature of FID and PID units, a complete chromatographic capture of all possible carbon compounds is typically generated by each detector. In the instances where compounds other than the target analytes were acquired (and possibly reported), these compounds were excluded from any statistical evaluation.

Table 2. Chemical Compounds Evaluated in the Field Deployment Phase

Compound	CAS Number
Benzene	71-43-2
1,3-Butadiene	106-99-0
n-Butane	106-97-8
1-Butene	106-98-6
cis-2-Butene	590-18-1
Carbon Tetrachloride	56-23-5
Ethane	74-84-0
Ethylbenzene	100-41-4
Ethylene	74-85-1
m-Ethyltoluene	620-14-4
o-Ethyltoluene	611-14-3
p-Ethyltoluene	622-96-8
n-Hexane	110-54-3
Isobutane	75-28-5
Isopentane	78-78-4
Isoprene	78-79-5
n-Pentane	109-66-0
Propane	74-98-6
Propylene	115-07-1
Styrene	100-42-5
Tetrachloroethylene	127-18-4
Toluene	108-88-3
trans-2-Butene	624-64-6
1,2,3-Trimethylbenzene	526-73-8
1,2,4-Trimethylbenzene	95-63-6
2,2,4-Trimethylpentane	540-84-1
o-Xylene	95-47-6
m-/p-Xylene	179601-23-1

Initially, the EPA technical team identified a set of “priority compounds” and a second set of “optional compounds” for the field deployment evaluation. In the 30-day test trial and the shakedown period, the vendors were requested to set up their auto-GC systems to detect and report as many of both sets of compounds as possible. However, after the shakedown, the WAM determined that only the priority compounds would be targeted in the final 45-day session. These are the compounds listed above in Table 2. The analyses of the results for these compounds are reported in Section 6 below.

5.0 Data Acquisition and Compilation

Because of the nature of the study, it was necessary to combine the data from the various auto-GC systems into a common database to allow comparative data analysis. In order to facilitate this goal, the system vendors were given a sample of a desired common data output format for the field deployment evaluation, and asked to adjust their system output files to be as close to it as possible. This was accomplished to varying degrees, detailed in Section 6.7 of this report along with additional system-specific details regarding data acquisition.

In addition to formatting issues, other factors also affected the process of collecting and compiling study data. These issues resulted from the nature of the study (comparing multiple systems), and might not arise in a real-world environment with a single system performing continuous monitoring. However, for the purposes of this study, it was critical to align the data from each system for each target compound with the hours in which standard VOC concentrations prepared with the TCEQ blend were delivered to the systems. This was less straightforward than might be expected due to following considerations:

- Compound naming - Each vendor employed different names for the target compounds for the study, often employing abbreviations. It was necessary to compile a standard list of names for chemical species and match them to the names used by each vendor when the data were compiled.
- System operation schedules - This was one of the most complicated factors influencing the preparation of a common database. Each system had a different operating schedule, and there were significant differences in the ways they collected and generated data:
 - Sampling frequency - Most systems collected samples once per hour, but one system collected samples twice hourly. After discussion with the vendor, it was decided to include only the second sample collected during each hour in statistical analyses (as opposed to averaging the two samples collected each hour.)
 - Sampling duration - Duration of sample collection varied significantly, with some systems collecting samples for 20-30 minutes and analyzing the sample immediately after collection, and other systems collecting samples lasting nearly an hour, and performing analysis during the subsequent hour. One system incorporated two sampling traps used alternately, and collected a sample for nearly an entire hour, then desorbed and analyzed that sample during the subsequent hour while collecting a sample using the second sampling trap.
 - Time-stamp assignment - The method by which systems assigned timestamps to data files also varied significantly among the different systems, with timestamps assigned corresponding to the beginning or the end of the sampling cycle, or to the beginning or the end of the analysis cycle. It was necessary to carefully study the operation cycle of each system and the timestamps assigned to its output files, as well as consult with the vendors, to ensure that the outputs from each system were processed correctly to align the data in the combined database with the hours in which standard VOC concentrations were being delivered to the systems.

Data from the auto-GC systems were collected remotely. All of the systems were accessible via the internet using a remote access program. This access allowed for regular collection and review of data, and remote troubleshooting. Remote data collection was relatively easy for all systems, with a few system-specific exceptions, described in Section 6.7 of this report. During the portion of the study when continuous ambient sampling was performed (the first, aborted 45-day session), data were collected on a daily basis. During the latter portion of the study when only targeted sampling was performed (the second 45-day session on which the statistical analysis is based), data were collected on an as-needed basis, generally shortly after the completion of each verification, precision, and MDL check.

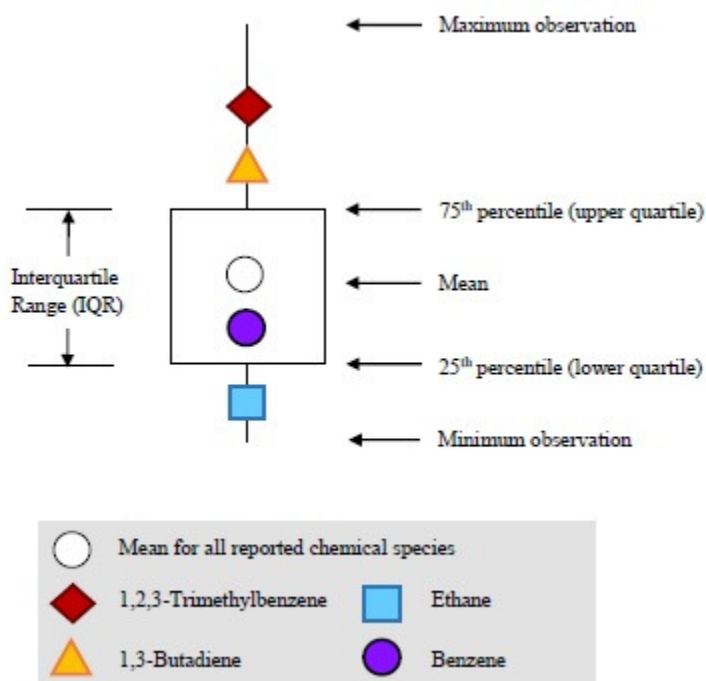
The data manipulation required to convert the individual system output files into a common database format was automated, and a system of programs was developed to allow relatively rapid processing of data after it was collected. Collection of a day's worth of data from all the systems, and transposition into the common database typically took over an hour. An additional program was developed to convert the common database format into

a crosstab file for import into the EPA's Data Analysis Reporting Tool (DART)¹ for visualization and graphical analysis.

¹ <http://www.airnowtech.org/>

6.0 Quantitative and Qualitative Results

Statistical analyses for the field deployment evaluation addressed the target compounds listed above in Table 2. To facilitate visual comparisons between vendors, distributions for the various statistical metrics are presented as box and whisker plots. A key to the features of these plots is provided below.



As shown above, these plots include the values for ethane, 1,3-butadiene, benzene, and 1,2,3-trimethylbenzene in addition to the statistics across all the compounds. Five of the six candidate auto-GC systems contain separate chromatographic columns to separate the lighter compounds (generally containing one to five carbon atoms) and heavier compounds (generally containing six or more carbon atoms). The values for these compounds have been included in the plots as example lighter (ethane and 1,3-butadiene) and heavier (benzene and 1,2,3-trimethylbenzene) compounds.

As an additional aid for visualization, the values of the various statistical metrics for the vendors are also presented by target compound. These plots are presented on a linear scale and, where useful, on a logarithmic scale to allow for greater resolution at different levels. These plots provide graphic information about the extremes for each vendor (the whiskers in the box and whisker plots), as well as showing whether there are trends across vendors for particular target compounds.

It should be noted that beginning with the second precision check, vendors generally were allowed to adjust their auto-GC systems after each precision check if their measured concentration for any compound was greater than ± 20 percent different from the target concentration, and also prior to and after the MDL setup run. Thus, the statistical analyses presented in Sections 6.1 through 6.6 do not reflect unattended operation over the course of the field deployment evaluation period, although the system adjustments made during the period varied by vendor. The occasions when the vendors took advantage of the opportunities to adjust the systems are discussed below in Section 6.8.

In addition, as noted previously, the cylinder of TCEQ blend was changed out between the second and third precision checks. To account for this change, the measured concentrations for each compound prior to the cylinder change were adjusted to be on a comparable basis with those measured after the change as follows:

$$Conc_{adj} = Conc \times \frac{Cylinder\ conc_{new}}{Cylinder\ conc_{old}}$$

The adjusted values were used with the concentrations measured after the TCEQ cylinder change for the statistical analyses presented in Section 6.1 through 6.6.

The data generally were used for the analyses as collected, with limited corrections or validation. Thus, some outliers may skew the analyses for some auto-GC system/target compound combinations.

6.1 Precision (Agreement between Replicate Measurements of the Same Sample)

For each vendor, precision was computed in terms of percent relative standard deviation (%RSD) for each target compound using the data reported for each of the 2 hours of the 3-ppb benzene standard point during the pre-verification check (corrected data), the six precision checks, the uncorrected post-verification check, and the setup run for the MDL check, according to the following formula:

$$\%RSD = \sqrt{\left[\frac{\sum (Meas - meas_i)^2}{N - 1} \right] \times \frac{100}{Meas}}$$

Only hours with reported measured values were included in this calculation. That is, hours when an auto-GC system did not detect a compound are not included, although such hours are used in the completeness calculations reported in Section 6.5 below.

The %RSD results for each vendor across all the target compounds are summarized in a box and whisker plot below in Figure 2. Figures 3 and 4 present the %RSD results for each target compound across vendors on linear and logarithmic scales, respectively. The results for each vendor for each compound are presented in tabular form in Appendix A-1.

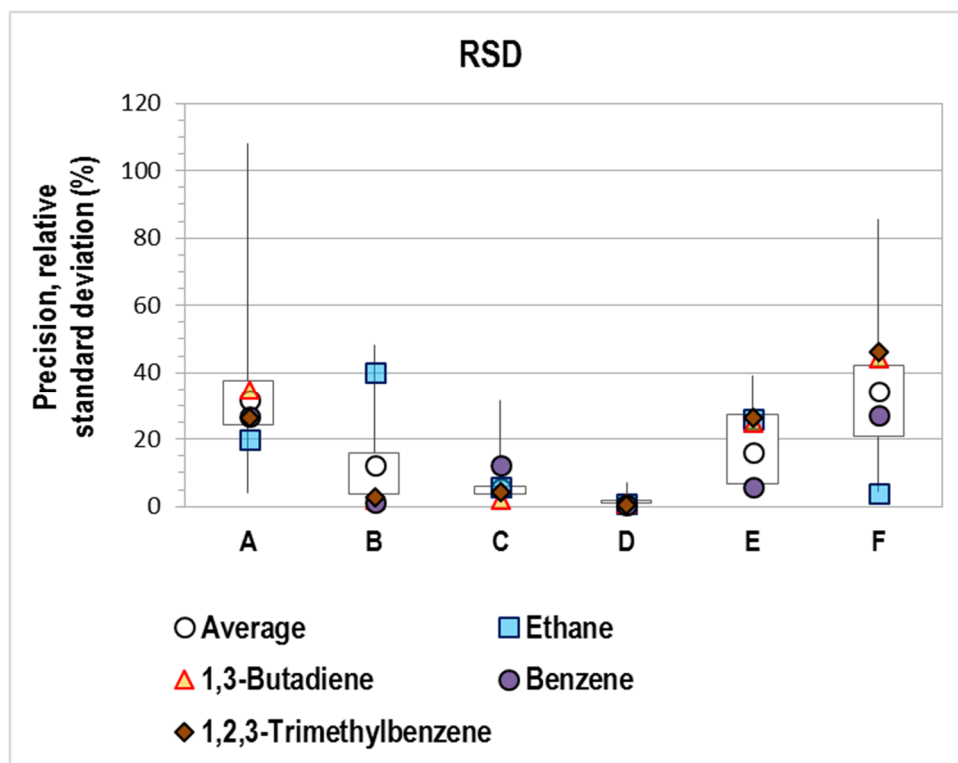


Figure 2. Distribution of %RSD by Vendor across All Target Compounds

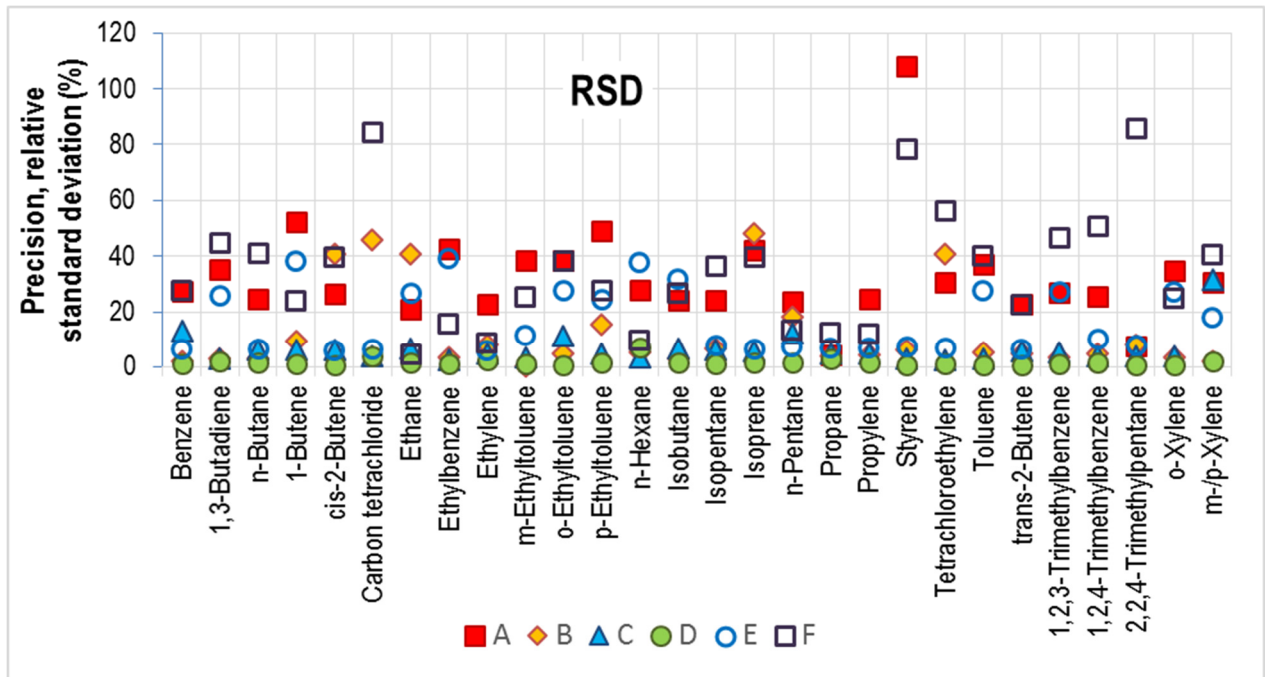


Figure 3. %RSD by Target Compound across Vendors

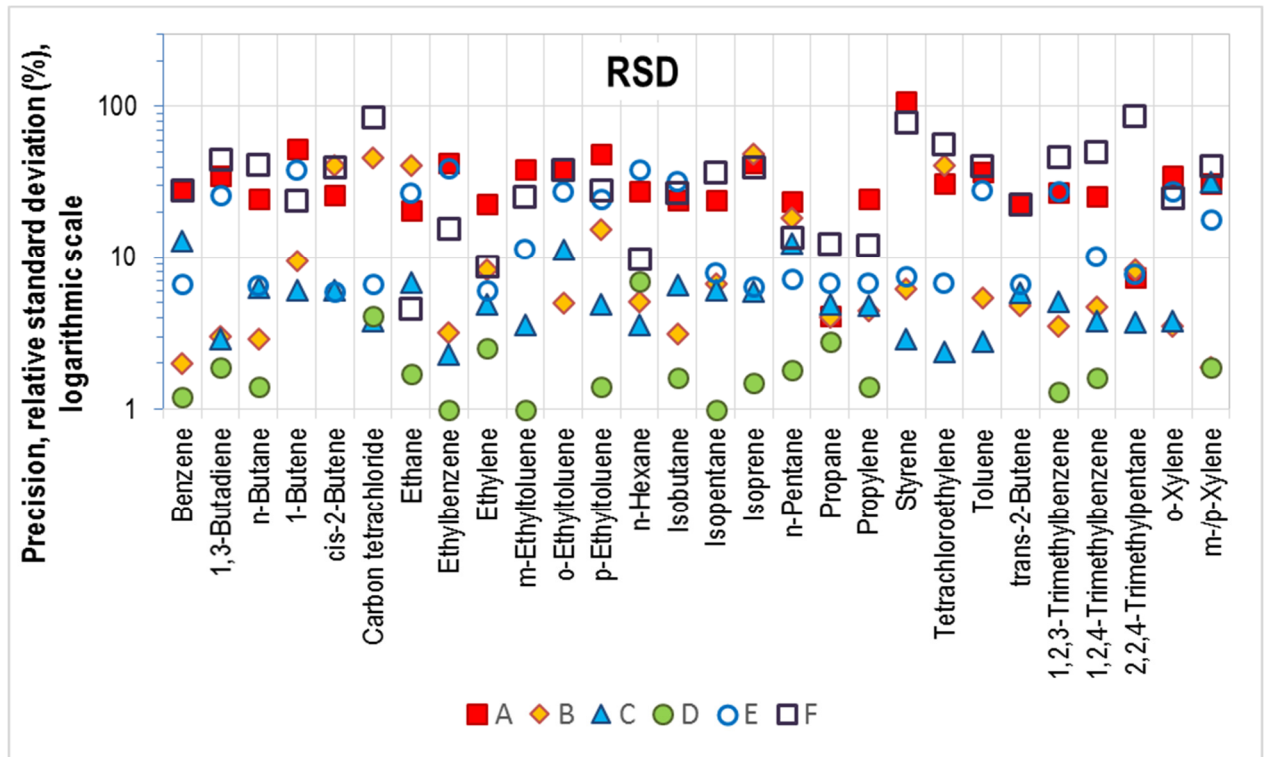


Figure 4. %RSD by Target Compound across Vendors, Logarithmic Scale

6.2 Bias (Quantitative Difference between Instrumental Measurement and Target Value)

For each vendor, normalized bias was computed for each compound using the data reported for each of the 2 hours of the 3-ppb benzene standard point during the pre-verification check (corrected data), the six precision checks, the uncorrected post-verification check, and the setup run for the MDL check, according to the following equation:

$$\text{Bias} = \sqrt{\frac{(\text{Vendor meas.} - \text{Challenge conc.})}{\text{Challenge conc.}}}$$

Thus, bias is defined in this section as the calculated difference between observed value and delivered concentration, normalized relative to the delivered concentration. Again, only hours with reported measured values were included in the calculation, although hours when an auto-GC system did not detect a compound are included in the completeness calculations reported in Section 6.5 below.

For each vendor, the mean normalized bias (MNB) was calculated for each compound, in terms of percent. In each case, the mean was calculated both signed and unsigned (i.e., using absolute values). The results for each vendor across all the compounds are summarized in box and whisker plots below in Figures 5 and 6 for signed and unsigned MNB, respectively. Figure 7 and 8 present the signed and unsigned MNB results, respectively, for each target compound across vendors on a linear scale; Figure 9 shows the unsigned MNB results on a logarithmic scale (zero and negative results cannot be displayed on a logarithmic scale). The results for each vendor for each compound are presented in tabular form in Appendix A-2.

In general, unsigned bias is a better representation of overall performance because a large positive value for one compound cannot be cancelled out by an equally large negative value for another. Figure 5 shows the tendency of bias to be positive or negative but can be slightly misleading in that positive biases can be nullified by negative biases. Figure 6 shows the magnitude of this metric without consideration of whether it is positive or negative.

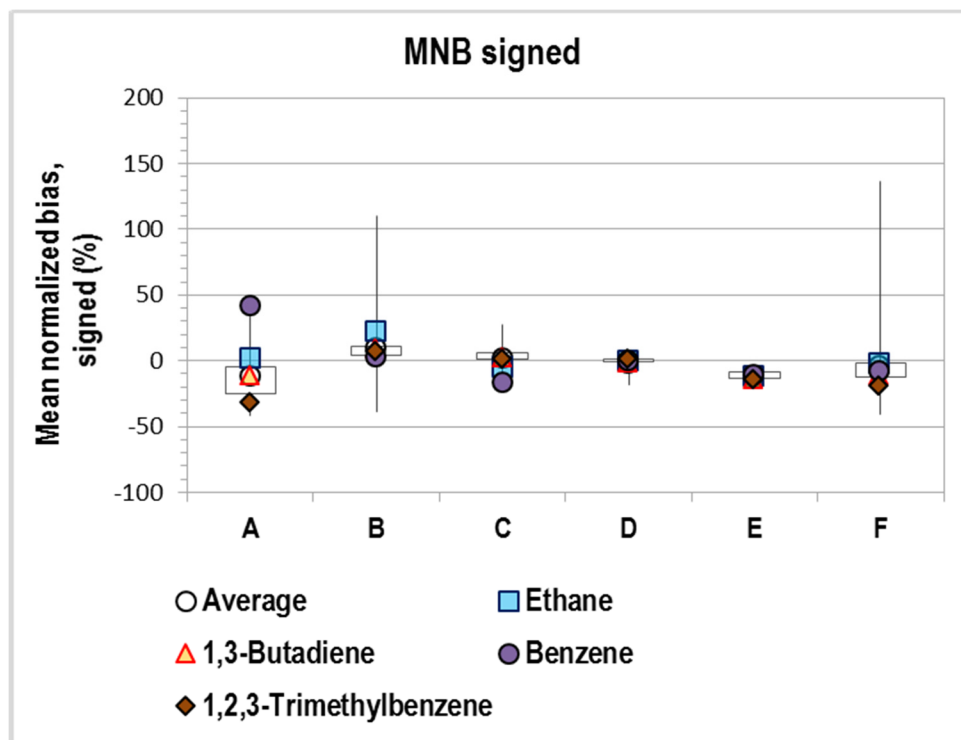


Figure 5. Distribution of Signed MNB by Vendor across All Target Compounds

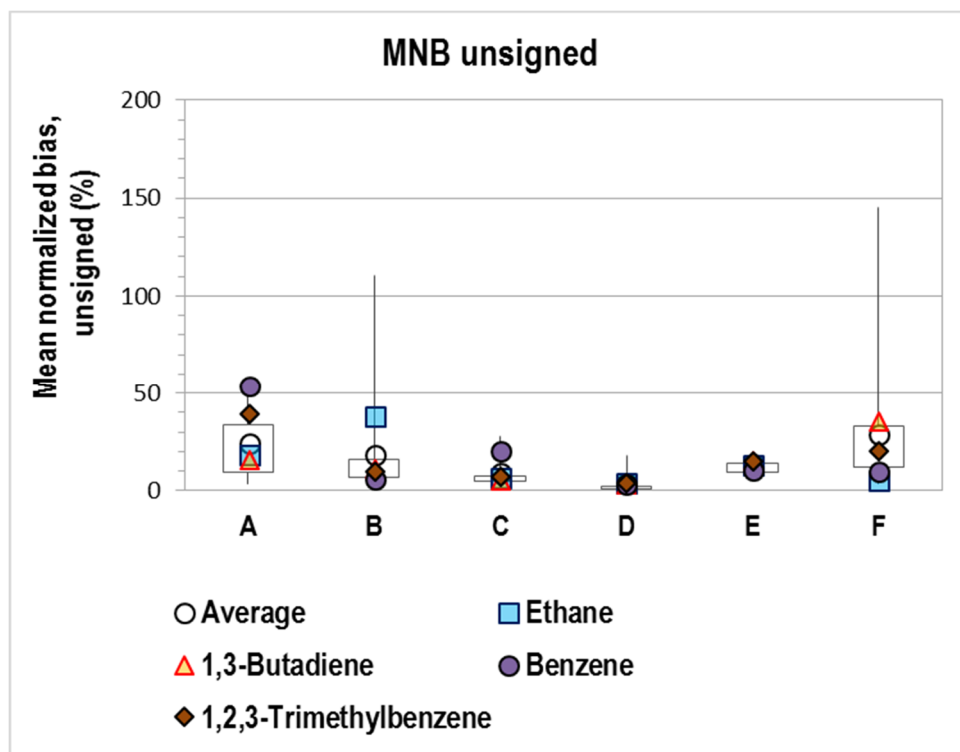


Figure 6. Distribution of Unsigned MNB by Vendor across All Target Compounds

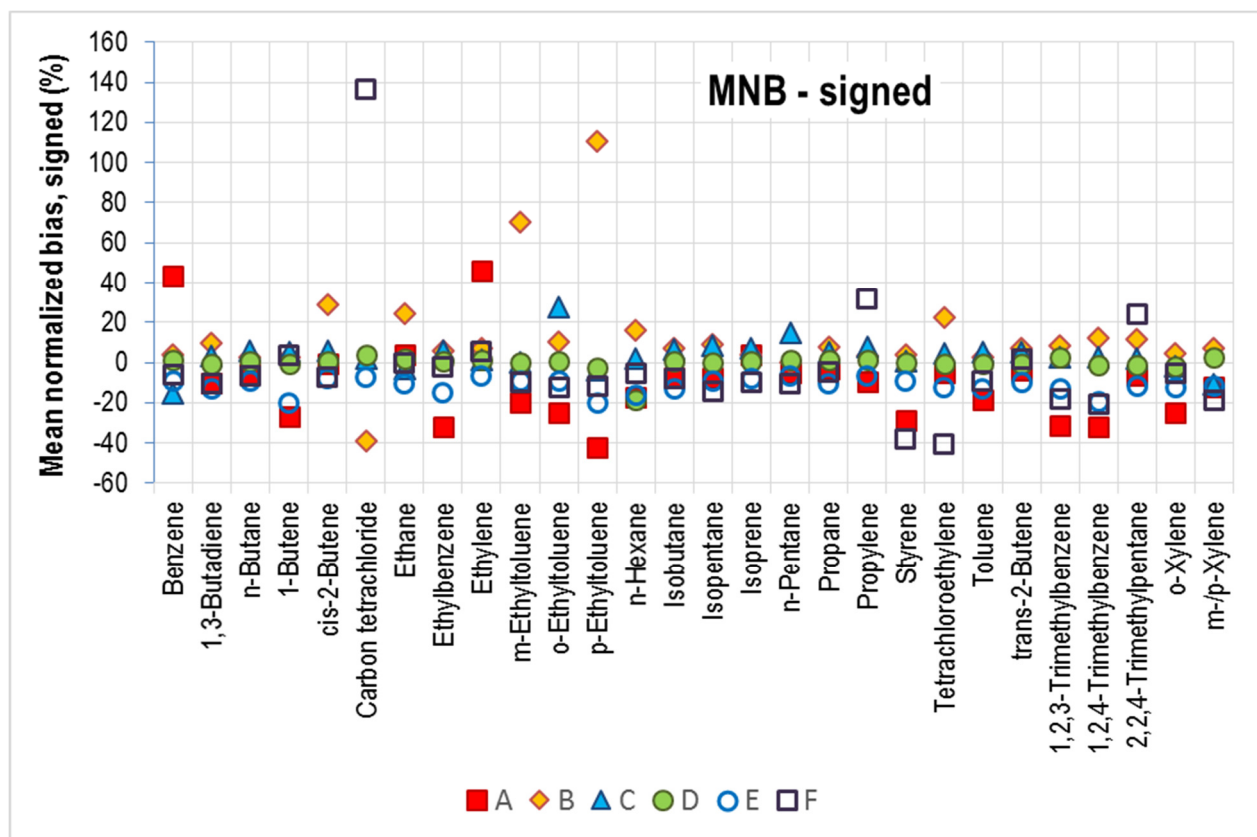


Figure 7. Signed MNB by Target Compound across Vendors

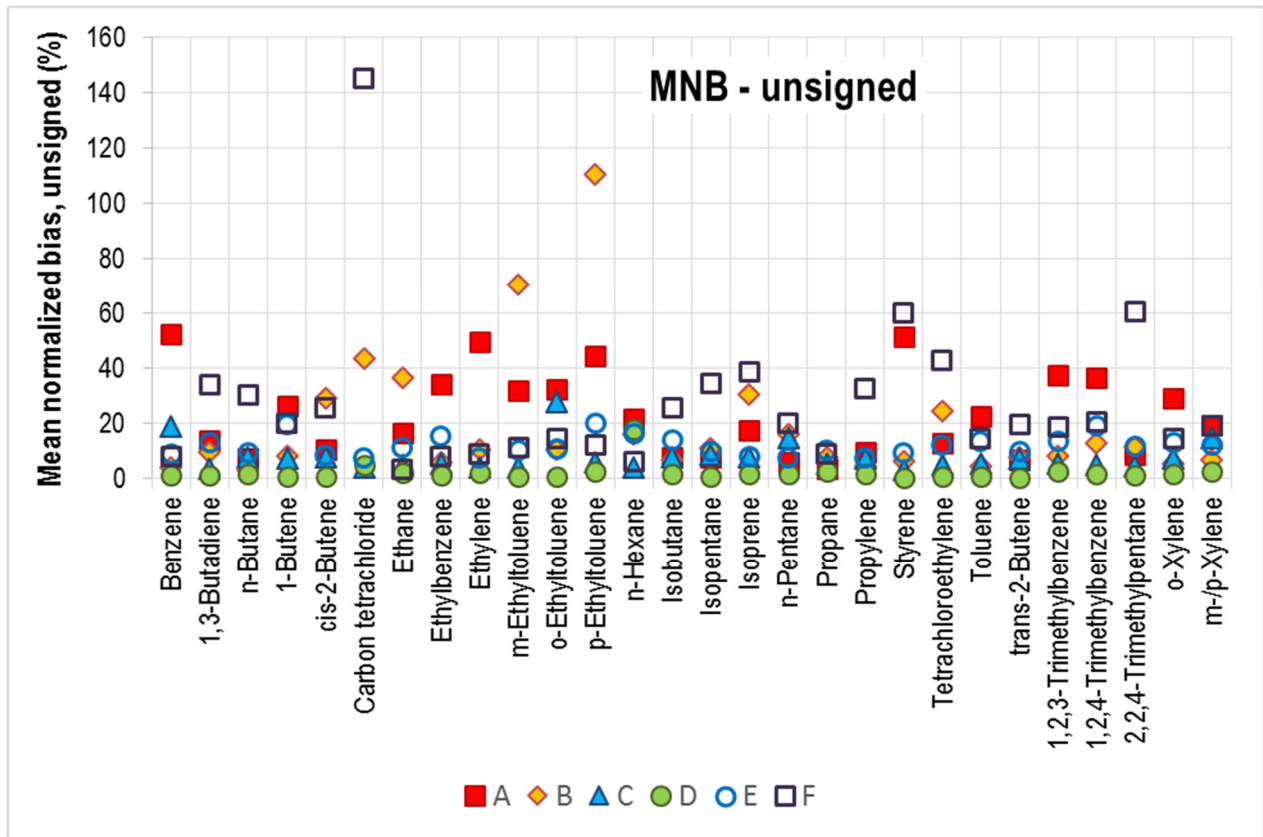


Figure 8. Unsigned MNB by Target Compound across Vendors

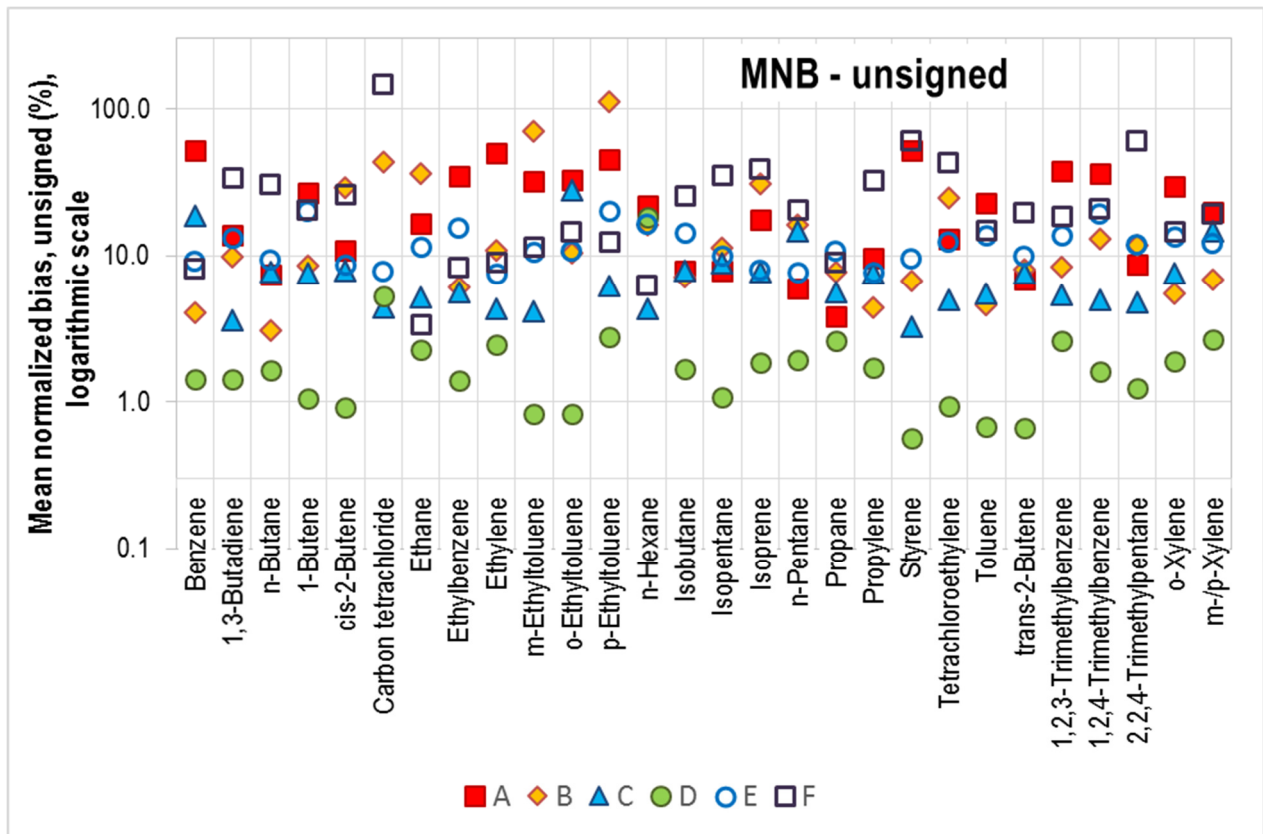


Figure 9. Unsigned MNB by Target Compound across Vendors, Logarithmic Scale

6.3 Drift (Variation in Bias over Time)

Drift is a metric reflecting the tendency of the measured value for a target compound to change systematically over time. For each vendor, drift was computed for each compound using the signed normalized bias determined for each of the 2 hours of the 3-ppb benzene standard point during the pre-verification check (corrected data), the six precision checks, the uncorrected post-verification check, and the setup run for the MDL check.

A linear regression analysis was performed on the data points, and the drift is the slope of the regression line, reported as the percent change in normalized bias per day. The closer to zero an auto-GC system's drift is for a particular target compound, the less overall drift that system exhibited for that compound. Positive values of drift indicate that the normalized bias tended to increase over time, and the larger the value, the greater the increase. Negative values indicate that the normalized bias tended to decrease over time, and the more negative the value, the greater the decrease. Drift was not computed for a compound when an auto-GC system recorded insufficient data for a linear regression, specifically for carbon tetrachloride where Vendor A had no measurements and for m-ethyltoluene. Vendor B recorded only one measurement in one instance. This is because the sum of m-ethyltoluene and p-ethyltoluene usually was reported as p-ethyltoluene. This comment applies to all tables in the appendices.

A linear regression analysis fits the best possible line to the data points, regardless of how consistent or scattered the points are. To assess the "goodness of fit," the analysis also computes the "correlation coefficient" (typically represented as "r") and the "coefficient of determination" (the square of the correlation coefficient, typically represented as "r²") for the regression line for each compound. These parameters are measures of the strength of the correlation between the dependent and independent variables in the regression analysis, in this case normalized bias and time, respectively. The value of r² can vary between 0 and 1, where 0 represents no correlation and 1 represents a perfect correlation (i.e., all data points fall precisely on the regression line). The value of r² can be thought of the fraction of the variation in the dependent variable (normalized bias) that is attributable to the variation in the independent variable (time); that is, in this case, how much of the calculated drift for a compound is systematic change associated with the passage of time versus variation due to other factors.

The drift results for each vendor across all the compounds are summarized in a box and whisker plot below in Figure 10. Figure 11 presents the results for each target compound across vendors on a linear scale. Figure 12 shows the absolute value of drift on a logarithmic scale; absolute value was used for this plot because zero and negative results cannot be displayed on a logarithmic scale. The results for each vendor for each compound are presented in tabular form in Appendix A-3, which also includes the correlation coefficient and coefficient of determination computed for each target compound. For all of the vendors, the values of r and r² were quite small for many of the target compounds, indicating that there was little systematic drift for those compounds.

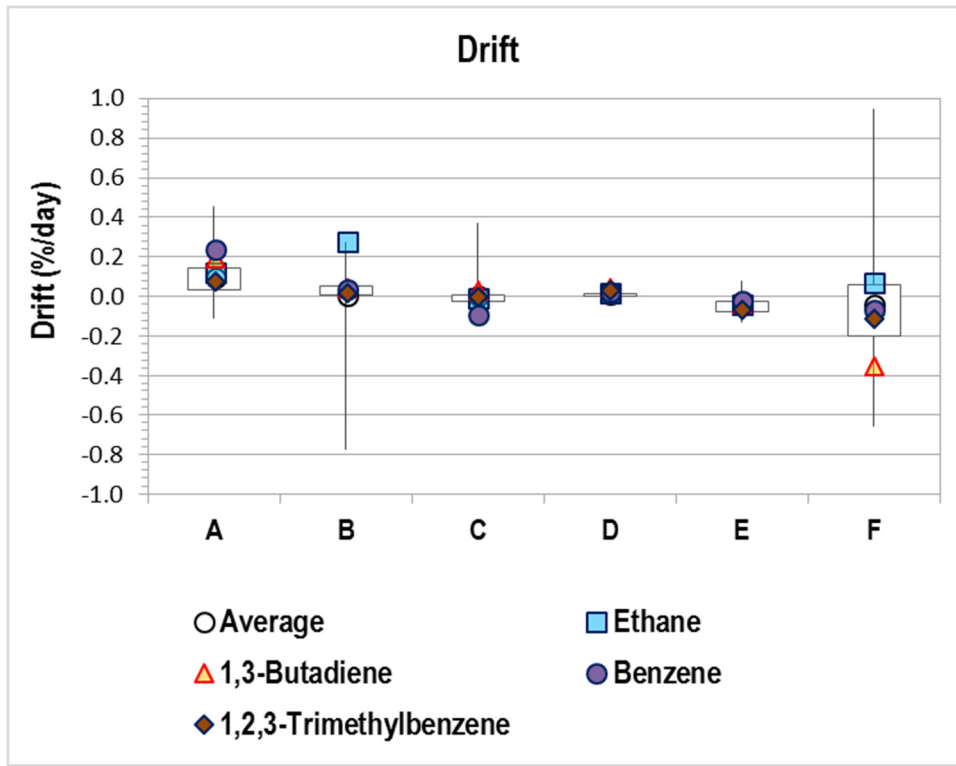


Figure 10. Distribution of Drift by Vendor across All Target Compounds

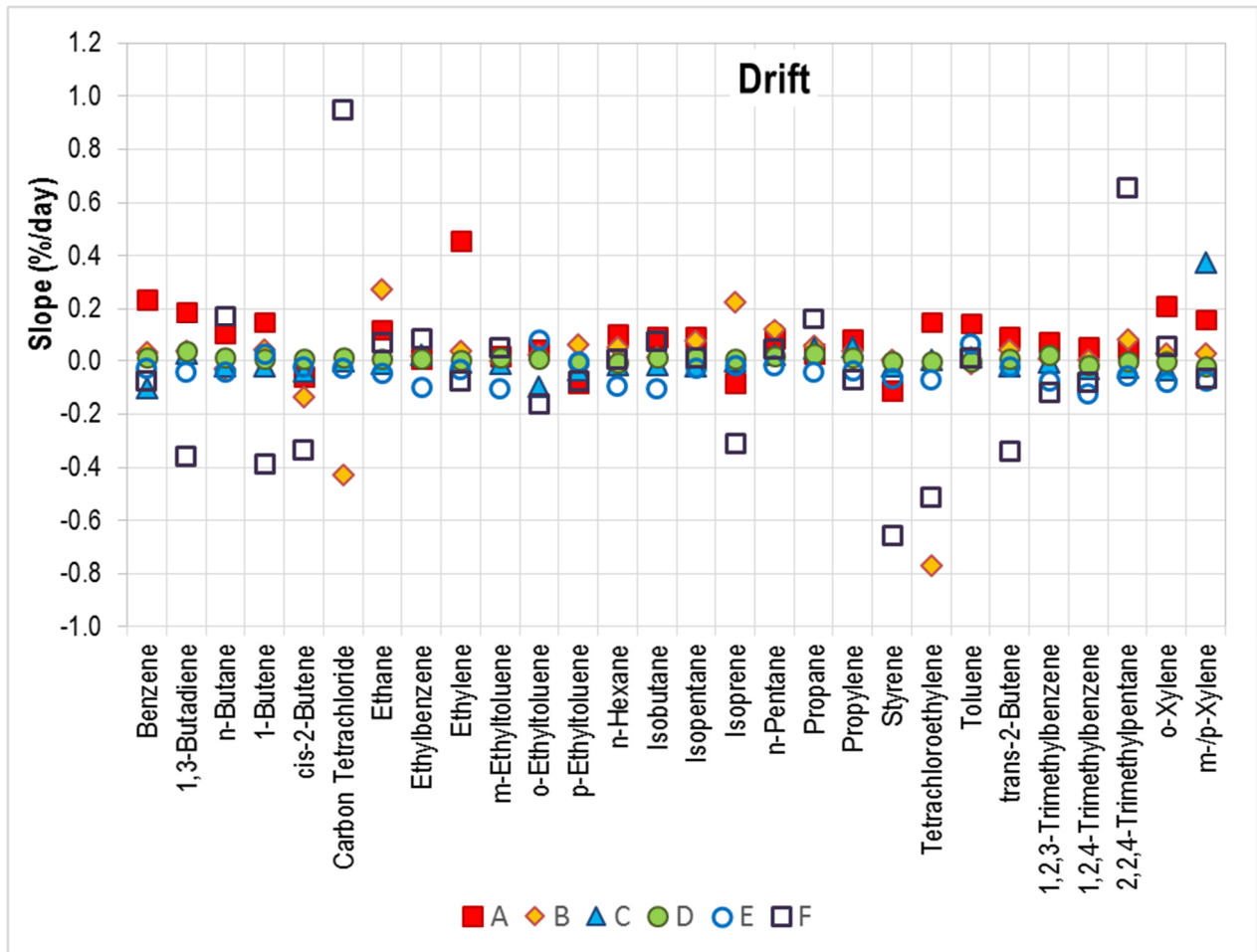


Figure 11. Drift by Target Compound across Vendors

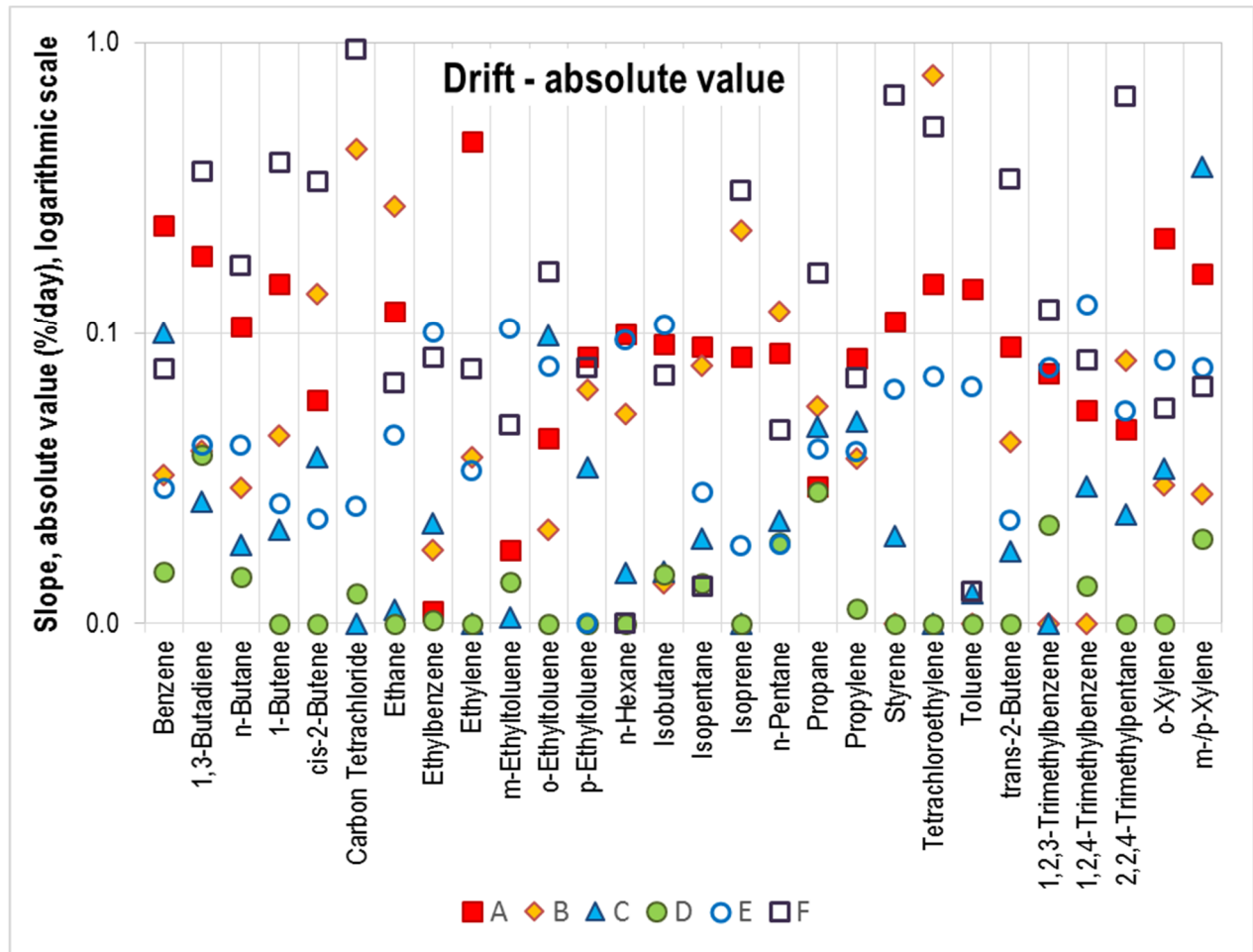


Figure 12. Absolute Value of Drift by Target Compound across Vendors, Logarithmic Scale

6.4 Linearity of System Measurements across Verification Check Standards

Linearity is a measure of how consistently the auto-GC systems responded over the range of the standard calibration points delivered to them during the pre- and post-verification tests that bracketed the 45-day session. For each vendor, linearity was computed for each compound using the values measured for each of the 2 hours at the 3-, 6-, 9-, and 12-ppb benzene standard points during the pre-verification check (corrected data), the values measured during the post-verification check (uncorrected data), and the combined data from both verification checks. The measured values were plotted against the target values for each compound, and a regression analysis was carried out. Linearity is reported as the slope of the regression line. Perfect linearity would result in a slope of exactly 1. Note that this would not imply perfect accuracy, only perfect linearity.

The linearity results for each vendor across all the compounds during the post-verification check (uncorrected) are summarized in a box and whisker plot below in Figure 13. Figure 14 presents the results for each target compound across vendors during the post-verification check (uncorrected). The results for each vendor for each compound for the pre-verification check, the post-verification check, and the combined data are presented in tabular form in Appendix A-4, which also includes the correlation coefficient and coefficient of determination computed for each target compound. Appendix A-4 also includes the intercept of the regression line for each compound, which would ideally be zero or very close to it.

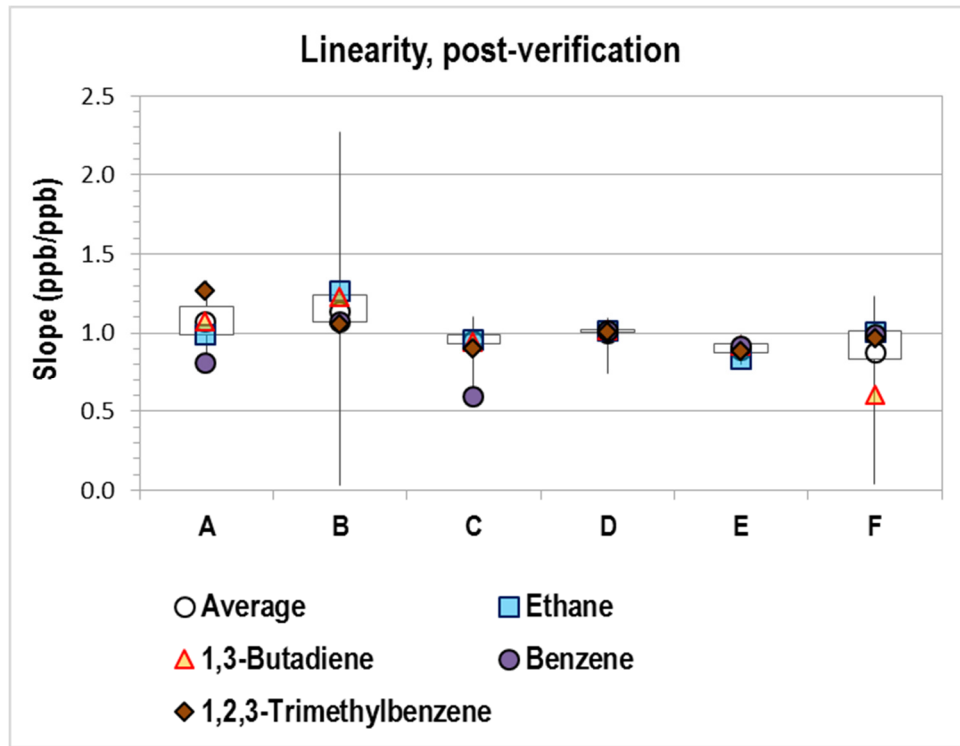


Figure 13. Distribution of Linearity by Vendor across All Target Compounds

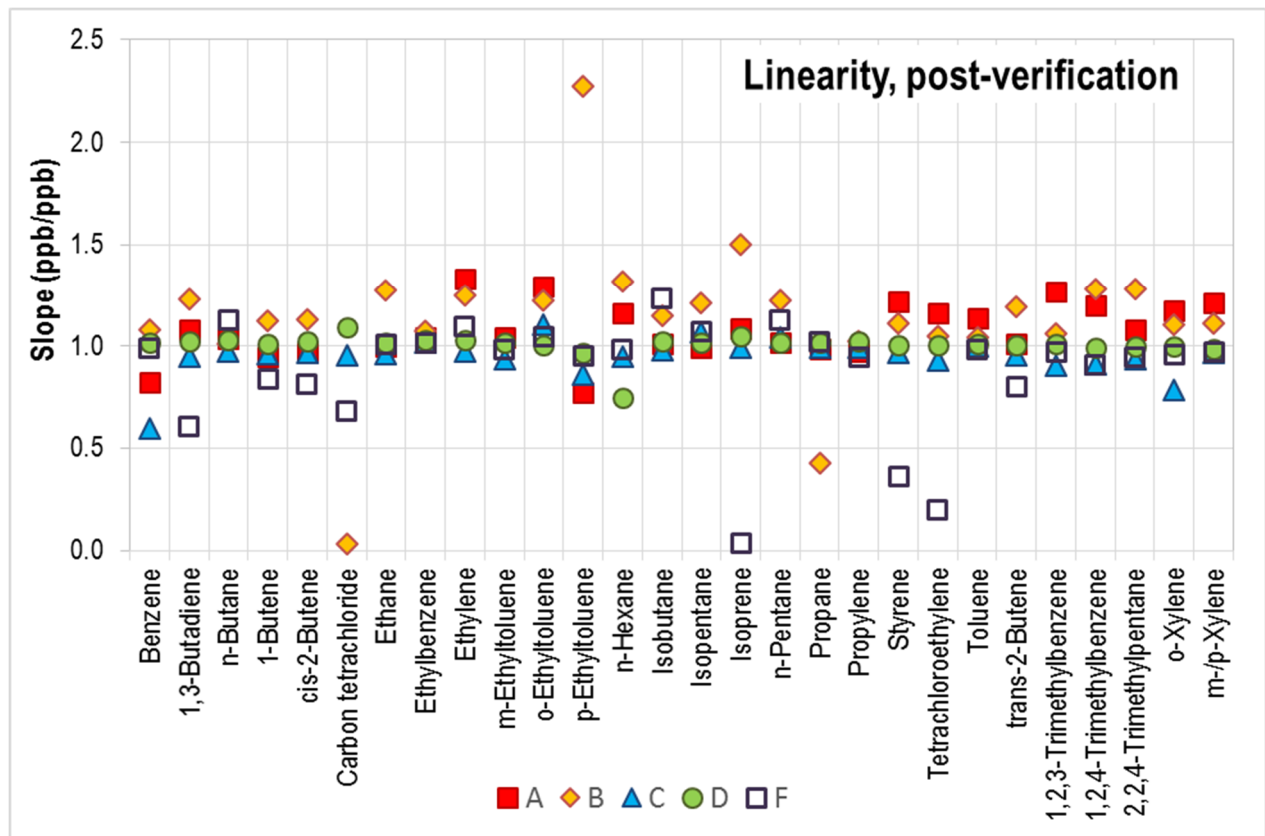


Figure 14. Linearity by Target Compound across Vendors

6.5 Completeness (Percent of All Target Compounds Reported across All Tests)

Completeness was computed as the percent of all target compounds reported across each hour at each concentration during the pre-verification check (corrected data), the six precision checks, the uncorrected post-verification check, and the setup run for the MDL check. The completeness results for each vendor across all the compounds are summarized in a box and whisker plot below in Figure 15. The results for each vendor for each compound are presented in tabular form in Appendix A-5. In Figure 15, Vendors A and B are seen to each have a very low minimum value, but in both cases there was only a single compound at such low levels. As can be seen in Appendix A-5, Vendor A's next lowest value was 79 percent and Vendor B's was 83 percent.

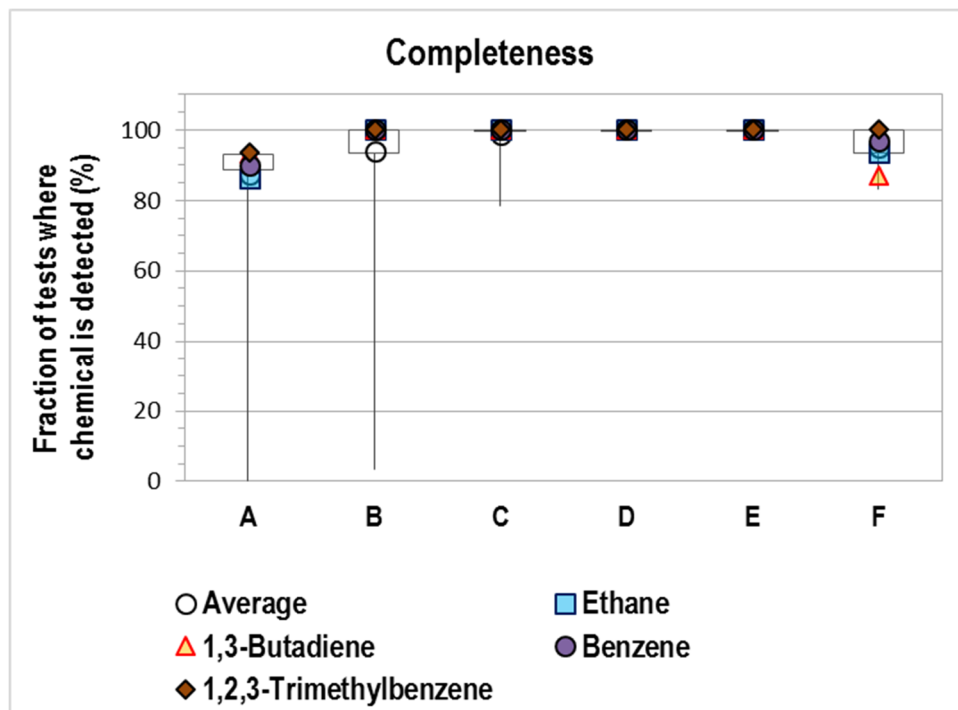


Figure 15. Distribution of Completeness by Vendor across All Target Compounds

6.6 Method Detection Limit (Determination of the Lowest Measurement that Can Be Distinguished from Zero)

The method detection limit (MDL) is defined as the lowest sample concentration that can be statistically distinguished from zero. Since larger sample collections result in greater analyte quantities delivered to the chromatographic column and detector, the MDL is highly dependent on the overall analytical method and not just the instrumental detector sensitivity. MDL is also highly dependent on the analytical precision.

For this study, MDLs were determined for each auto-GC system and target compound based on the procedure and calculations found in 40 CFR Part 136, Appendix B. In that procedure, the first step is to estimate the MDL, so that the procedure can be carried out with samples near that level. Because the field deployment phase involved 6 auto-GC systems each measuring 28 target compounds, and the actual instrumental limits of detection differ among auto-GC systems and target compounds, it was beyond the scope of this project to estimate the MDL for each system/compound combination and test them individually. Instead, a common challenge concentration was used for all auto-GC systems and target compounds.

The challenge concentration used for this determination was a 0.5-ppb benzene standard (the concentrations for the other compounds varied based on their perspective concentration in the standard gas, ranging from approximately 0.5 ppb to 1 ppb). Two MDL checks lasting 15 hours each at this concentration were conducted: (1) between the pre-verification check and the start of the 45-day session, and (2) as the final measurement of

the field deployment, after the post-verification check and the setup run for this MDL check. MDLs were determined for each auto-GC system and each target compound, for each of the two MDL checks. The two MDL estimates for each compound were averaged to give the final MDL estimate provided in Figures 16 to 21.

MDLs were computed for each target compound according to the expression:

where:

$$MDL = \sqrt{(t_{n-1, 1-\alpha=0.99}) \cdot s}$$

$t_{(n-1, 1-\alpha=0.99)}$ = the student's t statistic at the 99% confidence interval for n replicate measurements (n-1 degrees of freedom).

s = standard deviation of the multiple replicate measurements.

Thus, an MDL determined using this methodology is basically a measure of precision at the challenge concentration. In general, lower values of the MDL reflect better instrument performance and, hence, improved analyte detectability.

It should be noted, however, that an exception to this generality is the case where an instrument does not detect a compound and reports zeroes for every measurement. Because the standard deviation in such a case would be zero, the calculated MDL would likewise be zero. Similarly, a situation where most reported measurements are zeroes would likely have a deceptively low calculated MDL.

For this analysis, when an auto-GC system's dataset for a particular compound contained measured, non-zero values for 6 or more of the hours of the test, the MDL was calculated for that compound. Any zero or non-detect hours were not included in the MDL estimate. Conversely, when an auto-GC system's dataset for a particular compound contained less than 6 hours of non-zero or detected values, the MDL was not calculated. Instead, this is considered a non-detect for that compound.

The MDL results for each vendor across all the compounds based on the combination of both MDL checks are summarized in a box and whisker plot below in Figure 16. Figure 17 presents the results for each target compound across vendors for the averaged MDL checks on a linear scale, and Figure 18 shows the same MDL data on a logarithmic scale. The values in Figures 16, 17, and 18 are all on an "as compound" basis. Figures 19, 20, and 21 provide the same information on an "as carbon" basis, which was determined by multiplying the values "as compound" by the number of carbon atoms in each compound. Appendix A-6 presents results, in tabular form, for each vendor for each compound from the first and second MDL checks as well as the average MDL from both checks.

Additional notes on the data used in the MDL analysis:

- After the first MDL check, Vendor E explained that the system can detect all compounds at the MDL level but the integration parameters were set to the calibration range 3-12 ppb without the opportunity of seeing the integration results of an MDL standard. Because of this, the vendor asked to be allowed to integrate the peaks that were not identified in the MDL runs so that the analysis results would provide MDL's that reflect the capabilities of the system. The WAM permitted Vendor E to provide corrected data for the first MDL check, and all vendors were given the opportunity to do likewise. Vendor B also provided revised data for the first MDL check.
- Vendor A's auto-GC system developed problems prior to the second MDL check and registered non-detects for over half of the target compounds. Because these results are not considered indicative of the normal operation of the system, the data for these compounds from the second MDL check were not included in the analysis of the combined data from the two MDL checks.

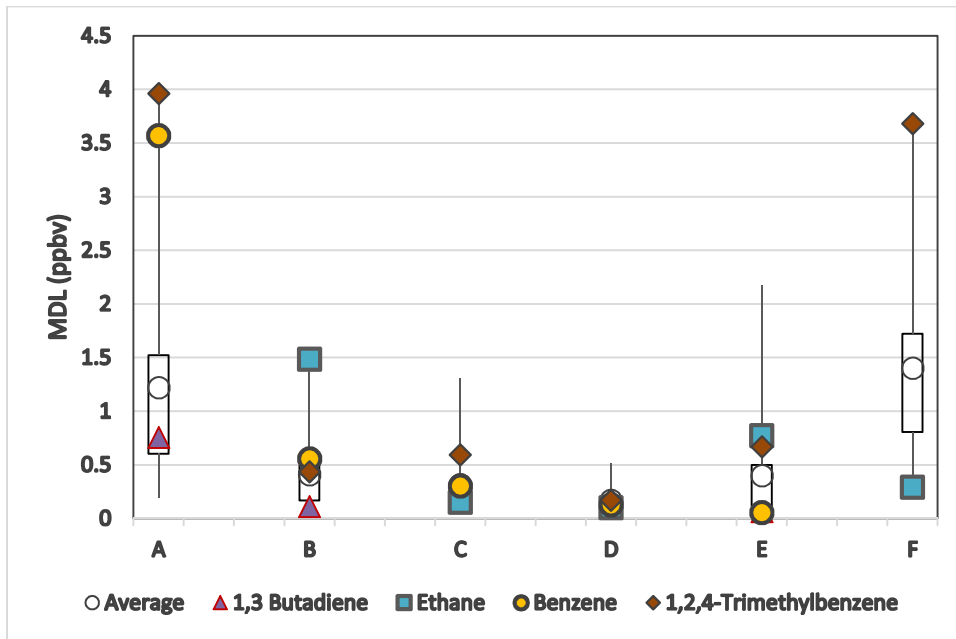


Figure 16. Distribution of MDL by Vendor across All Target Compounds, as Compound

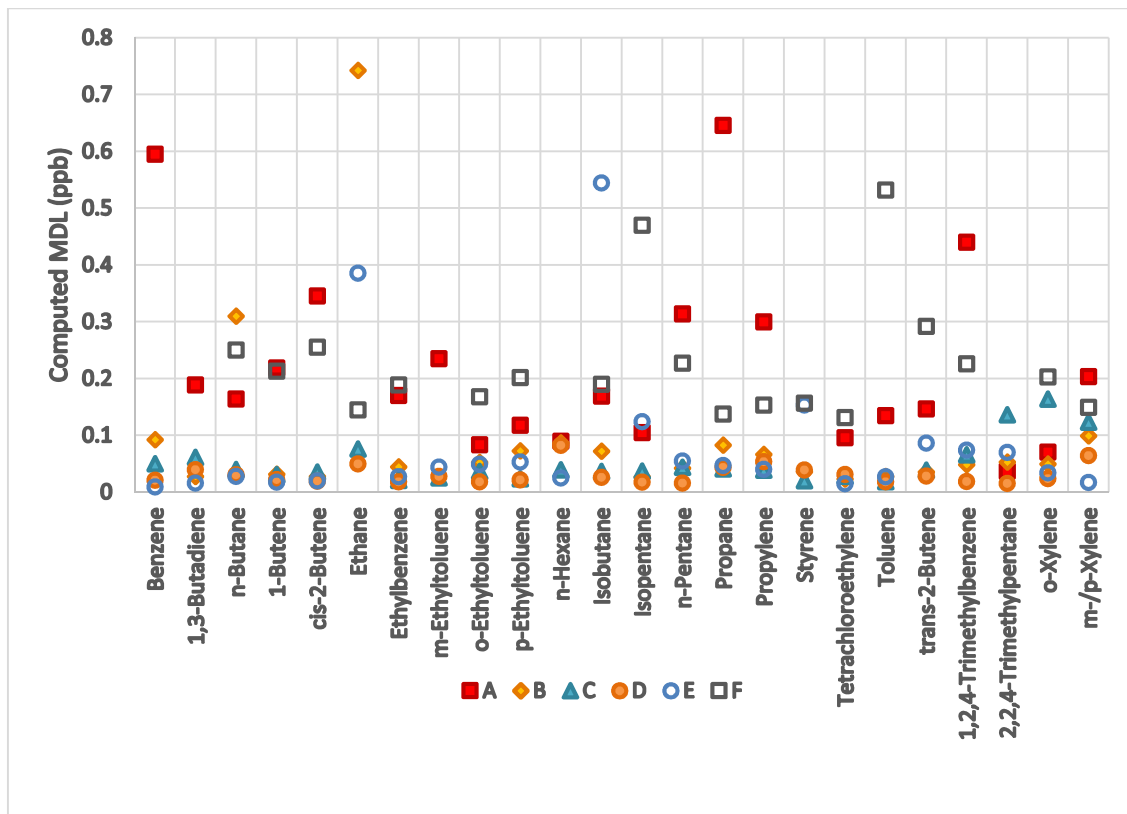


Figure 17. MDL by Target Compound across Vendors as Compound

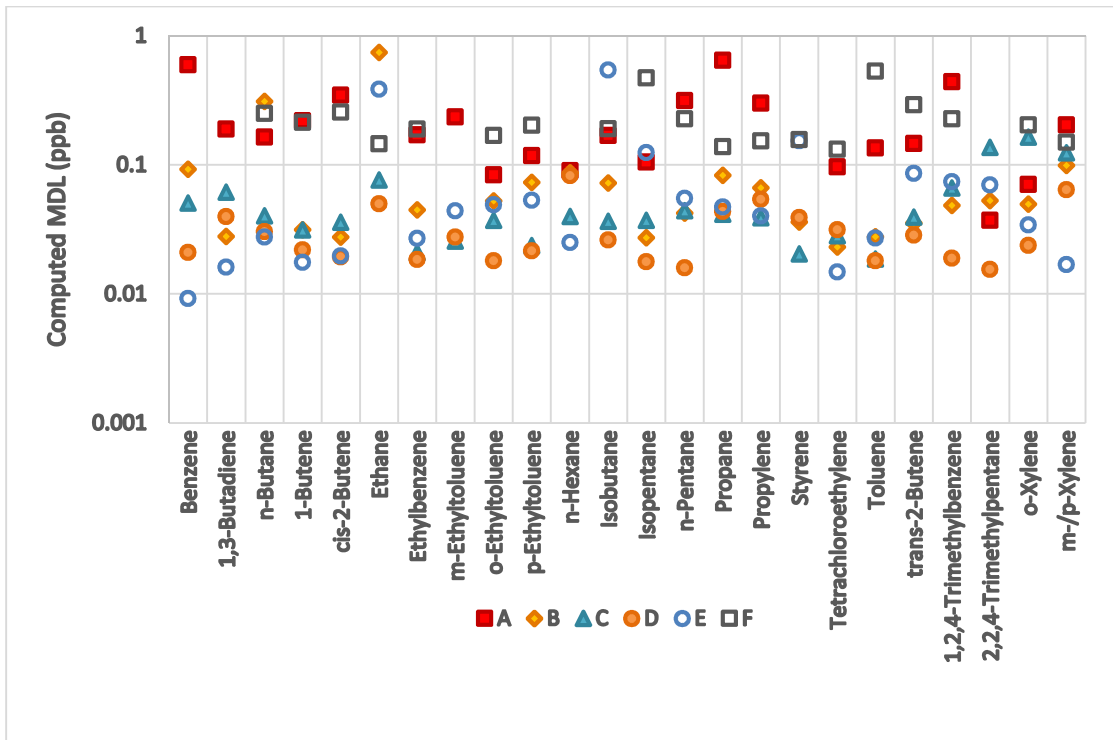


Figure 18. MDL by Target Compound across Vendors as Compound, Logarithmic Scale

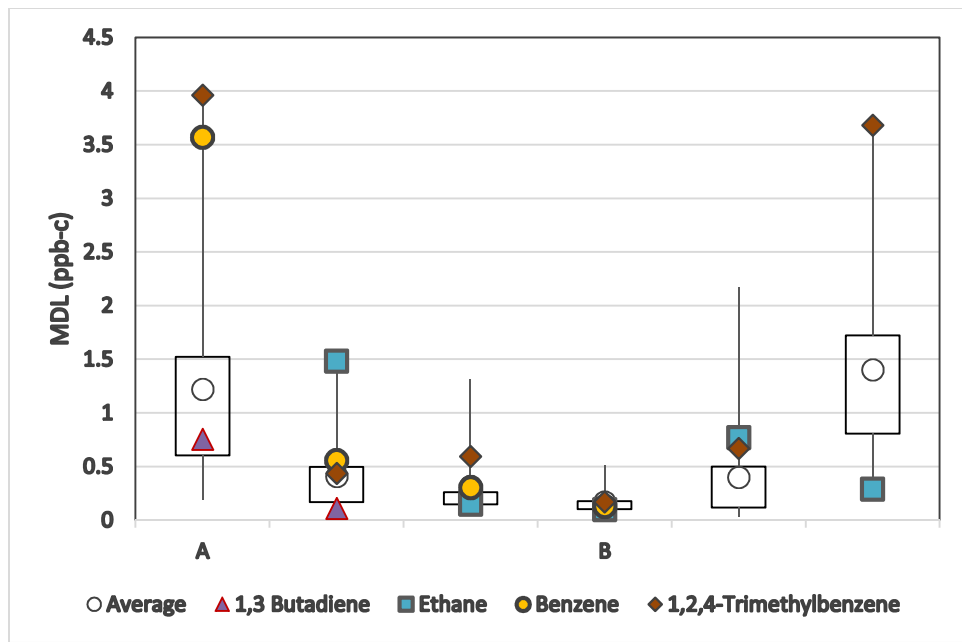


Figure 19. Distribution of MDL by Vendor across All Target Compounds, as Carbon

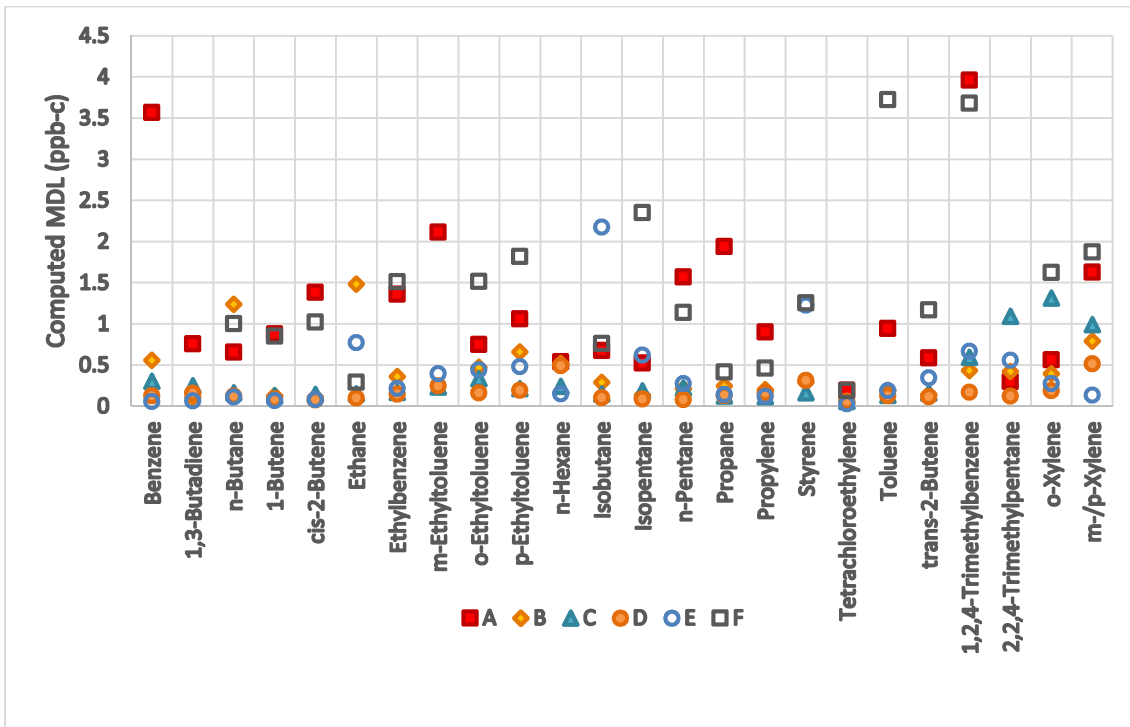


Figure 20. MDL by Target Compound across Vendors as Carbon

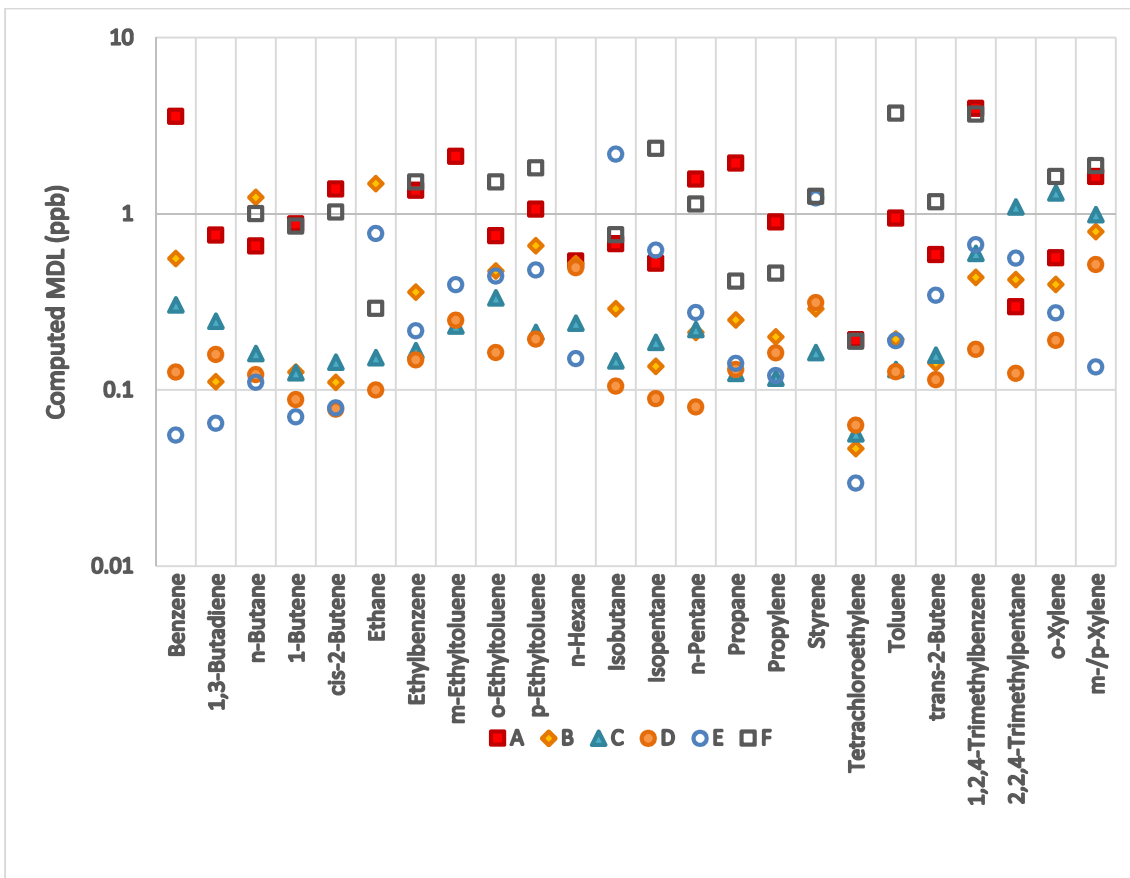


Figure 21. MDL by Target Compound across Vendors as Carbon, Logarithmic Scale

6.7 Intrinsic Data Processing Capabilities (Assessment of User Interface and Ease of File Export Procedures)

Information provided in this section is based on observations made by project team during the shakedown period, during which continuous ambient monitoring data were collected on a daily basis, and the 45-day session. Although the data collected during the early portion of the field study were not included in statistical analyses, the process of data generation and collection occurred regularly during this time and has been considered in this qualitative analysis of system operation and functionality.

The observations regarding each auto-GC system follow.

Vendor A

This system produced hourly data, as ASCII files. The files contained much of the information in the requested common format, but the format was quite different. Significant manipulation was necessary to convert the data into the common format, largely because the timestamp associated with the data was contained in the filename, rather than within the content of the file itself. The files were generated by the system hourly, as each analysis was completed.

This system uses an external laptop PC to collect data and communicate with the embedded computers operating the GC systems. Early in the study, recurring system problems were resulting at least partially from communication issues between these computers. This resulted in occasional data loss and need for user intervention. Eventually, the problems were solved by replacing the USB hub and RS-232-to-USB connectors used to connect the laptop PC and the GC systems. In some cases, it was possible to recover the lost data by re-exporting it from the system.

Vendor B

This system operated on a shorter cycle, performing two analyses each hour, and produced two monthly files (one for each GC.) The files were in ASCII format, and required manipulation to convert the data into the common format, primarily transposing rows and columns and combining the files for the two GCs. The files were updated by the system twice hourly, as each analysis was completed.

The data is stored in a format that can be copied and pasted into MS Excel as tab- or comma-delimited CSV file, and can be reconfigured with a column to row transposition. The system also allows for direct data retrieval through standard serial ports via Modbus communication protocol, as most commonly used at ambient air monitoring stations deployed by the USEPA and local agencies.

Vendor C

This system produced hourly files, in ASCII format, and required considerable manipulation to convert the data into the common format, primarily due to formatting issues. The output files were not automatically generated by the system. Significant and tedious user interaction was necessary to produce machine-readable output files, requiring the user to manually generate each hourly file.

It is also worth noting that while this system operates continuously, it does require a programmed GC sequence, which has a maximum of 999 lines (about 40 days, assuming one line per hour, and continuous 24 hour sampling.) A new sampling sequence may be created remotely, but user intervention is necessary.

Vendor D

This system produced hourly data, as MS excel files in a format very similar to the requested common format. The files were generated by the system hourly, as each analysis was completed.

This system experienced occasional issues with failure to write data to the data output folder. In all instances but one, the data could be recovered by regeneration of the output files from raw system files. This issue was determined to be a result of an over-full data export folder.

Vendor E

This system produced hourly data, as MS excel files in a format similar to the requested common format. The files were not automatically generated by the system without user interaction, but could be generated via a batch process for large blocks of time, as needed.

One issue worth noting for this system is that sampling and analysis occur via programmed batches, which can contain a maximum of 501 samples (about 20 days, assuming continuous 24 hour sampling.) Multiple batches may be queued to allow for longer periods of continuous sampling. When a new batch is created, if it does not include verification (calibration) standards, it must be linked to a batch with verification standards.

Vendor F

This system produced two monthly files (one for each GC), in ASCII format, and required significant manipulation to convert the data into the common format, primarily transposing rows and columns and combining the files for the two GCs. The files were updated by the system hourly, as each analysis was completed.

6.8 Unattended Operation (Assessment of Duration of Operation without Compromise in Data Integrity)

Information provided in this section is based on observations made by the project team during the 45-day session of the field deployment, and does not cover the shakedown period. As described previously, due to issues external to the operation of the individual auto-GC systems, the data collected during the shakedown period were not included in the statistical analyses performed for this study. Similarly, these issues affected the concentration of the measured samples delivered to the systems, and thus the necessity for system adjustments and calibrations.

Generally, it was observed that all of the candidates were able to successfully record data over a period of unattended operation. However, some systems required more frequent intervention than others to maintain proper calibration, and some systems had regular problems with specific pollutants.

During the 45-day session, vendors were not allowed unrestricted remote access to their systems. After precision checks, vendors were briefly allowed remote access to their systems to make adjustments if the measured concentration reported for any compound differed from the target concentration by ± 20 percent or more. Records were maintained of the frequency and nature of adjustments reported by each vendor.

During the 45-day session, vendors were given six opportunities to review their data and perform system corrections as necessary:

- January 21, 2016 – After the January 12 and 19 precision checks,
- February 5, 2016 – After the January 26 and February 2 precision checks,
- February 11, 2016 – After the February 9 precision check,
- February 18, 2016 – After the February 16 precision check,
- February 25, 2016 – After the February 23 post-verification check, and
- March 2, 2016 – After the March 1 MDL setup run, prior to the final MDL check. Note that this was the vendors' first opportunity to calibrate their systems at the 0.5-ppb benzene standard MDL level.

Given these parameters, the following system-specific observations were made:

Vendor A

During the 45-day session, this auto-GC system regularly reported concentrations for 10 or more compounds that differed from the target concentrations by ± 20 percent or more, including in the vendor's adjusted data for 3-ppb benzene standard during the pre-verification check. In the pre- and post-verification checks, this system tended to have fewer compounds outside this range at the higher concentrations.

The vendor accessed the auto-GC system after the January 19 precision check (during which only two compounds were within the ± 20 percent range, for 1 hour each) and made unspecified adjustments, which returned the system to more typical performance in the January 26 precision check. The vendor also accessed the system after the February 2 precision check, noting that the problem compounds were all analyzed by one of the two system GCs. The vendor suggested that the issue was because a component in the system needed cleaning or was showing its age because the field deployment phase had lasted longer than originally planned. The vendor representative noted that he would normally recommend cleaning and recalibrating under these circumstances. Rather than perform these actions during the study, the vendor made other adjustments to the system, noting that this was "a bit outside their SOP." The system's performance showed marginal improvement at the next precision check after this adjustment.

Vendor B

During the 45-day session, this auto-GC system reported concentrations for only three compounds that differed from the target concentrations by ≥ 20 percent in over half of the six precision checks, with another four compounds outside this range in three of the six precision checks. Six other compounds were outside this range in one or two precision checks. Thus, on the whole, the system's performance was relatively consistent over precision checks. In the pre- and post-verification checks, this system tended to have more compounds outside the ± 20 percent range at the higher concentrations.

The vendor reported accessing the system after the January 19 precision check and noted that some retention times shifted slightly, and reported not making any adjustments. The vendor also reported accessing the system after the February 23 post-verification check, and reported making an adjustment for one compound. The vendor attributed results that were out of line at that time to the system operating continuously for almost a full year with minimal maintenance.

Vendor C

During the 45-day session, this auto-GC system reported concentrations for one compound that regularly differed from the target concentrations by ± 20 percent or more, due to a co-elution issue with another compound not on the list of target compounds for the study. The system was also outside this range occasionally for six other compounds; four of these compounds were out of range for only 1 hour each across all the precision checks for which data were reported. (It should be noted that this system reported data for only five of the six precision checks, as discussed in the next section.) The system's performance was consistent with this pattern across the range of concentrations in the pre- and post-verification checks.

The vendor reported accessing the system four times: (1) after the January 19 precision check to correct target values for m- and p-xylenes, which the system does not resolve; (2) after the February 2 precision check, due to a communication port issue resulting in lost data (no adjustments were made to system parameters); (3) after the February 9 precision check, to correct an erroneous value in the calibration table; and (4) after the March 1 MDL setup run, to adjust processing method parameters and calibration curves in advance of the final MDL check. With the exception of adjustments to deal with compounds for which erroneous values were entered in calibration tables, little adjustment or calibration was required to maintain consistent operation of this system over the testing period.

Vendor D

This auto-GC system required little intervention to maintain performance during the study period. During the 45-day session, concentrations for only one compound differed from the target concentrations by ± 20 percent or more, and this occurred for only 3 hours across the six precision checks. The system showed similar performance across concentrations during the pre- and post-verification checks. The vendor accessed the system only once, after the March 1 MDL setup run, to adjust integration parameters and recalibrate prior to the second MDL check.

Vendor E

During the 45-day session, concentrations reported by this auto-GC were generally within ± 20 percent of the challenge concentration, with the exception of the February 9 precision check. During this check, 11 compounds differed from the target concentration by ± 20 percent or more for at least one of the two hours of that test. However, over the rest of the 45-day session, the system reported three compounds outside the range during the January 12 precision check and one compound outside the range during the January 19 precision check. Three of these four compounds were out of range for only 1 of the 2 hours of the precision check. The system's performance during the pre- and post-verification checks was very good across all concentrations.

The vendor accessed the system twice: after the January 19 and February 9 precision checks to adjust retention times and detector gain.

Vendor F

During the 45-day study, this auto-GC system regularly reported concentrations for 10 or more compounds that differed from the target concentrations by ± 20 percent or more during the precision checks. The system tended to have fewer compounds out of this range at the higher concentration of the verification checks, particularly in the corrected pre-verification check results.

The vendor accessed the system three times: after February 2 precision check to adjust the calibration and correct peak windows and after the February 9 and 16 precision checks to adjust peak windows.

6.9 Robustness (Physical Sensitivity to Non-Laboratory Environmental Conditions and General System Maintenance Issues)

Information provided in this section is based on observations made by the project team during the entire field deployment, including the 30-day test trial, the shakedown period, and the 45-day session. Although the data collected during the earlier portion of the field study were not included in statistical analyses due to issues previously described, the systems were located in a field environment and operational for most of the time during the entire study period (from April 2015 through the beginning of March 2016) and this qualitative analysis of issues affecting system performance covers the entire study period.

During the 30-day test trial, several auto-GC systems experienced occasional issues related to variation in the temperature within the mobile laboratory housing the instruments. These issues were deemed to be a result of problems with the mobile laboratory air conditioning system, exacerbated by the fact that there were six systems producing heat in very tight quarters within the laboratory. During this time, ambient temperatures outside the laboratory sometimes reached 90° F² (not atypical for North Carolina in May) and the laboratory was in direct sunlight all day, with the result that temperatures in the laboratory sometimes exceeded 90° F. Repair of the AC system for the trailer solved this problem before the beginning of the shakedown period and 45-day session, and no system showed permanent damage.

Although these issues resulted from external factors, it is worth noting the effects of this situation – several of the systems sometimes experienced delays in operating cycles because of the elevated temperatures in the mobile laboratory. Typically, this occurred when GC ovens were unable to complete their cool-down cycles in

² <https://www.wunderground.com/history/airport/KRDU/2015/5/31/MonthlyHistory.html>

time for the next sample injection. The result was that hourly sampling and analysis could not be completed during the hot afternoon hours, although cycle times generally returned to normal as temperatures cooled overnight.

Another external factor that affected the operation of multiple systems was the electrical system in the mobile laboratory. The trailer electrical system was operating near its peak capacity, and was supporting the air conditioning system, an auxiliary AC unit, several fans, a gas dilution system used to deliver samples to the systems, and six GC systems, plus their ancillary equipment (zero-air generators, hydrogen generators, etc.). On one occasion, a power spike occurred, which interrupted operation of all the systems except Vendor B's, which is equipped, in its standard configuration, with a battery backup system.

The following system-specific observations were made:

Vendor A

During the early part of the study prior to the two 45-day sessions, this system experienced a data loss resulting from low zero air pressure due to a failure of the air compressor. The compressor was replaced and system operation returned to normal. This problem recurred at the very end of the study, resulting in loss of data for the final precision check. The final MDL check was performed using bottled zero air, and it is expected that the compressor may need to be replaced before the system will be fully operational again.

At another point during the early portion of the study, high noise levels in the baseline signal were detected, and were suspected to be a result of moisture in the sample lines. Sample lines were cleared of moisture, air pressure from the compressor was temporarily increased, the FID was checked for moisture, and electrical connections to the detectors were checked. No specific problems were identified, but the problem did not recur.

Vendor B

During the initial portion of the study, odd results from one of the system GC's were noted, which were determined to be a result of damage to the adsorbent trap resulting from ice created in the Peltier cooler, due to air conditioning failure and the resulting high humidity. The trap was replaced by the vendor and normal operation was resumed.

Later in the study, shifts for some peaks were identified, leading to suggestions from the vendor that there might be system leaks or a problem with the dryer. Flow from the dryer was investigated at the request of the vendor and was determined to be correct. No further action was taken, and the retention times returned to normal. Because there were no further shifts in the peak positions, the vendor attributed this anomaly to possible temperature or humidity irregularities in the trailer.

Vendor C

During the shakedown period, this system reported several error messages for the GC and sample injector, resulting in system stoppage and data loss. A vendor service technician indicated that a valve inside the unit appeared to be leaking or stuck in an open position. After some time, the system was re-started and resumed normal operation. This issue recurred at least two additional times during the remainder of the study. The vendor stated the belief that the problem is the result of a solenoid that is sticking intermittently, and that it is difficult to identify the specific component unless it fails completely. Data for one of the precision checks during the 45-day session were lost, either due to a recurrence of this issue, or operator error.

Vendor D

This system experienced some difficulties with a third-party gas generator that was purchased for use with this system. Eventually the gas generator failed and was replaced with gas from cylinders.

Another third-party gas generator purchased for use with the system, and also used to supply this gas to Vendor E's system, proved to have insufficient capacity for both instruments. Flow of this gas was also increased during the course of the study, resulting in higher-than expected consumption of this gas from cylinders.

Vendor E

During the 30-day test trial, this auto-GC system failed an automated leak check and stopped operating. A subsequent remote leak check performed by the vendor passed with no errors. Later, during the shakedown period, the system stopped collecting data, accompanied by a crashed interface program. It was unclear whether this was a problem with the system itself or the PC and software managing it, but after remote troubleshooting and a system restart performed by the vendor, the problem was resolved.

Between the shakedown period and the 45-day session, the vendor replaced a component of a detector, resulting in the need for a re-calibration.

Vendor F

During the shakedown period, this system experienced data loss due to a faulty regulator on a gas generator unit. After troubleshooting, the regulator was replaced, and normal operation resumed. During the period between the shakedown period and the 45-day session, the system experienced problems with humidity control, and rapidly depleted drier tubes. Soon thereafter, system operating pressures were observed to be very low. The vendor replaced a different gas generator unit to address these issues.

During the 45-day session, the system experienced occasional issues during which the system could not be accessed remotely. The situation appeared to be a result of errors occurring with the remote-access software (which was used to access all the other systems, with no such issues arising). Multiple software errors would accumulate, resulting in the remote-access program taking up nearly 100 percent of CPU capacity, and preventing remote access. System error lights accompanied these events, but remote troubleshooting by the vendor did not reveal any system issues. No data were lost due to these events, but continuous testing was not being performed during this phase of the study.

6.10 Cost

As noted previously, the EPA purchased three of the auto-GC systems that took part in the field deployment phase, and the other three were lent by the vendors for the study. The costs listed below in Table 3 represent the total actual costs charged by the vendors for the three purchased systems and cost estimates that were obtained during the laboratory evaluation phase for the three systems lent for the field evaluation phase. These costs include the base price for the system as well as any ancillary/add-on equipment and any cost for installation and setup of the systems. Detailed information on the gas generators included in the price of some systems cannot be given in this report because of the possibility of compromising anonymity. Sales taxes are not included.

Table 3. Cost for the Candidate Auto-GC Systems

Vendor	Cost	Notes
A	\$114,029	Includes the cost of gas generators for some or all of the gases used.
B	\$161,202	Includes the cost of calibration gas generator, battery backup system, training, and gas generators for all of the gases used.
C	\$92,269	Includes the cost of gas generators for some or all of the gases used.
D	\$93,306	Includes the cost of gas generators for some or all of the gases used.
E	\$117,419	No gas generators included in cost.
F	\$92,600	Includes the cost of gas generators for some or all of the gases used.

It should be noted that the costs in Table 3 do not include the costs of preventive maintenance, maintenance kits, and replacement parts. These can be significant factors in the cost of ownership, and should be understood prior to purchasing an auto-GC system.

6.11 Summary of Results

Table 4 provides a summary of the various statistics for which the auto-GC systems were evaluated. Based on these results and those of the earlier laboratory evaluations, the following conclusions and recommendations for network deployment of auto-GC systems into the PAMS network can be made:

- Several auto-GC systems exist that can provide semi-continuous measurements of the PAMS target VOCs with typical precision and bias of 20-30 percent or better.
- Typical MDLs for the auto-GC systems evaluated are on the order of 1 ppb as carbon, with several systems capable of MDLs as low as 0.5 ppb as carbon or lower.
- All instruments evaluated had linear response at the concentrations used in the evaluation.
- All instruments evaluated were capable of very high rates of completeness for the PAMS target VOCs.

Table 4. Mean Values for Each Quantitative Evaluation by Vendor across All Target Compounds^a

Test	Vendor					
	A	B	C	D	E	F
Precision (%RSD)	32.3	13.1	6.3	1.6	16.7	34.9
Bias (MNB, % unsigned)	23	17	8	2	12	27
Drift (%/day)	0.09	0.00	0.00	0.01	-0.04	-0.05
Linearity (slope, ppb/ppb)	1.07	1.14	0.95	1.01	0.90	0.88
Completeness (%)	87.1	93.7	98.6	100.0	100.0	95.0
MDL (ppb as carbon)	1.22	0.41	0.32	0.17	0.40	1.40

^a The mean values presented in this table are based on the same datasets that are the bases for the figures presented in the sections above.

In addition to the results of the performance testing discussed above, a number of observations can be made based on the experience provided from the evaluation.

- Careful control of moisture in carrier gases is needed to prevent shifts in peaks which can adversely impact performance of the auto-GC system.
- Sample and calibration lines should be limited in length to prevent retention of “sticky” compounds in the sample lines and be of a small enough diameter to ensure short retention times in the delivery system.
- Sample and calibration lines should be constructed of chromatography grade silica treated stainless steel or other materials which have been shown to not degrade sample delivery.
- If stainless steel lines are used, calibration gases may need to be humidified to ensure proper delivery.
- PTFE sample lines (and other Teflon based sample lines) may be an option to eliminate the need for humidification and simplify the calibration system, however, additional evaluations are needed to ensure the PTFE lines do not create other problems in the sample delivery system.
- The auto-GC systems can be successfully operated remotely where internet access is available with minimal onsite interaction.
- Once installed and operating, onsite operator interaction can be periodic (on the order of once per week).

- Monthly or weekly precision checks should be conducted with all target species to help identify problems including shifts in peaks. Automation of the checks should be considered to reduce the burden. More frequent checks (e.g., daily) would likely be impractical due to the length of time needed to conduct a test (approximately 2-3 hours) and the resulting loss of ambient data that could be collected.
- While the systems have automated much of the data collection and peak integration processes, significant effort is still needed to process the data into a format suitable for submission of the data to EPA's Air Quality System (AQS). Additional efforts to integrate auto-GC systems into data management systems commonly used by monitoring agencies should be explored.
- Typical capital costs for complete auto-GC systems (including support equipment, if needed) is on the order of \$100,000, and does not vary greatly between vendors.
- Generators can be used to produce hydrogen and nitrogen of suitable quality to operate the auto-GC systems, however moisture control must be maintained for carrier gases.

7.0 References

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Appendices

Appendix A-1: Statistics on Precision

Appendix A-1. Statistics on precision for priority chemicals, by vendor and chemical.

Chemical	Relative standard deviation, by vendor ID (%)					
	A	B	C	D	E	F
Benzene	27.4	2.0	13.0	1.2	6.6	27.8
1,3-Butadiene	35.3	3.0	2.9	1.9	25.6	44.7
n-Butane	24.7	2.9	6.3	1.4	6.5	41.1
1-Butene	52.2	9.4	6.0	0.9	38.4	23.9
cis-2-Butene	26.3	40.9	6.0	0.7	5.9	39.8
Carbon tetrachloride		45.6	3.8	4.1	6.6	84.5
Ethane	20.8	40.7	6.8	1.7	26.7	4.6
Ethylbenzene	42.5	3.2	2.3	1.0	39.1	15.6
Ethylene	22.9	8.2	4.9	2.5	6.0	8.6
m-Ethyltoluene	38.6	0.0	3.6	1.0	11.4	25.3
o-Ethyltoluene	38.3	5.0	11.4	0.8	27.4	38.3
p-Ethyltoluene	48.9	15.3	4.9	1.4	24.6	27.7
n-Hexane	27.8	5.1	3.6	7.0	37.8	9.8
Isobutane	24.3	3.1	6.6	1.6	31.7	26.9
Isopentane	24.2	6.7	6.0	1.0	7.9	36.4
Isoprene	42.4	48.3	5.9	1.5	6.4	39.7
n-Pentane	23.6	18.2	12.4	1.8	7.2	13.5
Propane	4.1	4.0	4.9	2.8	6.7	12.4
Propylene	24.6	4.4	4.8	1.4	6.7	12.0
Styrene	108.1	6.2	2.9	0.8	7.5	78.3
Tetrachloroethylene	30.8	40.8	2.4	0.9	6.8	56.1
Toluene	36.9	5.4	2.8	0.7	27.8	40.1
trans-2-Butene	23.0	4.8	5.8	0.6	6.6	22.6
1,2,3-Trimethylbenzene	27.0	3.5	5.1	1.3	27.2	46.7
1,2,4-Trimethylbenzene	25.7	4.7	3.8	1.6	10.1	50.5
2,2,4-Trimethylpentane	7.4	8.2	3.7	0.8	7.7	85.7
o-Xylene	34.7	3.5	3.8	0.6	27.3	24.7
m-/p-Xylene	30.8	1.9	31.4	1.9	17.8	40.7

Summary of precision based on relative standard deviation (RSD), distribution across priority chemicals for each vendor

Vendor ID	Average of the RSD (%) for priority chemicals	Standard deviation (%)	Distribution of RSD across the priority chemicals					Examples of RSD for specific chemicals			
			Minimum	25th percentile	Median	75th percentile	Maximum	Ethane	1,3-Butadiene	Benzene	1,2,3-Tri-methyl-benzene
A	32.3	96.3	4.1	24.2	27.4	37.6	108.1	20.8	35.3	27.4	27.0
B	13.1	79.9	1.9	3.5	5.2	16.0	48.3	40.7	3.0	2.0	3.5
C	6.3	29.8	2.3	3.7	4.9	6.1	31.4	6.8	2.9	13.0	5.1
D	1.6	6.9	0.6	0.9	1.3	1.7	7.0	1.7	1.9	1.2	1.3
E	16.7	62.8	5.9	6.7	9.0	27.2	39.1	26.7	25.6	6.6	27.2
F	34.9	115.0	4.6	20.8	32.1	42.0	85.7	4.6	44.7	27.8	46.7

Appendix A-2: Statistics on Bias

Appendix A-2. Statistics on signed and unsigned bias, by vendor ID and chemical.

Vendor ID	Chemical	Signed bias	Standard deviation	Unsigned bias	Standard deviation	Number of obs.
A	Benzene	43.8	41.0	52.4	28.5	19
	1,3-Butadiene	-10.2	26.4	13.9	24.6	20
	n-Butane	-5.5	19.1	7.4	18.4	19
	1-Butene	-26.6	31.1	26.6	31.1	20
	cis-2-Butene	-0.8	22.5	10.9	19.5	19
	Carbon tetrachloride					
	Ethane	3.9	19.7	16.6	10.6	18
	Ethylbenzene	-32.1	27.4	34.5	24.2	19
	Ethylene	46.1	28.0	49.9	20.1	18
	m-Ethyltoluene	-19.9	36.5	31.9	26.0	20
	o-Ethyltoluene	-25.1	31.7	32.6	23.4	20
	p-Ethyltoluene	-42.1	28.0	44.7	23.2	20
	n-Hexane	-17.3	23.5	22.0	19.0	19
	Isobutane	-7.4	18.5	7.9	18.3	19
	Isopentane	-7.8	18.2	7.8	18.2	19
	Isoprene	4.1	33.5	17.6	28.4	16
	n-Pentane	-5.2	18.8	6.0	18.5	18
	Propane	-3.4	3.5	3.8	3.0	18
	Propylene	-9.5	18.2	9.6	18.1	19
	Styrene	-28.8	58.1	51.5	38.1	20
	Tetrachloroethylene	-5.1	24.6	12.9	21.3	18
	Toluene	-18.7	27.2	22.6	23.8	20
	trans-2-Butene	-4.1	18.2	6.8	17.3	20
	1,2,3-Trimethylbenzene	-31.2	29.8	37.7	20.3	20
	1,2,4-Trimethylbenzene	-31.9	27.1	36.5	20.0	20
	2,2,4-Trimethylpentane	-6.1	9.0	8.6	6.3	18
	o-Xylene	-25.2	27.1	29.4	22.3	20
	m-/p-Xylene	-11.9	25.6	19.6	20.0	20

Appendix A-2. Statistics on signed and unsigned bias, by vendor ID and chemical, cont.

Vendor ID	Chemical	Signed bias	Standard deviation	Unsigned bias	Standard deviation	Number of obs.
B	Benzene	4.0	2.7	4.0	2.7	22
	1,3-Butadiene	9.8	6.9	9.8	6.8	22
	n-Butane	2.3	2.7	3.1	1.4	19
	1-Butene	2.6	9.7	8.5	5.0	22
	cis-2-Butene	28.9	47.9	29.2	47.7	20
	Carbon tetrachloride	-39.0	50.7	43.8	46.3	16
	Ethane	24.3	42.5	36.5	32.1	22
	Ethylbenzene	6.0	3.0	6.0	3.0	22
	Ethylene	7.2	11.3	10.7	7.9	22
	m-Ethyltoluene	70.7	0.0	70.7	0.0	1
	o-Ethyltoluene	10.5	7.5	10.5	7.5	22
	p-Ethyltoluene	110.6	27.0	110.6	27.0	19
	n-Hexane	16.2	9.4	16.2	9.4	22
	Isobutane	6.8	5.0	7.1	4.6	18
	Isopentane	9.3	9.2	11.3	6.3	20
	Isoprene	3.6	42.5	30.6	28.8	18
	n-Pentane	0.0	18.9	16.3	8.9	22
	Propane	7.6	7.1	7.8	6.9	22
	Propylene	3.0	3.7	4.4	1.7	19
	Styrene	3.8	6.3	6.7	2.8	22
	Tetrachloroethylene	22.5	46.1	24.7	44.9	22
	Toluene	2.9	4.6	4.5	2.8	22
	trans-2-Butene	6.8	7.6	8.0	6.2	22
	1,2,3-Trimethylbenzene	8.3	3.6	8.3	3.6	22
	1,2,4-Trimethylbenzene	12.4	9.2	13.0	8.3	22
	2,2,4-Trimethylpentane	11.7	11.3	11.7	11.3	22
	o-Xylene	4.8	4.0	5.5	3.0	22
	m-/p-Xylene	6.8	2.5	6.8	2.5	22

Appendix A-2. Statistics on signed and unsigned bias, by vendor ID and chemical, cont.

Vendor ID	Chemical	Signed bias	Standard deviation	Unsigned bias	Standard deviation	Number of obs.
C	Benzene	-15.2	16.9	18.8	12.5	20
	1,3-Butadiene	3.3	3.3	3.6	2.8	20
	n-Butane	6.0	8.1	7.8	6.4	20
	1-Butene	5.4	8.0	7.6	5.9	20
	cis-2-Butene	5.7	8.1	7.9	5.8	20
	Carbon tetrachloride	2.1	5.3	4.4	3.5	20
	Ethane	-3.4	6.2	5.2	5.0	20
	Ethylbenzene	5.6	2.8	5.6	2.8	20
	Ethylene	1.1	5.8	4.3	4.0	20
	m-Ethyltoluene	0.3	5.0	4.1	2.7	20
	o-Ethyltoluene	27.8	14.7	27.8	14.7	15
	p-Ethyltoluene	-4.0	7.0	6.2	5.0	20
	n-Hexane	2.1	5.3	4.3	3.6	20
	Isobutane	6.4	8.1	7.8	6.6	20
	Isopentane	8.6	6.6	8.9	6.2	14
	Isoprene	7.1	7.1	7.7	6.4	20
	n-Pentane	14.8	13.4	14.8	13.4	20
	Propane	5.4	4.9	5.6	4.7	20
	Propylene	7.6	5.7	7.6	5.7	20
	Styrene	0.9	3.6	3.3	1.7	20
	Tetrachloroethylene	4.3	3.9	5.0	2.8	20
	Toluene	5.3	3.7	5.5	3.5	20
	trans-2-Butene	5.2	8.1	7.5	5.8	20
	1,2,3-Trimethylbenzene	2.8	6.4	5.4	4.2	19
	1,2,4-Trimethylbenzene	2.7	5.4	4.9	3.3	20
	2,2,4-Trimethylpentane	1.7	5.7	4.8	3.5	20
	o-Xylene	-1.8	9.5	7.6	5.8	20
	m-/p-Xylene	-10.8	23.0	14.7	20.6	20

Appendix A-2. Statistics on signed and unsigned bias, by vendor ID and chemical, cont.

Vendor ID	Chemical	Signed bias	Standard deviation	Unsigned bias	Standard deviation	Number of obs.
D	Benzene	1.1	1.4	1.4	1.0	21
	1,3-Butadiene	-0.3	2.0	1.4	1.4	21
	n-Butane	0.7	1.7	1.6	1.0	22
	1-Butene	-0.7	1.4	1.1	1.0	21
	cis-2-Butene	0.4	1.0	0.9	1.0	22
	Carbon tetrachloride	3.8	4.9	5.2	3.3	22
	Ethane	1.9	1.4	2.2	1.0	22
	Ethylbenzene	1.0	1.4	1.4	1.0	22
	Ethylene	1.6	2.5	2.4	1.4	21
	m-Ethyltoluene	-0.1	1.0	0.8	0.0	22
	o-Ethyltoluene	0.5	1.0	0.8	0.0	21
	p-Ethyltoluene	-2.8	1.0	2.8	1.0	22
	n-Hexane	-18.3	6.3	18.3	6.3	22
	Isobutane	1.0	1.7	1.7	1.0	21
	Isopentane	0.3	1.4	1.1	1.0	22
	Isoprene	0.8	2.2	1.9	1.4	22
	n-Pentane	1.3	1.7	1.9	1.0	21
	Propane	1.2	2.5	2.6	1.0	21
	Propylene	1.4	1.4	1.7	1.0	21
	Styrene	0.1	0.0	0.6	0.0	22
	Tetrachloroethylene	-0.7	1.0	0.9	1.0	22
	Toluene	-0.4	1.0	0.7	1.0	20
	trans-2-Butene	-0.4	0.0	0.7	0.0	21
	1,2,3-Trimethylbenzene	2.6	1.0	2.6	1.0	20
	1,2,4-Trimethylbenzene	-1.4	1.4	1.6	1.0	22
	2,2,4-Trimethylpentane	-1.2	0.0	1.2	0.0	21
	o-Xylene	-1.9	1.0	1.9	1.0	21
	m-/p-Xylene	2.4	2.0	2.7	1.7	22

Appendix A-2. Statistics on signed and unsigned bias, by vendor ID and chemical, cont.

Vendor ID	Chemical	Signed bias	Standard deviation	Unsigned bias	Standard deviation	Number of obs.
E	Benzene	-8.9	5.2	9.2	4.6	22
	1,3-Butadiene	-13.2	18.7	13.2	18.7	22
	n-Butane	-9.2	5.1	9.3	5.0	21
	1-Butene	-19.8	26.2	19.8	26.2	21
	cis-2-Butene	-8.1	4.9	8.5	4.1	21
	Carbon tetrachloride	-7.5	5.2	7.9	4.6	22
	Ethane	-10.3	20.6	11.4	20.0	22
	Ethylbenzene	-14.7	27.7	15.6	27.2	22
	Ethylene	-6.9	5.4	7.4	4.5	22
	m-Ethyltoluene	-9.4	9.3	10.5	8.0	22
	o-Ethyltoluene	-9.4	20.8	10.8	20.2	22
	p-Ethyltoluene	-20.1	17.0	20.2	16.9	21
	n-Hexane	-16.2	26.3	16.4	26.2	22
	Isobutane	-13.0	23.0	14.2	22.3	22
	Isopentane	-9.5	6.9	9.8	6.3	21
	Isoprene	-7.7	5.5	8.0	4.9	22
	n-Pentane	-6.7	5.8	7.6	4.6	22
	Propane	-10.6	5.1	10.6	5.1	22
	Propylene	-6.9	5.3	7.7	4.0	22
	Styrene	-9.1	5.9	9.5	5.4	21
	Tetrachloroethylene	-12.3	5.1	12.3	5.1	22
	Toluene	-13.1	20.8	13.7	20.4	21
	trans-2-Butene	-9.8	5.5	9.9	5.2	21
	1,2,3-Trimethylbenzene	-13.1	19.8	13.8	19.3	22
	1,2,4-Trimethylbenzene	-19.2	7.0	19.2	7.0	22
	2,2,4-Trimethylpentane	-11.9	6.0	12.0	5.9	21
	o-Xylene	-12.7	20.0	13.3	19.5	22
	m-/p-Xylene	-11.7	13.2	12.1	12.8	22

Appendix A-2. Statistics on signed and unsigned bias, by vendor ID and chemical, cont.

Vendor ID	Chemical	Signed bias	Standard deviation	Unsigned bias	Standard deviation	Number of obs.
F	Benzene	-6.3	21.6	8.1	21.6	21
	1,3-Butadiene	-10.4	43.7	34.0	28.3	18
	n-Butane	-6.4	36.9	30.4	20.9	20
	1-Butene	3.5	25.7	20.4	15.3	20
	cis-2-Butene	-7.4	33.3	25.9	21.4	20
	Carbon tetrachloride	136.8	226.0	145.2	220.4	22
	Ethane	-0.3	4.1	3.4	2.2	20
	Ethylbenzene	-2.0	13.2	8.3	10.3	21
	Ethylene	5.4	8.0	9.0	3.2	20
	m-Ethyltoluene	-10.0	19.4	11.3	19.3	22
	o-Ethyltoluene	-12.7	27.6	14.5	26.6	20
	p-Ethyltoluene	-12.0	20.6	12.3	20.5	22
	n-Hexane	-5.7	8.5	6.3	8.1	22
	Isobutane	-8.2	28.4	25.7	13.6	20
	Isopentane	-14.3	36.2	34.8	15.8	20
	Isoprene	-9.8	53.2	38.9	36.7	20
	n-Pentane	-10.2	20.3	20.4	9.0	20
	Propane	-4.8	11.3	9.0	8.1	20
	Propylene	31.6	23.2	32.6	21.7	20
	Styrene	-38.1	49.1	60.1	12.4	22
	Tetrachloroethylene	-40.5	37.5	43.0	34.4	16
	Toluene	-9.1	30.2	14.7	27.8	22
	trans-2-Butene	1.4	24.8	19.7	14.4	18
	1,2,3-Trimethylbenzene	-18.1	31.7	18.7	31.4	22
	1,2,4-Trimethylbenzene	-20.5	32.7	20.6	32.6	21
	2,2,4-Trimethylpentane	24.2	97.7	60.8	79.2	21
	o-Xylene	-5.7	19.5	14.6	13.8	21
	m-/p-Xylene	-19.1	27.8	19.1	27.8	22

Summary by vendor of the distribution of mean normalized bias (MNB) across priority chemicals.

Vendor ID	Average of the MNB (%) for priority chemicals	Standard deviation (%)	Distribution of MNB across the priority chemicals					Examples of MNB for specific chemicals				
			Minimum	25th percentile	Median	75th percentile	Maximum	Ethane	1,3-Butadiene	Benzene	1,2,3-Tri-methyl-benzene	
Unsigned bias (absolute value)												
A	23	79	4	9	20	34	52	17	14	52	38	
B	17	112	3	7	10	16	111	36	10	4	8	
C	8	28	3	5	6	8	28	5	4	19	5	
D	2	17	1	1	2	2	18	2	1	1	3	
E	12	20	7	9	11	14	20	11	13	9	14	
F	27	145	3	12	20	33	145	3	34	8	19	
Signed bias												
A	-10	104	-42	-25	-10	-5	46	4	-10	44	-31	
B	11	120	-39	4	7	11	111	24	10	4	8	
C	3	40	-15	1	4	6	28	-3	3	-15	3	
D	0	20	-18	0	0	1	4	2	0	1	3	
E	-11	20	-20	-13	-10	-9	-7	-10	-13	-9	-13	
F	-2	163	-40	-12	-8	-2	137	0	-10	-6	-18	

Appendix A-3: Statistics on Drift

Appendix A-3. Statistics for measurement drift (target chemicals by vendor ID)

Vendor ID	Chemical	Slope (%/day)	Correlation coefficient, r	Coefficient of determination, r ²
A	Benzene	0.23	0.30	0.09
	1,3-Butadiene	0.18	0.34	0.12
	n-Butane	0.10	0.26	0.07
	1-Butene	0.15	0.23	0.05
	cis-2-Butene	-0.06	-0.12	0.01
	Carbon Tetrachloride	ND		
	Ethane	0.12	0.30	0.09
	Ethylbenzene	0.01	0.02	0.00
	Ethylene	0.46	0.72	0.52
	m-Ethyltoluene	0.02	0.03	0.00
	o-Ethyltoluene	0.04	0.10	0.01
	p-Ethyltoluene	-0.08	-0.16	0.03
	n-Hexane	0.10	0.27	0.08
	Isobutane	0.09	0.23	0.05
	Isopentane	0.09	0.23	0.05
	Isoprene	-0.08	-0.12	0.01
	n-Pentane	0.08	0.21	0.05
	Propane	0.03	0.42	0.17
	Propylene	0.08	0.21	0.04
	Styrene	-0.11	-0.09	0.01
	Tetrachloroethylene	0.15	0.32	0.10
	Toluene	0.14	0.28	0.08
	trans-2-Butene	0.09	0.22	0.05
	1,2,3-Trimethylbenzene	0.07	0.28	0.08
	1,2,4-Trimethylbenzene	0.05	0.21	0.04
	2,2,4-Trimethylpentane	0.05	0.40	0.16
	o-Xylene	0.21	0.50	0.25
	m-/p-Xylene	0.16	0.36	0.13

Appendix A-3. Statistics for measurement drift (target chemicals by vendor ID), cont.

Vendor ID	Chemical	Slope (%/day)	Correlation coefficient, r	Coefficient of determination, r ²
B	Benzene	0.03	0.74	0.55
	1,3-Butadiene	0.04	0.60	0.36
	n-Butane	-0.03	-0.63	0.39
	1-Butene	0.04	0.29	0.08
	cis-2-Butene	-0.14	-0.15	0.02
	Carbon Tetrachloride	-0.43	-0.58	0.34
	Ethane	0.27	0.34	0.12
	Ethylbenzene	0.02	0.28	0.08
	Ethylene	0.04	0.27	0.07
	m-Ethyltoluene	ND		
	o-Ethyltoluene	0.02	0.23	0.05
	p-Ethyltoluene	0.06	0.14	0.02
	n-Hexane	0.05	0.52	0.28
	Isobutane	0.01	0.24	0.06
	Isopentane	0.08	0.69	0.47
	Isoprene	0.23	0.37	0.13
	n-Pentane	0.12	0.41	0.17
	Propane	0.06	0.72	0.52
	Propylene	0.04	0.44	0.20
	Styrene	0.01	0.06	0.00
	Tetrachloroethylene	-0.77	-0.79	0.62
	Toluene	-0.01	-0.09	0.01
	trans-2-Butene	0.04	0.51	0.26
	1,2,3-Trimethylbenzene	0.01	0.14	0.02
	1,2,4-Trimethylbenzene	0.00	0.03	0.00
	2,2,4-Trimethylpentane	0.08	0.53	0.28
	o-Xylene	0.03	0.48	0.23
	m-/p-Xylene	0.03	0.64	0.40

Appendix A-3. Statistics for measurement drift (target chemicals by vendor ID), cont.

Vendor ID	Chemical	Slope (%/day)	Correlation coefficient, r	Coefficient of determination, r ²
C	Benzene	-0.10	-0.52	0.27
	1,3-Butadiene	0.03	0.49	0.24
	n-Butane	-0.02	-0.17	0.03
	1-Butene	-0.02	-0.20	0.04
	cis-2-Butene	-0.04	-0.37	0.13
	Carbon Tetrachloride	0.00	-0.04	0.00
	Ethane	-0.01	-0.11	0.01
	Ethylbenzene	0.02	0.50	0.25
	Ethylene	-0.01	-0.08	0.01
	m-Ethyltoluene	-0.01	-0.18	0.03
	o-Ethyltoluene	-0.10	-0.36	0.13
	p-Ethyltoluene	-0.03	-0.45	0.21
	n-Hexane	-0.01	-0.25	0.06
	Isobutane	-0.02	-0.13	0.02
	Isopentane	-0.02	-0.19	0.04
	Isoprene	0.00	-0.03	0.00
	n-Pentane	0.02	0.10	0.01
	Propane	0.05	0.54	0.29
	Propylene	0.05	0.56	0.32
	Styrene	-0.02	-0.43	0.19
	Tetrachloroethylene	0.01	0.15	0.02
	Toluene	0.01	0.26	0.07
	trans-2-Butene	-0.02	-0.18	0.03
	1,2,3-Trimethylbenzene	-0.01	-0.07	0.00
	1,2,4-Trimethylbenzene	-0.03	-0.47	0.22
	2,2,4-Trimethylpentane	-0.02	-0.39	0.15
	o-Xylene	-0.03	-0.52	0.27
	m-/p-Xylene	0.37	0.81	0.66

Appendix A-3. Statistics for measurement drift (target chemicals by vendor ID), cont.

Vendor ID	Chemical	Slope (%/day)	Correlation coefficient, r	Coefficient of determination, r ²
D	Benzene	0.02	0.59	0.35
	1,3-Butadiene	0.04	0.90	0.82
	n-Butane	0.01	0.54	0.29
	1-Butene	0.01	0.51	0.26
	cis-2-Butene	0.01	0.48	0.23
	Carbon Tetrachloride	0.01	0.17	0.03
	Ethane	0.01	0.26	0.07
	Ethylbenzene	0.01	0.45	0.20
	Ethylene	0.00	0.09	0.01
	m-Ethyltoluene	0.01	0.59	0.35
	o-Ethyltoluene	0.01	0.46	0.21
	p-Ethyltoluene	-0.01	-0.26	0.07
	n-Hexane	-0.01	-0.07	0.00
	Isobutane	0.01	0.49	0.24
	Isopentane	0.01	0.64	0.40
	Isoprene	0.01	0.25	0.06
	n-Pentane	0.02	0.53	0.28
	Propane	0.03	0.53	0.28
	Propylene	0.01	0.40	0.16
	Styrene	0.00	-0.12	0.02
	Tetrachloroethylene	0.00	-0.16	0.02
	Toluene	0.00	-0.03	0.00
	trans-2-Butene	0.01	0.77	0.59
	1,2,3-Trimethylbenzene	0.02	0.61	0.37
	1,2,4-Trimethylbenzene	-0.01	-0.46	0.22
	2,2,4-Trimethylpentane	0.00	-0.15	0.02
	o-Xylene	0.00	0.14	0.02
	m-/p-Xylene	-0.02	-0.62	0.38

Appendix A-3. Statistics for measurement drift (target chemicals by vendor ID), cont.

Vendor ID	Chemical	Slope (%/day)	Correlation coefficient, r	Coefficient of determination, r ²
E	Benzene	-0.03	-0.27	0.07
	1,3-Butadiene	-0.04	-0.11	0.01
	n-Butane	-0.04	-0.38	0.15
	1-Butene	0.03	0.05	0.00
	cis-2-Butene	-0.02	-0.24	0.06
	Carbon Tetrachloride	-0.03	-0.24	0.06
	Ethane	-0.04	-0.11	0.01
	Ethylbenzene	-0.10	-0.18	0.03
	Ethylene	-0.03	-0.33	0.11
	m-Ethyltoluene	-0.10	-0.56	0.31
	o-Ethyltoluene	0.08	0.19	0.03
	p-Ethyltoluene	0.00	-0.01	0.00
	n-Hexane	-0.09	-0.18	0.03
	Isobutane	-0.11	-0.23	0.05
	Isopentane	-0.03	-0.23	0.05
	Isoprene	-0.02	-0.18	0.03
	n-Pentane	-0.02	-0.16	0.03
	Propane	-0.04	-0.38	0.14
	Propylene	-0.04	-0.36	0.13
	Styrene	-0.06	-0.52	0.27
	Tetrachloroethylene	-0.07	-0.61	0.37
	Toluene	0.07	0.16	0.03
	trans-2-Butene	-0.02	-0.19	0.04
	1,2,3-Trimethylbenzene	-0.08	-0.19	0.04
	1,2,4-Trimethylbenzene	-0.13	-0.74	0.55
	2,2,4-Trimethylpentane	-0.05	-0.42	0.18
	o-Xylene	-0.08	-0.20	0.04
	m-/p-Xylene	-0.08	-0.28	0.08

Appendix A-3. Statistics for measurement drift (target chemicals by vendor ID), cont.

Vendor ID	Chemical	Slope (%/day)	Correlation coefficient, r	Coefficient of determination, r ²
F	Benzene	-0.08	-0.18	0.03
	1,3-Butadiene	-0.36	-0.56	0.31
	n-Butane	0.17	0.30	0.09
	1-Butene	-0.39	-0.86	0.73
	cis-2-Butene	-0.33	-0.50	0.25
	Carbon Tetrachloride	0.95	0.22	0.05
	Ethane	0.07	0.85	0.73
	Ethylbenzene	0.08	0.31	0.10
	Ethylene	-0.08	-0.50	0.25
	m-Ethyltoluene	0.05	0.13	0.02
	o-Ethyltoluene	-0.16	-0.33	0.11
	p-Ethyltoluene	-0.08	-0.19	0.04
	n-Hexane	0.01	0.04	0.00
	Isobutane	0.07	0.20	0.04
	Isopentane	0.01	0.03	0.00
	Isoprene	-0.31	-0.43	0.18
	n-Pentane	0.05	0.26	0.07
	Propane	0.16	0.82	0.68
	Propylene	-0.07	-0.26	0.07
	Styrene	-0.66	-0.66	0.43
	Tetrachloroethylene	-0.52	-0.78	0.60
	Toluene	0.01	0.02	0.00
	trans-2-Butene	-0.34	-0.85	0.72
	1,2,3-Trimethylbenzene	-0.12	-0.21	0.04
	1,2,4-Trimethylbenzene	-0.08	-0.13	0.02
	2,2,4-Trimethylpentane	0.65	0.34	0.11
	o-Xylene	0.06	0.14	0.02
	m-/p-Xylene	-0.07	-0.13	0.02

Vendor ID	Average drift slope (%/day) for priority chemicals	Standard deviation	Distribution of drift slope (%/day) across the target chemicals					Example slopes for specific chemicals			
			Minimum	25th percentile	Median	75th percentile	Maximum	Ethane	1,3-Butadiene	Benzene	1,2,3-Tri-methyl-benzene
A	0.09	0.59	-0.11	0.04	0.09	0.14	0.46	0.12	0.18	0.23	0.07
B	0.00	1.01	-0.77	0.01	0.03	0.05	0.27	0.27	0.04	0.03	0.01
C	0.00	0.42	-0.10	-0.02	-0.01	0.01	0.37	-0.01	0.03	-0.10	-0.01
D	0.01	0.06	-0.02	0.00	0.01	0.01	0.04	0.01	0.04	0.02	0.02
E	-0.04	0.25	-0.13	-0.07	-0.04	-0.02	0.08	-0.04	-0.04	-0.03	-0.08
F	-0.05	1.68	-0.66	-0.20	-0.07	0.06	0.95	0.07	-0.36	-0.08	-0.12

Appendix A-4: Statistics on Linearity

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²	
A	Both tests	Benzene	0.78	2.73	0.99	0.98	
		1,3-Butadiene	1.06	-0.28	1.00	1.00	
		n-Butane	1.03	-0.12	1.00	1.00	
		1-Butene	0.98	-0.13	1.00	1.00	
		cis-2-Butene	1.03	-0.24	0.99	0.99	
		Carbon tetrachloride					
		Ethane	0.88	0.60	0.95	0.90	
		Ethylbenzene	1.11	-0.92	0.98	0.96	
		Ethylene	1.13	0.65	0.95	0.90	
		m-Ethyltoluene	1.29	-1.29	0.86	0.74	
		o-Ethyltoluene	1.32	-1.61	0.99	0.97	
		p-Ethyltoluene	0.87	-0.49	0.87	0.75	
		n-Hexane	1.18	-0.92	0.99	0.99	
		Isobutane	1.01	-0.09	1.00	1.00	
		Isopentane	1.01	-0.15	1.00	1.00	
		Isoprene	1.08	-0.23	1.00	1.00	
		n-Pentane	1.02	-0.10	1.00	1.00	
		Propane	1.00	-0.11	1.00	1.00	
		Propylene	1.01	-0.18	1.00	0.99	
		Styrene	1.30	-2.09	0.98	0.95	
		Tetrachloroethylene	1.14	-0.44	0.99	0.99	
		Toluene	1.14	-0.70	1.00	0.99	
		trans-2-Butene	1.00	0.08	1.00	1.00	
		1,2,3-Trimethylbenzene	1.29	-1.54	0.99	0.97	
		1,2,4-Trimethylbenzene	1.27	-1.65	0.99	0.97	
		2,2,4-Trimethylpentane	1.10	-0.42	1.00	0.99	
o-Xylene	1.21	-1.37	0.99	0.98			
m-/p-Xylene	1.21	-1.80	0.99	0.98			
A	Post-verification	Benzene	0.82	2.78	1.00	0.99	
		1,3-Butadiene	1.08	-0.17	1.00	1.00	
		n-Butane	1.04	-0.09	1.00	1.00	
		1-Butene	0.95	-0.07	1.00	1.00	
		cis-2-Butene	0.97	-0.04	1.00	1.00	
		Carbon tetrachloride					
		Ethane	1.00	0.36	0.97	0.94	
		Ethylbenzene	1.04	-0.71	0.97	0.94	
		Ethylene	1.33	0.49	1.00	0.99	
		m-Ethyltoluene	1.04	-0.39	0.88	0.77	
		o-Ethyltoluene	1.29	-1.26	0.98	0.97	

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		p-Ethyltoluene	0.77	-0.38	0.85	0.72
		n-Hexane	1.16	-0.67	0.99	0.99
		Isobutane	1.01	-0.06	1.00	1.00
		Isopentane	0.99	-0.05	1.00	1.00
		Isoprene	1.09	-0.05	1.00	1.00
		n-Pentane	1.02	-0.05	1.00	1.00
		Propane	0.99	-0.03	1.00	1.00
		Propylene	0.98	-0.07	1.00	1.00
		Styrene	1.22	-1.56	0.97	0.94
		Tetrachloroethylene	1.16	-0.35	1.00	0.99
		Toluene	1.14	-0.55	0.99	0.99
		trans-2-Butene	1.01	0.05	1.00	1.00
		1,2,3-Trimethylbenzene	1.27	-1.18	0.98	0.97
		1,2,4-Trimethylbenzene	1.20	-1.17	0.98	0.97
		2,2,4-Trimethylpentane	1.08	-0.27	1.00	1.00
		o-Xylene	1.17	-0.92	0.99	0.98
		m-/p-Xylene	1.21	-1.37	0.99	0.99
		A	Pre-verification	Benzene	0.76	2.50
1,3-Butadiene	1.07			-0.64	1.00	1.00
n-Butane	1.03			-0.24	1.00	1.00
1-Butene	1.03			-0.23	1.00	1.00
cis-2-Butene	1.13			-0.68	1.00	1.00
Carbon tetrachloride						
Ethane	0.73			1.11	0.96	0.92
Ethylbenzene	1.22			-1.40	1.00	0.99
Ethylene	0.92			0.78	1.00	1.00
m-Ethyltoluene	1.68			-3.50	0.88	0.78
o-Ethyltoluene	1.41			-2.59	1.00	1.00
p-Ethyltoluene	0.98			-0.63	0.90	0.80
n-Hexane	1.24			-1.64	1.00	0.99
Isobutane	1.02			-0.18	1.00	1.00
Isopentane	1.04			-0.42	1.00	0.99
Isoprene	1.12			-0.74	1.00	1.00
n-Pentane	1.04			-0.22	1.00	1.00
Propane	1.03			-0.34	1.00	1.00
Propylene	1.05			-0.46	0.99	0.99
Styrene	1.47			-3.51	0.99	0.98
Tetrachloroethylene	1.14			-0.76	1.00	0.99
Toluene	1.18			-1.14	1.00	1.00

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		trans-2-Butene	0.98	0.15	1.00	1.00
		1,2,3-Trimethylbenzene	1.38	-2.56	1.00	0.99
		1,2,4-Trimethylbenzene	1.42	-2.91	1.00	0.99
		2,2,4-Trimethylpentane	1.14	-0.80	1.00	0.99
		o-Xylene	1.34	-2.63	1.00	1.00
		m-/p-Xylene	1.25	-3.07	0.99	0.99
B	Both tests	Benzene	1.07	-0.09	1.00	1.00
		1,3-Butadiene	1.18	-0.20	1.00	0.99
		n-Butane	1.00	0.15	1.00	1.00
		1-Butene	1.10	-0.08	1.00	1.00
		cis-2-Butene	1.10	-0.12	1.00	1.00
		Carbon tetrachloride	0.62	0.25	0.51	0.26
		Ethane	0.96	1.10	0.85	0.72
		Ethylbenzene	1.19	-0.28	0.99	0.98
		Ethylene	1.17	-0.15	0.99	0.99
		m-Ethyltoluene				
		o-Ethyltoluene	1.21	-0.26	1.00	1.00
		p-Ethyltoluene	2.26	-0.32	1.00	1.00
		n-Hexane	1.25	-0.18	1.00	0.99
		Isobutane	1.12	-0.11	1.00	1.00
		Isopentane	1.10	0.04	0.99	0.98
		Isoprene	1.44	-0.40	0.99	0.99
		n-Pentane	1.15	-0.10	0.99	0.99
		Propane	0.64	4.10	0.64	0.41
		Propylene	0.99	0.25	1.00	1.00
		Styrene	1.13	-0.19	1.00	1.00
		Tetrachloroethylene	1.66	-0.19	0.85	0.72
		Toluene	1.07	-0.12	1.00	1.00
		trans-2-Butene	1.15	-0.15	1.00	1.00
		1,2,3-Trimethylbenzene	1.11	-0.07	1.00	1.00
		1,2,4-Trimethylbenzene	1.27	-0.28	1.00	1.00
		2,2,4-Trimethylpentane	1.36	-0.66	0.99	0.98
o-Xylene	1.10	-0.15	1.00	1.00		
m-/p-Xylene	1.14	-0.39	1.00	1.00		
B	Post-verification	Benzene	1.08	-0.06	1.00	1.00
		1,3-Butadiene	1.23	-0.22	1.00	1.00
		n-Butane	1.01	0.12	1.00	1.00
		1-Butene	1.13	-0.07	1.00	1.00
		cis-2-Butene	1.13	-0.13	1.00	1.00

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		Carbon tetrachloride	0.03	0.13	0.91	0.82
		Ethane	1.27	1.22	0.99	0.97
		Ethylbenzene	1.07	-0.08	1.00	1.00
		Ethylene	1.25	-0.24	1.00	1.00
		m-Ethyltoluene				
		o-Ethyltoluene	1.23	-0.23	1.00	1.00
		p-Ethyltoluene	2.27	-0.30	1.00	1.00
		n-Hexane	1.32	-0.23	1.00	1.00
		Isobutane	1.15	-0.11	1.00	1.00
		Isopentane	1.21	-0.11	1.00	1.00
		Isoprene	1.50	-0.71	1.00	0.99
		n-Pentane	1.23	-0.19	1.00	1.00
		Propane	0.43	6.62	0.42	0.18
		Propylene	1.02	0.21	1.00	1.00
		Styrene	1.11	-0.19	1.00	1.00
		Tetrachloroethylene	1.05	-0.05	1.00	1.00
		Toluene	1.04	-0.12	1.00	1.00
		trans-2-Butene	1.19	-0.16	1.00	1.00
		1,2,3-Trimethylbenzene	1.06	-0.01	1.00	1.00
		1,2,4-Trimethylbenzene	1.28	-0.23	1.00	1.00
		2,2,4-Trimethylpentane	1.28	-0.31	1.00	1.00
o-Xylene	1.11	-0.15	1.00	1.00		
m-/p-Xylene	1.11	-0.25	1.00	1.00		
B	Pre-verification	Benzene	1.06	-0.11	1.00	1.00
		1,3-Butadiene	1.14	-0.19	1.00	1.00
		n-Butane	0.99	0.19	1.00	1.00
		1-Butene	1.07	-0.10	1.00	1.00
		cis-2-Butene	1.07	-0.11	1.00	1.00
		Carbon tetrachloride	1.27	-0.41	1.00	1.00
		Ethane	0.64	0.98	0.99	0.98
		Ethylbenzene	1.30	-0.48	1.00	0.99
		Ethylene	1.08	-0.07	1.00	1.00
		m-Ethyltoluene				
		o-Ethyltoluene	1.19	-0.28	1.00	1.00
		p-Ethyltoluene	2.25	-0.34	1.00	1.00
		n-Hexane	1.18	-0.13	1.00	1.00
		Isobutane	1.10	-0.11	1.00	1.00
		Isopentane	0.99	0.20	1.00	1.00
Isoprene	1.38	-0.09	0.99	0.99		

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		n-Pentane	1.07	-0.01	1.00	1.00
		Propane	0.85	1.59	0.97	0.95
		Propylene	0.95	0.29	1.00	1.00
		Styrene	1.15	-0.20	1.00	1.00
		Tetrachloroethylene	2.27	-0.34	1.00	1.00
		Toluene	1.09	-0.11	1.00	1.00
		trans-2-Butene	1.11	-0.13	1.00	1.00
		1,2,3-Trimethylbenzene	1.15	-0.13	1.00	1.00
		1,2,4-Trimethylbenzene	1.26	-0.33	1.00	1.00
		2,2,4-Trimethylpentane	1.45	-1.00	0.99	0.98
		o-Xylene	1.10	-0.15	1.00	1.00
		m-/p-Xylene	1.17	-0.54	1.00	1.00
C	Both tests	Benzene	0.78	0.22	0.93	0.87
		1,3-Butadiene	0.96	0.26	1.00	1.00
		n-Butane	0.97	0.16	0.99	0.99
		1-Butene	0.96	0.17	0.99	0.99
		cis-2-Butene	0.97	0.16	0.99	0.99
		Carbon tetrachloride	0.97	0.12	1.00	0.99
		Ethane	1.00	-0.05	1.00	0.99
		Ethylbenzene	1.01	0.08	1.00	1.00
		Ethylene	1.00	-0.02	1.00	0.99
		m-Ethyltoluene	0.96	0.06	1.00	1.00
		o-Ethyltoluene	1.13	0.44	1.00	0.99
		p-Ethyltoluene	0.92	0.09	0.99	0.99
		n-Hexane	0.97	0.14	1.00	0.99
		Isobutane	0.97	0.16	0.99	0.99
		Isopentane	0.97	0.12	1.00	1.00
		Isoprene	0.99	0.16	1.00	0.99
		n-Pentane	1.01	0.16	0.99	0.99
		Propane	0.99	0.11	1.00	1.00
		Propylene	1.01	0.13	1.00	1.00
		Styrene	0.99	0.03	1.00	1.00
		Tetrachloroethylene	0.96	0.33	1.00	1.00
		Toluene	1.00	0.11	1.00	1.00
		trans-2-Butene	0.96	0.17	0.99	0.99
		1,2,3-Trimethylbenzene	0.94	0.34	1.00	1.00
		1,2,4-Trimethylbenzene	0.96	0.28	1.00	0.99
		2,2,4-Trimethylpentane	0.96	0.12	1.00	0.99
		o-Xylene	0.88	0.35	0.99	0.98
m-/p-Xylene	0.73	0.08	0.87	0.76		

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
C	Post-verification	Benzene	0.60	0.37	0.99	0.98
		1,3-Butadiene	0.95	0.47	1.00	1.00
		n-Butane	0.97	0.18	0.99	0.98
		1-Butene	0.96	0.20	0.99	0.98
		cis-2-Butene	0.97	0.18	0.99	0.98
		Carbon tetrachloride	0.95	0.15	1.00	0.99
		Ethane	0.96	-0.01	1.00	0.99
		Ethylbenzene	1.02	0.11	1.00	1.00
		Ethylene	0.97	0.04	1.00	0.99
		m-Ethyltoluene	0.94	0.08	1.00	1.00
		o-Ethyltoluene	1.11	0.52	0.99	0.99
		p-Ethyltoluene	0.86	0.13	1.00	0.99
		n-Hexane	0.95	0.17	0.99	0.99
		Isobutane	0.98	0.18	0.99	0.98
		Isopentane	1.07	0.00	1.00	1.00
		Isoprene	0.99	0.20	0.99	0.99
		n-Pentane	1.04	0.21	0.99	0.98
		Propane	0.99	0.20	1.00	1.00
		Propylene	0.99	0.26	1.00	1.00
		Styrene	0.97	0.04	1.00	1.00
		Tetrachloroethylene	0.93	0.58	1.00	1.00
		Toluene	1.00	0.15	1.00	1.00
		trans-2-Butene	0.96	0.21	0.99	0.98
		1,2,3-Trimethylbenzene	0.90	0.46	1.00	1.00
1,2,4-Trimethylbenzene	0.91	0.51	1.00	1.00		
2,2,4-Trimethylpentane	0.94	0.14	1.00	0.99		
o-Xylene	0.78	0.60	0.99	0.99		
m-/p-Xylene	0.97	0.12	1.00	1.00		
C	Pre-verification	Benzene	0.96	0.08	1.00	1.00
		1,3-Butadiene	0.98	0.04	1.00	1.00
		n-Butane	0.96	0.14	1.00	1.00
		1-Butene	0.96	0.14	1.00	1.00
		cis-2-Butene	0.97	0.14	1.00	1.00
		Carbon tetrachloride	0.98	0.09	1.00	1.00
		Ethane	1.04	-0.09	1.00	1.00
		Ethylbenzene	0.99	0.05	1.00	1.00
		Ethylene	1.04	-0.09	1.00	1.00
		m-Ethyltoluene	0.98	0.04	1.00	1.00

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²		
		o-Ethyltoluene	1.14	0.40	1.00	0.99		
		p-Ethyltoluene	0.98	0.05	1.00	1.00		
		n-Hexane	0.98	0.12	1.00	1.00		
		Isobutane	0.96	0.14	1.00	1.00		
		Isopentane	0.97	0.12	1.00	1.00		
		Isoprene	0.98	0.12	1.00	1.00		
		n-Pentane	0.98	0.11	1.00	1.00		
		Propane	0.99	0.01	1.00	1.00		
		Propylene	1.02	0.01	1.00	1.00		
		Styrene	1.01	0.03	1.00	1.00		
		Tetrachloroethylene	1.00	0.08	1.00	1.00		
		Toluene	1.00	0.07	1.00	1.00		
		trans-2-Butene	0.97	0.13	1.00	1.00		
		1,2,3-Trimethylbenzene	0.97	0.22	1.00	1.00		
		1,2,4-Trimethylbenzene	1.01	0.05	1.00	1.00		
		2,2,4-Trimethylpentane	0.99	0.10	1.00	1.00		
		o-Xylene	0.97	0.09	1.00	1.00		
		m-/p-Xylene	0.50	0.04	1.00	1.00		
		D	Both tests	Benzene	1.01	0.01	1.00	1.00
				1,3-Butadiene	1.01	-0.05	1.00	1.00
n-Butane	1.02			-0.03	1.00	1.00		
1-Butene	1.01			-0.05	1.00	1.00		
cis-2-Butene	1.02			-0.04	1.00	1.00		
Carbon tetrachloride	1.05			-0.08	1.00	0.99		
Ethane	1.02			-0.02	1.00	1.00		
Ethylbenzene	1.02			-0.04	1.00	1.00		
Ethylene	1.03			-0.03	1.00	1.00		
m-Ethyltoluene	1.01			-0.04	1.00	1.00		
o-Ethyltoluene	1.01			0.00	1.00	1.00		
p-Ethyltoluene	0.98			-0.02	1.00	1.00		
n-Hexane	0.88			-0.11	0.98	0.95		
Isobutane	1.02			-0.03	1.00	1.00		
Isopentane	1.01			-0.03	1.00	1.00		
Isoprene	1.03			-0.07	1.00	1.00		
n-Pentane	1.01			-0.02	1.00	1.00		
Propane	1.00			-0.01	1.00	1.00		
Propylene	1.02			-0.04	1.00	1.00		
Styrene	1.02			-0.03	1.00	1.00		
Tetrachloroethylene	1.01	-0.03	1.00	1.00				
Toluene	1.01	-0.04	1.00	1.00				

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		trans-2-Butene	1.01	-0.03	1.00	1.00
		1,2,3-Trimethylbenzene	1.01	0.02	1.00	1.00
		1,2,4-Trimethylbenzene	1.01	-0.05	1.00	1.00
		2,2,4-Trimethylpentane	1.00	-0.03	1.00	1.00
		o-Xylene	1.00	-0.05	1.00	1.00
		m-/p-Xylene	1.00	0.16	1.00	1.00
D	Post-verification	Benzene	1.02	0.06	1.00	1.00
		1,3-Butadiene	1.02	-0.04	1.00	1.00
		n-Butane	1.03	-0.03	1.00	1.00
		1-Butene	1.01	-0.03	1.00	1.00
		cis-2-Butene	1.02	-0.03	1.00	1.00
		Carbon tetrachloride	1.09	-0.05	1.00	1.00
		Ethane	1.02	0.02	1.00	1.00
		Ethylbenzene	1.03	-0.03	1.00	1.00
		Ethylene	1.03	0.00	1.00	1.00
		m-Ethyltoluene	1.01	-0.03	1.00	1.00
		o-Ethyltoluene	1.01	0.07	1.00	1.00
		p-Ethyltoluene	0.97	-0.01	1.00	1.00
		n-Hexane	0.75	0.07	1.00	1.00
		Isobutane	1.03	-0.01	1.00	1.00
		Isopentane	1.02	-0.01	1.00	1.00
		Isoprene	1.05	-0.07	1.00	1.00
		n-Pentane	1.02	0.01	1.00	1.00
		Propane	1.02	0.04	1.00	1.00
		Propylene	1.02	-0.01	1.00	1.00
		Styrene	1.00	0.01	1.00	1.00
		Tetrachloroethylene	1.00	-0.02	1.00	1.00
		Toluene	1.01	-0.03	1.00	1.00
		trans-2-Butene	1.01	-0.02	1.00	1.00
		1,2,3-Trimethylbenzene	1.01	0.09	1.00	1.00
1,2,4-Trimethylbenzene	0.99	-0.04	1.00	1.00		
2,2,4-Trimethylpentane	1.00	-0.02	1.00	1.00		
o-Xylene	1.00	-0.03	1.00	1.00		
m-/p-Xylene	0.99	0.28	1.00	1.00		
D	Pre-verification	Benzene	1.00	-0.05	1.00	1.00
		1,3-Butadiene	0.99	-0.07	1.00	1.00
		n-Butane	1.00	-0.03	1.00	1.00
		1-Butene	1.01	-0.06	1.00	1.00

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		cis-2-Butene	1.02	-0.06	1.00	1.00
		Carbon tetrachloride	1.00	-0.12	1.00	1.00
		Ethane	1.02	-0.05	1.00	1.00
		Ethylbenzene	1.02	-0.06	1.00	1.00
		Ethylene	1.02	-0.06	1.00	1.00
		m-Ethyltoluene	1.00	-0.05	1.00	1.00
		o-Ethyltoluene	1.02	-0.06	1.00	1.00
		p-Ethyltoluene	1.00	-0.04	1.00	1.00
		n-Hexane	1.01	-0.30	1.00	0.99
		Isobutane	1.01	-0.05	1.00	1.00
		Isopentane	1.01	-0.04	1.00	1.00
		Isoprene	1.02	-0.07	1.00	1.00
		n-Pentane	1.01	-0.04	1.00	1.00
		Propane	0.99	-0.06	1.00	1.00
		Propylene	1.03	-0.07	1.00	1.00
		Styrene	1.03	-0.07	1.00	1.00
		Tetrachloroethylene	1.01	-0.04	1.00	1.00
		Toluene	1.01	-0.05	1.00	1.00
		trans-2-Butene	1.00	-0.04	1.00	1.00
		1,2,3-Trimethylbenzene	1.01	-0.06	1.00	1.00
		1,2,4-Trimethylbenzene	1.04	-0.07	1.00	1.00
		2,2,4-Trimethylpentane	1.01	-0.03	1.00	1.00
		o-Xylene	1.01	-0.07	1.00	1.00
m-/p-Xylene	1.01	0.03	1.00	1.00		
E	Both tests	Benzene	0.96	0.02	1.00	1.00
		1,3-Butadiene	0.95	0.03	1.00	1.00
		n-Butane	0.96	-0.01	1.00	1.00
		1-Butene	0.94	0.05	1.00	0.99
		cis-2-Butene	0.97	0.04	1.00	1.00
		Carbon tetrachloride	0.97	-0.03	1.00	1.00
		Ethane	0.93	0.15	0.99	0.98
		Ethylbenzene	0.97	0.03	1.00	1.00
		Ethylene	0.93	0.15	0.99	0.99
		m-Ethyltoluene	1.03	-0.31	0.99	0.98
		o-Ethyltoluene	0.98	0.06	1.00	0.99
		p-Ethyltoluene	0.91	0.04	0.99	0.99
		n-Hexane	0.96	0.04	1.00	1.00
		Isobutane	0.87	0.70	0.99	0.99
		Isopentane	0.98	-0.02	1.00	1.00
		Isoprene	0.97	0.03	1.00	1.00

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		n-Pentane	0.97	0.02	1.00	1.00
		Propane	0.94	-0.01	1.00	0.99
		Propylene	0.96	0.04	1.00	0.99
		Styrene	0.95	0.04	0.99	0.99
		Tetrachloroethylene	0.93	0.04	0.99	0.98
		Toluene	0.96	0.02	1.00	0.99
		trans-2-Butene	0.95	0.11	1.00	1.00
		1,2,3-Trimethylbenzene	0.95	0.02	1.00	0.99
		1,2,4-Trimethylbenzene	0.90	-0.07	0.98	0.96
		2,2,4-Trimethylpentane	0.96	-0.04	1.00	0.99
		o-Xylene	0.94	0.04	1.00	0.99
		m-/p-Xylene	0.95	0.07	1.00	0.99
E	Post-verification	Benzene	0.92	0.06	1.00	1.00
		1,3-Butadiene	0.92	0.05	1.00	1.00
		n-Butane	0.92	0.01	1.00	1.00
		1-Butene	0.88	0.06	1.00	1.00
		cis-2-Butene	0.93	0.06	1.00	1.00
		Carbon tetrachloride	0.94	-0.01	1.00	1.00
		Ethane	0.84	0.30	1.00	1.00
		Ethylbenzene	0.92	0.05	1.00	1.00
		Ethylene	0.86	0.26	1.00	1.00
		m-Ethyltoluene	0.99	-0.46	0.99	0.99
		o-Ethyltoluene	0.93	0.09	1.00	1.00
		p-Ethyltoluene	0.85	0.03	1.00	1.00
		n-Hexane	0.92	0.06	1.00	1.00
		Isobutane	0.86	0.43	1.00	1.00
		Isopentane	0.97	-0.06	1.00	1.00
		Isoprene	0.93	0.09	1.00	1.00
		n-Pentane	0.95	0.04	1.00	1.00
		Propane	0.88	0.04	1.00	1.00
		Propylene	0.92	0.04	1.00	1.00
		Styrene	0.89	0.07	1.00	1.00
		Tetrachloroethylene	0.86	0.06	1.00	1.00
		Toluene	0.91	0.05	1.00	1.00
		trans-2-Butene	0.94	0.01	1.00	1.00
		1,2,3-Trimethylbenzene	0.89	0.04	1.00	1.00
		1,2,4-Trimethylbenzene	0.80	-0.11	1.00	1.00
2,2,4-Trimethylpentane	0.91	-0.02	1.00	1.00		
o-Xylene	0.89	0.06	1.00	1.00		

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		m-/p-Xylene	0.90	0.13	1.00	1.00
E	Pre-verification	Benzene	1.00	-0.02	1.00	1.00
		1,3-Butadiene	0.98	0.01	1.00	1.00
		n-Butane	1.00	-0.02	1.00	1.00
		1-Butene	0.99	0.03	1.00	1.00
		cis-2-Butene	1.00	0.01	1.00	1.00
		Carbon tetrachloride	1.00	-0.04	1.00	1.00
		Ethane	1.02	0.01	1.00	1.00
		Ethylbenzene	1.01	0.01	1.00	1.00
		Ethylene	1.01	0.03	1.00	1.00
		m-Ethyltoluene	1.08	-0.16	0.99	0.99
		o-Ethyltoluene	1.03	0.02	1.00	1.00
		p-Ethyltoluene	0.97	0.06	1.00	1.00
		n-Hexane	1.00	0.02	1.00	1.00
		Isobutane	0.88	0.97	1.00	0.99
		Isopentane	1.00	0.01	1.00	1.00
		Isoprene	1.01	-0.03	1.00	1.00
		n-Pentane	1.00	0.00	1.00	1.00
		Propane	0.99	-0.05	1.00	1.00
		Propylene	1.01	0.03	1.00	1.00
		Styrene	1.02	0.01	1.00	1.00
		Tetrachloroethylene	1.00	0.02	1.00	1.00
		Toluene	1.01	-0.01	1.00	1.00
		trans-2-Butene	0.97	0.22	1.00	1.00
		1,2,3-Trimethylbenzene	1.00	0.00	1.00	1.00
1,2,4-Trimethylbenzene	1.00	-0.03	1.00	0.99		
2,2,4-Trimethylpentane	1.01	-0.06	1.00	1.00		
o-Xylene	0.99	0.02	1.00	1.00		
m-/p-Xylene	1.01	0.01	1.00	1.00		
F	Both tests	Benzene	1.01	-0.14	1.00	1.00
		1,3-Butadiene	0.76	0.83	0.77	0.59
		n-Butane	1.08	-0.25	0.93	0.86
		1-Butene	0.86	0.45	0.98	0.95
		cis-2-Butene	0.85	0.43	0.97	0.94
		Carbon tetrachloride	0.84	0.79	0.95	0.90
		Ethane	1.02	-0.05	1.00	1.00
		Ethylbenzene	1.04	-0.16	1.00	0.99
		Ethylene	1.03	0.20	1.00	0.99
		m-Ethyltoluene	1.02	-0.21	1.00	0.99

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²		
		o-Ethyltoluene	1.07	-0.26	1.00	1.00		
		p-Ethyltoluene	1.00	-0.17	1.00	0.99		
		n-Hexane	1.01	-0.15	1.00	1.00		
		Isobutane	1.13	-0.42	0.94	0.89		
		Isopentane	1.06	-0.49	0.88	0.78		
		Isoprene	0.45	1.70	0.50	0.25		
		n-Pentane	1.09	-0.42	0.95	0.89		
		Propane	1.03	-0.09	1.00	0.99		
		Propylene	0.92	0.79	0.99	0.98		
		Styrene	1.26	-0.49	0.66	0.43		
		Tetrachloroethylene	0.64	0.31	0.70	0.48		
		Toluene	1.02	-0.17	1.00	1.00		
		trans-2-Butene	0.85	0.50	0.97	0.95		
		1,2,3-Trimethylbenzene	1.02	-0.17	1.00	0.99		
		1,2,4-Trimethylbenzene	0.97	-0.11	1.00	0.99		
		2,2,4-Trimethylpentane	1.03	-0.44	0.98	0.97		
		o-Xylene	1.00	-0.21	1.00	1.00		
		m-/p-Xylene	1.01	-0.38	1.00	1.00		
		F	Post-verification	Benzene	0.99	0.06	1.00	1.00
				1,3-Butadiene	0.61	1.06	0.59	0.35
n-Butane	1.13			-0.15	0.88	0.78		
1-Butene	0.84			0.02	0.99	0.99		
cis-2-Butene	0.81			-0.02	0.99	0.99		
Carbon tetrachloride	0.68			1.65	0.94	0.88		
Ethane	1.01			0.08	1.00	1.00		
Ethylbenzene	1.01			0.17	1.00	1.00		
Ethylene	1.10			0.01	1.00	1.00		
m-Ethyltoluene	0.98			0.05	1.00	1.00		
o-Ethyltoluene	1.05			-0.12	1.00	1.00		
p-Ethyltoluene	0.95			0.05	1.00	1.00		
n-Hexane	0.99			0.05	1.00	1.00		
Isobutane	1.24			-0.58	0.92	0.85		
Isopentane	1.07			-0.56	0.80	0.64		
Isoprene	0.04			2.25	0.06	0.00		
n-Pentane	1.13			-0.46	0.91	0.83		
Propane	1.02			0.20	1.00	1.00		
Propylene	0.94			0.74	0.99	0.97		
Styrene	0.36			0.25	0.99	0.99		
Tetrachloroethylene	0.20	-0.07	1.00	0.99				

Appendix A-4. Statistics for the linearity of response during verification tests (target chemicals by vendor ID)

Vendor ID	Test	Chemical	Slope	Intercept	Correlation coefficient, r	Coefficient of determination, r ²
		Toluene	0.98	0.08	1.00	1.00
		trans-2-Butene	0.80	0.09	0.99	0.98
		1,2,3-Trimethylbenzene	0.97	0.12	1.00	1.00
		1,2,4-Trimethylbenzene	0.91	0.25	1.00	0.99
		2,2,4-Trimethylpentane	0.94	0.17	0.99	0.98
		o-Xylene	0.96	-0.03	1.00	1.00
		m-/p-Xylene	0.97	0.07	1.00	1.00
F	Pre-verification	Benzene	1.04	-0.34	1.00	1.00
		1,3-Butadiene	0.91	0.60	0.99	0.99
		n-Butane	1.04	-0.34	1.00	0.99
		1-Butene	0.89	0.88	0.98	0.97
		cis-2-Butene	0.90	0.87	0.99	0.97
		Carbon tetrachloride	0.99	-0.07	0.98	0.95
		Ethane	1.03	-0.18	1.00	1.00
		Ethylbenzene	1.06	-0.49	1.00	0.99
		Ethylene	0.97	0.39	1.00	0.99
		m-Ethyltoluene	1.05	-0.47	1.00	0.99
		o-Ethyltoluene	1.09	-0.40	1.00	1.00
		p-Ethyltoluene	1.05	-0.38	1.00	0.99
		n-Hexane	1.04	-0.36	1.00	1.00
		Isobutane	1.03	-0.26	1.00	1.00
		Isopentane	1.04	-0.42	0.99	0.99
		Isoprene	0.86	1.15	0.97	0.95
		n-Pentane	1.05	-0.38	1.00	0.99
		Propane	1.03	-0.38	1.00	1.00
		Propylene	0.91	0.85	0.99	0.98
		Styrene	2.17	-1.23	1.00	0.99
		Tetrachloroethylene	1.00	0.09	1.00	1.00
		Toluene	1.05	-0.41	1.00	1.00
		trans-2-Butene	0.89	0.91	0.99	0.98
		1,2,3-Trimethylbenzene	1.06	-0.47	1.00	0.99
		1,2,4-Trimethylbenzene	1.03	-0.48	1.00	0.99
		2,2,4-Trimethylpentane	1.11	-1.05	0.99	0.97
		o-Xylene	1.04	-0.40	1.00	1.00
m-/p-Xylene	1.05	-0.82	1.00	1.00		

Summary of linearity in the verification tests, distribution across target chemicals for each vendor.

Test and vendor ID	Average slope (ppb/ppb) for priority chemicals	Standard deviation	Distribution of slope (ppb/ppb) across the priority chemicals					Example slopes for specific chemicals			
			Minimum	25th percentile	Median	75th percentile	Maximum	Ethane	1,3-Butadiene	Benzene	1,2,3-Tri-methyl-benzene
Post-verification											
A	1.07	0.69	0.77	0.99	1.04	1.17	1.33	1.00	1.08	0.82	1.27
B	1.14	1.86	0.03	1.07	1.13	1.24	2.27	1.27	1.23	1.08	1.06
C	0.95	0.49	0.60	0.94	0.96	0.99	1.11	0.96	0.95	0.60	0.90
D	1.01	0.29	0.75	1.00	1.02	1.02	1.09	1.02	1.02	1.02	1.01
E	0.90	0.21	0.80	0.88	0.92	0.93	0.99	0.84	0.92	0.92	0.89
F	0.88	1.46	0.04	0.83	0.97	1.01	1.24	1.01	0.61	0.99	0.97
Pre-verification											
A	1.14	1.10	0.73	1.03	1.12	1.24	1.68	0.73	1.07	0.76	1.38
B	1.20	1.79	0.64	1.07	1.11	1.23	2.27	0.64	1.14	1.06	1.15
C	0.97	0.53	0.50	0.97	0.98	1.00	1.14	1.04	0.98	0.96	0.97
D	1.01	0.05	0.99	1.00	1.01	1.02	1.04	1.02	0.99	1.00	1.01
E	0.99	0.16	0.88	0.99	1.00	1.01	1.08	1.02	0.98	1.00	1.00
F	1.05	1.22	0.86	0.99	1.04	1.05	2.17	1.03	0.91	1.04	1.06
Both pre- and post-verification											
A	1.09	0.72	0.78	1.01	1.08	1.20	1.32	0.88	1.06	0.78	1.29
B	1.17	1.54	0.62	1.08	1.13	1.20	2.26	0.96	1.18	1.07	1.11
C	0.96	0.38	0.73	0.96	0.97	0.99	1.13	1.00	0.96	0.78	0.94
D	1.01	0.15	0.88	1.01	1.01	1.02	1.05	1.02	1.01	1.01	1.01
E	0.95	0.15	0.87	0.94	0.96	0.97	1.03	0.93	0.95	0.96	0.95
F	0.97	0.84	0.45	0.91	1.01	1.03	1.26	1.02	0.76	1.01	1.02

Appendix A-5: Statistics on Completeness

Appendix A-5. Statistics on completeness, by vendor, for target chemicals

Chemical	CAS No	Completeness (% of tests where chemical is detected), by vendor ID					
		A	B	C	D	E	F
Benzene	71-43-2	90	100	100	100	100	97
1,3-Butadiene	106-99-0	93	100	100	100	100	87
n-Butane	106-97-8	90	93	100	100	100	93
1-Butene	106-98-6	93	100	100	100	100	93
cis-2-Butene	590-18-1	93	93	100	100	100	93
Carbon tetrachloride	56-23-5	0	83	100	100	100	100
Ethane	74-84-0	86	100	100	100	100	93
Ethylbenzene	100-41-4	90	100	100	100	100	97
Ethylene	74-85-1	86	100	100	100	100	93
m-Ethyltoluene	620-14-4	93	3	100	100	100	100
o-Ethyltoluene	611-14-3	93	100	82	100	100	93
p-Ethyltoluene	622-96-8	93	90	100	100	100	100
n-Hexane	110-54-3	90	100	100	100	100	100
Isobutane	75-28-5	90	90	100	100	100	93
Isopentane	78-78-4	90	93	79	100	100	93
Isoprene	78-79-5	79	87	100	100	100	93
n-Pentane	109-66-0	90	100	100	100	100	93
Propane	74-98-6	86	100	100	100	100	93
Propylene	115-07-1	90	90	100	100	100	93
Styrene	100-42-5	93	100	100	100	100	100
Tetrachloroethylene	127-18-4	86	100	100	100	100	83
Toluene	108-88-3	93	100	100	100	100	100
trans-2-Butene	624-64-6	93	100	100	100	100	87
1,2,3-Trimethylbenzene	526-73-8	93	100	100	100	100	100
1,2,4-Trimethylbenzene	95-63-6	93	100	100	100	100	97
2,2,4-Trimethylpentane	540-84-1	86	100	100	100	100	97
o-Xylene	95-47-6	93	100	100	100	100	97
m-/p-Xylene	1330-20-7	93	100	100	100	100	100

Vendor	Average completeness for target chemicals (% of tests)	Standard deviation across target chemicals (%)	Distribution of completeness across the target chemicals (% of tests where chemical is detected)					Examples of completeness for specific chemicals			
			Minimum	25th percentile	Median	75th percentile	Maximum	Ethane	1,3-Butadiene	Benzene	1,2,3-Tri-methyl-benzene
A	87.1	92.1	0.0	88.8	89.7	93.1	93.1	86	93	89.7	93.1
B	93.7	97.2	3.3	93.3	100.0	100.0	100.0	100	100	100.0	100.0
C	98.6	27.4	78.6	100.0	100.0	100.0	100.0	100	100	100.0	100.0
D	100.0	0.0	100.0	100.0	100.0	100.0	100.0	100	100	100.0	100.0
E	100.0	0.0	100.0	100.0	100.0	100.0	100.0	100	100	100.0	100.0
F	95.0	23.3	83.3	93.3	93.3	100.0	100.0	93	87	96.7	100.0

Appendix A-6: Statistics on MDL

Appendix A-6. Results of MDL Tests - ppbv																		
Compound	A			B			C			D			E			F		
	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg
Benzene	1.09	0.10	0.59	0.12	0.07	0.09	0.07	0.03	0.05	0.02	0.02	0.02	0.01	0.01	0.01			
1,3-Butadiene	0.16	0.22	0.19	0.03	0.02	0.03	0.09	0.04	0.06	0.02	0.06	0.04	0.02	0.02	0.02			
n-Butane	0.20	0.13	0.16	0.59	0.03	0.31	0.03	0.05	0.04	0.03	0.03	0.03	0.03	0.03	0.03	0.25	0.39	0.25
1-Butene	0.18	0.26	0.22	0.02	0.04	0.03	0.03	0.04	0.03	0.02	0.02	0.02	0.02	0.01	0.02	0.21	0.22	0.21
cis-2-Butene	0.19	0.50	0.35	0.02	0.03	0.03	0.03	0.04	0.04	0.01	0.03	0.02	0.02	0.02	0.02	0.26	0.26	0.26
Ethane				0.73	0.76	0.74	0.08	0.07	0.08	0.02	0.05	0.05	0.31	0.47	0.39	0.15	0.16	0.15
Ethylbenzene	0.17		0.17	0.06	0.03	0.04	0.02	0.02	0.02	0.02	0.02	0.02	0.03	0.03	0.03	0.19	0.34	0.19
m-Ethyltoluene	0.23		0.23				0.03	0.03	0.03	0.03	0.02	0.03	0.03	0.06	0.04			
o-Ethyltoluene	0.08		0.08	0.07	0.03	0.05	0.03	0.04	0.04	0.02	0.01	0.02	0.04	0.06	0.05	0.17	0.29	0.17
p-Ethyltoluene	0.12		0.12	0.06	0.09	0.07	0.02	0.02	0.02	0.02	0.02	0.02	0.07	0.03	0.05	0.20	0.23	0.20
n-Hexane	0.09		0.09	0.13	0.04	0.09	0.03	0.05	0.04	0.13	0.04	0.08	0.02	0.03	0.03			
Isobutane	0.19	0.15	0.17	0.05	0.09	0.07	0.03	0.04	0.04	0.04	0.02	0.03	0.68	0.41	0.54	0.19	0.27	0.19
Isopentane	0.13	0.08	0.10	0.02	0.04	0.03	0.02	0.05	0.04	0.01	0.02	0.02	0.09	0.16	0.12	0.47	0.84	0.47
n-Pentane	0.52	0.10	0.31	0.06	0.03	0.04	0.06	0.03	0.04	0.01	0.03	0.02	0.05	0.06	0.06	0.23	0.29	0.23
Propane	1.10	0.19	0.65	0.11	0.06	0.08	0.04	0.04	0.04	0.05	0.04	0.04	0.04	0.06	0.05	0.14	0.18	0.14
Propylene	0.37	0.23	0.30	0.05	0.08	0.07	0.04	0.04	0.04	0.05	0.06	0.05	0.04	0.05	0.04	0.15	0.11	0.15
Styrene				0.05	0.02	0.04	0.02	0.03	0.02	0.02	0.06	0.04	0.04	0.27	0.15	0.16	0.25	0.16
Tetrachloroethylene	0.10		0.10	0.02	0.02	0.02	0.03	0.02	0.03	0.03	0.04	0.03	0.01	0.02	0.01	0.13	0.09	0.13
Toluene	0.13		0.13	0.03	0.03	0.03	0.02	0.02	0.02	0.01	0.02	0.02	0.02	0.03	0.03	0.53	0.53	0.53
trans-2-Butene	0.16	0.13	0.15	0.03	0.04	0.04	0.03	0.04	0.04	0.03	0.02	0.03	0.05	0.13	0.09	0.29	0.29	0.29
1,2,4-Trimethylbenzene	0.03	0.85	0.44	0.05	0.05	0.05	0.07	0.06	0.07	0.02	0.02	0.02	0.08	0.07	0.07	0.23	0.41	0.23
2,2,4-Trimethylpentane	0.04		0.04	0.06	0.05	0.05	0.20	0.07	0.14	0.01	0.02	0.02	0.10	0.04	0.07			
o-Xylene	0.07		0.07	0.08	0.02	0.05	0.02	0.30	0.16	0.03	0.02	0.02	0.04	0.03	0.03	0.20	0.24	0.20
m-/p-Xylene	0.20		0.20	0.15	0.05	0.10	0.09	0.15	0.12	0.03	0.10	0.06	0.01	0.02	0.02	0.15	0.23	0.15

Appendix A-6. Results of MDL Tests - ppb-c																		
Compound	A			B			C			D			E			F		
	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg	Test 1	Test 2	Avg
Benzene	6.53	0.60	3.57	0.71	0.41	0.56	0.44	0.16	0.30	0.11	0.14	0.13	0.06	0.06	0.06			
1,3-Butadiene	0.64	0.87	0.76	0.13	0.09	0.11	0.35	0.15	0.25	0.09	0.23	0.16	0.06	0.07	0.06			
n-Butane	0.79	0.52	0.66	2.35	0.12	1.24	0.12	0.20	0.16	0.12	0.12	0.12	0.11	0.11	0.11	0.43	1.57	1.00
1-Butene	0.73	1.02	0.88	0.08	0.18	0.13	0.10	0.15	0.13	0.10	0.08	0.09	0.09	0.05	0.07	0.84	0.87	0.85
cis-2-Butene	0.77	2.00	1.38	0.10	0.12	0.11	0.13	0.16	0.14	0.05	0.10	0.08	0.08	0.07	0.08	1.00	1.04	1.02
Ethane				1.45	1.52	1.49	0.17	0.14	0.15	0.09	0.10	0.10	0.61	0.93	0.77	0.25	0.33	0.29
Ethylbenzene	1.36		1.36	0.51	0.21	0.36	0.16	0.17	0.17	0.15	0.15	0.15	0.21	0.22	0.22	0.34	2.68	1.51
m-Ethyltoluene	2.11		2.11				0.23	0.23	0.23	0.29	0.21	0.25	0.29	0.51	0.40			
o-Ethyltoluene	0.75		0.75	0.66	0.29	0.47	0.27	0.40	0.33	0.20	0.12	0.16	0.36	0.52	0.44	0.41	2.62	1.51
p-Ethyltoluene	1.06		1.06	0.52	0.80	0.66	0.21	0.22	0.21	0.19	0.20	0.19	0.66	0.29	0.48	1.61	2.03	1.82
n-Hexane	0.54		0.54	0.80	0.24	0.52	0.16	0.32	0.24	0.78	0.21	0.49	0.14	0.16	0.15			
Isobutane	0.75	0.60	0.68	0.21	0.37	0.29	0.12	0.17	0.15	0.14	0.07	0.10	2.72	1.63	2.18	0.43	1.08	0.76
Isopentane	0.66	0.39	0.52	0.10	0.18	0.14	0.12	0.25	0.19	0.07	0.10	0.09	0.44	0.80	0.62	0.48	4.22	2.35
n-Pentane	2.62	0.52	1.57	0.29	0.14	0.21	0.29	0.15	0.22	0.03	0.13	0.08	0.23	0.32	0.28	0.84	1.43	1.14
Propane	3.31	0.57	1.94	0.33	0.17	0.25	0.13	0.12	0.12	0.15	0.11	0.13	0.11	0.17	0.14	0.29	0.54	0.41
Propylene	1.10	0.70	0.90	0.16	0.24	0.20	0.12	0.11	0.12	0.14	0.18	0.16	0.11	0.14	0.12	0.59	0.33	0.46
Styrene				0.42	0.16	0.29	0.12	0.20	0.16	0.14	0.49	0.31	0.30	2.16	1.23	0.54	1.97	1.25
Tetrachloroethylene	0.19		0.19	0.05	0.05	0.05	0.07	0.04	0.06	0.05	0.07	0.06	0.03	0.03	0.03		0.19	0.19
Toluene	0.94		0.94	0.21	0.18	0.19	0.11	0.15	0.13	0.10	0.16	0.13	0.16	0.22	0.19		3.72	3.72
trans-2-Butene	0.66	0.52	0.59	0.11	0.18	0.14	0.14	0.18	0.16	0.13	0.09	0.11	0.18	0.51	0.34	1.18	1.16	1.17
1,2,4-Trimethylbenzene	0.24	7.68	3.96	0.43	0.45	0.44	0.64	0.56	0.60	0.17	0.17	0.17	0.71	0.63	0.67		3.68	3.68
2,2,4-Trimethylpentane	0.30		0.30	0.44	0.40	0.42	1.59	0.59	1.09	0.10	0.15	0.12	0.83	0.29	0.56			
o-Xylene	0.56		0.56	0.61	0.19	0.40	0.19	2.43	1.31	0.21	0.17	0.19	0.31	0.24	0.27	1.34	1.91	1.62
m-/p-Xylene	1.63		1.63	1.17	0.42	0.79	0.75	1.23	0.99	0.22	0.81	0.51	0.10	0.17	0.14	0.00	1.87	1.87

