Gas Chromatograph (GC) Evaluation Study

Laboratory Evaluation Phase Report

Prepared by
RTI International and EC/R Incorporated
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Table of Contents

Table of Figures

Table of Tables

1.0 Introduction

1.1 Background

On February 12, 1993, the US 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 (O_3), oxides of nitrogen (NO_x), volatile organic compounds (VOCs), selected carbonyl compounds, and monitoring of meteorological parameters. The revisions required States and local monitoring agencies to establish Photochemical Assessment Monitoring Stations (PAMS) in ozone nonattainment areas classified as serious, severe, or extreme.

Monitoring agencies are 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. 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.

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 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, Work Assignment (WA) 2-01. EC/R designated their subcontractor, RTI International the role of accomplishing the tasks described in Automated GC Evaluation WA. These tasks consisted of a literature search of auto-GC vendors; developing a test plan and Quality Assurance Project Plan (QAPP) for the laboratory and field deployment phases; conducting a laboratory evaluation; and conducting a field deployment evaluation at PAMS locations throughout the US.

1.2 Identification of Candidate Instrument Vendors

The first task completed by the RTI team was to develop an approach to locate vendor candidates of auto-GC units. This approach consisted of generating a comprehensive list of potential candidates both domestically and internationally. RTI staff conducted an initial search on Internet sites such as www.chromatographyonline.com; trade publications including LC/GC that lead to gas chromatograph vendors; and Exhibitor lists from recent meetings of the American Chemical Society, Pittcon, and the Air & Waste Management Association. Further information was congregated by conducting Google searches on the Internet utilizing truncated forms of the "*" wildcard character with key search terms such as "gas chromatography system" combined with descriptors indicating more application-specific terms, such as "field", "portable", "automated", "on-line", and "process". The EPA also directly provided a few potential candidates that were not located by RTI staff using the above search.

Where possible, the website of each vendor was visited to verify an auto-GC unit was commercially available and that it was not a re-branded device from another manufacturer. Contact information was requested and compiled into a spreadsheet to be used for direct contact with the manufacturer. Through these processes, over 40 potential vendors were identified and contacted.

In order to evaluate and collect the same type of information from each vendor candidate, a detailed questionnaire was developed and sent to each candidate to complete. Direct contact by telephone was attempted with a representative of each vendor, otherwise, e-mails were sent to a point of contact indicated on the website.

The purpose and general design of the study, as well as the criteria for inclusion, were described and the vendor was asked to complete and return the completed questionnaire. Information from the questionnaire was transferred back into the spreadsheet, and any missing information was obtained by follow-up conversations with the vendor. Information for all vendors who indicated an interest in participating was then forwarded to EPA for final selection of the laboratory phase participants. Based on the information provided from the list of interested candidate participants, the EPA technical team reviewed the detailed specifications of each vendor's auto-GC unit and reduced the number of candidates down to fewer than 10 participants for the laboratory evaluation phase. Details regarding the selected and participating vendors can be found in Section 3.

1.3 Test Plan and QAPP Development

Prior to conducting the Laboratory Evaluation Phase, the RTI team developed a test plan and QAPP that was 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 was developed by RTI, working closely with the EPA Work Assignment Manager (WAM), and described the activities to be conducted during an RTI-based laboratory evaluation phase, as well as a subsequent field deployment phase at selected PAMS locations. During both implementation phases, the overall objective was to challenge the candidate automated-GC units with a breadth of technical and environmental conditions in a manner sufficiently rigorous to reveal performance and capability differences between 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 and was prepared based on EPA guidelines for collecting environmental data, which are detailed in the guidance document entitled "*Guidance for Quality Assurance Project Plans (QA/G-5)*". RTI worked with the EPA 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 evaluation phases.

1.4 Laboratory Evaluation Phase

The laboratory evaluation phase was conducted at RTI's Air Monitoring Laboratory (Building 3, Room 219) over the course of a four month period. The steps involved and the subsequent results are discussed in Section 2. 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 vendor candidates performed the installation, setup, and calibration of their auto-GC units. During the evaluation, the candidates operated their equipment and provided data to RTI staff overseeing the evaluation. At the conclusion of the laboratory evaluation phase, RTI prepared and submitted data packets back to each vendor for validation so that it could be used to prepare this report.

1.5 Field Deployment Phase

Based on the results contained in the laboratory evaluation report, the EPA WAM will select four candidate auto-GC units to be installed in a mobile laboratory. This laboratory will be moved to each of the PAMS locations in the next WA. A 30-day test study will be performed at each of the field locations. At the conclusion of the field evaluation phase, RTI will analyze the field data and prepare a summary report of the field activities and results. The mobile laboratory and all equipment, supplies, and materials will be returned to EPA at the conclusion of the field deployment study.

2.0 Overview of Laboratory Evaluation Phase

2.1 Schedule of Activities

The laboratory evaluation phase of the GC study was initially scheduled to be completed near the end of the 2013 calendar year, however due to unforeseen circumstances and beyond the control of the EPA and RTI, the schedule was pushed back to the first quarter of 2014. The Laboratory Evaluation was comprised of four key phases: a laboratory setup, the candidate vendors shipping and setting up their equipment, the laboratory evaluation, and the vendor candidates removing their units at the completion of the study. These four phases occurred over a four month time span (January through April 2014).

Prior to the laboratory evaluation, the RTI team worked with the EPA WAM and EPA QA Officer to develop a test plan and QAPP as described in Section 1.3. An initial draft test plan and QAPP were submitted to EPA for review on February 24, 2014. These documents were revised based on recommended changes from EPA and time restrictions to complete the laboratory evaluation study by April 30, 2014. The revised documents were submitted the EPA WAM and EPA QA Officer for review on March 6 and were later approved for the laboratory evaluation phase on March 11, 2014. The QAPP with the test plan as an appendix was electronically submitted to each vendor candidate on March 11.

2.2 Laboratory Setup

The RTI team began implementing a plan to arrange the Air Monitoring Laboratory in Building 3 (Room 219) on RTI's campus for the GC Laboratory Evaluation Phase in early January 2014. The plan was developed to ensure the testing system provided equal distribution of deliverable concentration gas under controlled temperature and relative humidity to each of the sampling ports. The basic overview of the laboratory setup is displayed in **Figure 2-1**. A 10-port glass manifold (constructed by URG Corporation, Chapel Hill, NC) and dilution system (Environics® Series 2014 Computerized VOC Gas Dilution System and Environics® Series 7000 Zero Air Generator) were configured to deliver standard gas mixtures to candidate auto-GC units. Two VOC blends (Spectra VOC Standards US EPA PAMS and USA 112 VOC Standards) prepared by Linde Electronic and Specialty Gases were used to make dilutions over a range of evaluation concentrations by proportionating the flows of the standard mixture with high-purity zero air. The VOC Standards US EPA PAMS mixture contains 56 VOCs ranging in concentrations from 20 to 60 ppb carbon (ppbC). The initial intent was to use the Spectra VOC Standards TCEQ (Texas Commission on Environmental Quality) that contains 102 VOCs. The planned TCEQ mixture contains all 56 of the VOCs also contained in the PAMS blend at concentrations typically near 100 ppb volume/volume (ppbV) as well as some VOCs that occur in certain locations in the US. Electronic copies of the CoA documents are maintained on the RTI secure server under the Project Folder.

Prior to any setup, each piece of equipment and all supplies were confirmed to be in working order, or in satisfactory condition for use in testing. Equipment was tested thoroughly, and general troubleshooting activities were performed as needed. The laboratory space was cleaned and shelving was configured or removed as needed to ensure dilution system could function as intended. All nonessential equipment was relocated to allow for adequate vendor instrument space.

By the end of January (January 27), RTI had received the dilution system, zero air generator, NIST-traceable gas mixtures, and necessary materials and supplies to construct the overall testing system for the laboratory evaluation. The supply lines for the testing system were made of ¼" 316 stainless steel (SS) tubing with Swagelok fittings. Each stainless steel line used in the dilution system was cut to length and cleaned by actively pulling approximately 300mL of hexane followed by 300mL of Isopropyl Alcohol through each line using vacuum filtration. To distribute the sample ports, each line was bent at varying spots and angles to reach designated areas of the laboratory. The manifold and each sample line were affixed to various points in the lab using metal clips to ensure components did not detach during testing. All SS tubing, fittings, and manifold were wrapped with thermostat-controlled heating tapes. The complete system was covered with insulation wrap.

To incorporate moisture into the challenge gas line, an RH system was created and placed downstream of the gas dilution system and upstream of the manifold.

As shown in Figure 2-1, the test concentration exited the gas dilution system and enters the relative humidity (RH) system. The RH system consisted of a sample intake line which was split into two. One of the lines forced flow through a borosilicate glass bubbler filled with deionized water. The second line bypassed the bubbler system and had a variable flow control valve attached to it. Both lines were connected immediately after the bubbler system and the amount of moisture in the line was controlled by portioning the flow allowed to bypass the bubbler (if the variable valve was completely "open", all flow went around the bubbler and the moisture in the line was near zero). An additional line was fixed to the setup prior to the bubbler to allow for passive collection of sorbent tubes to be used as a control sample (same concentration of gas in system with no significant temperature or RH change from gas dilution system). The test concentration gas left the RH system and enters the 10-port borosilicate manifold. SS lines ran from the manifold to each of the sampling ports where the vendor candidate collected the test samples.

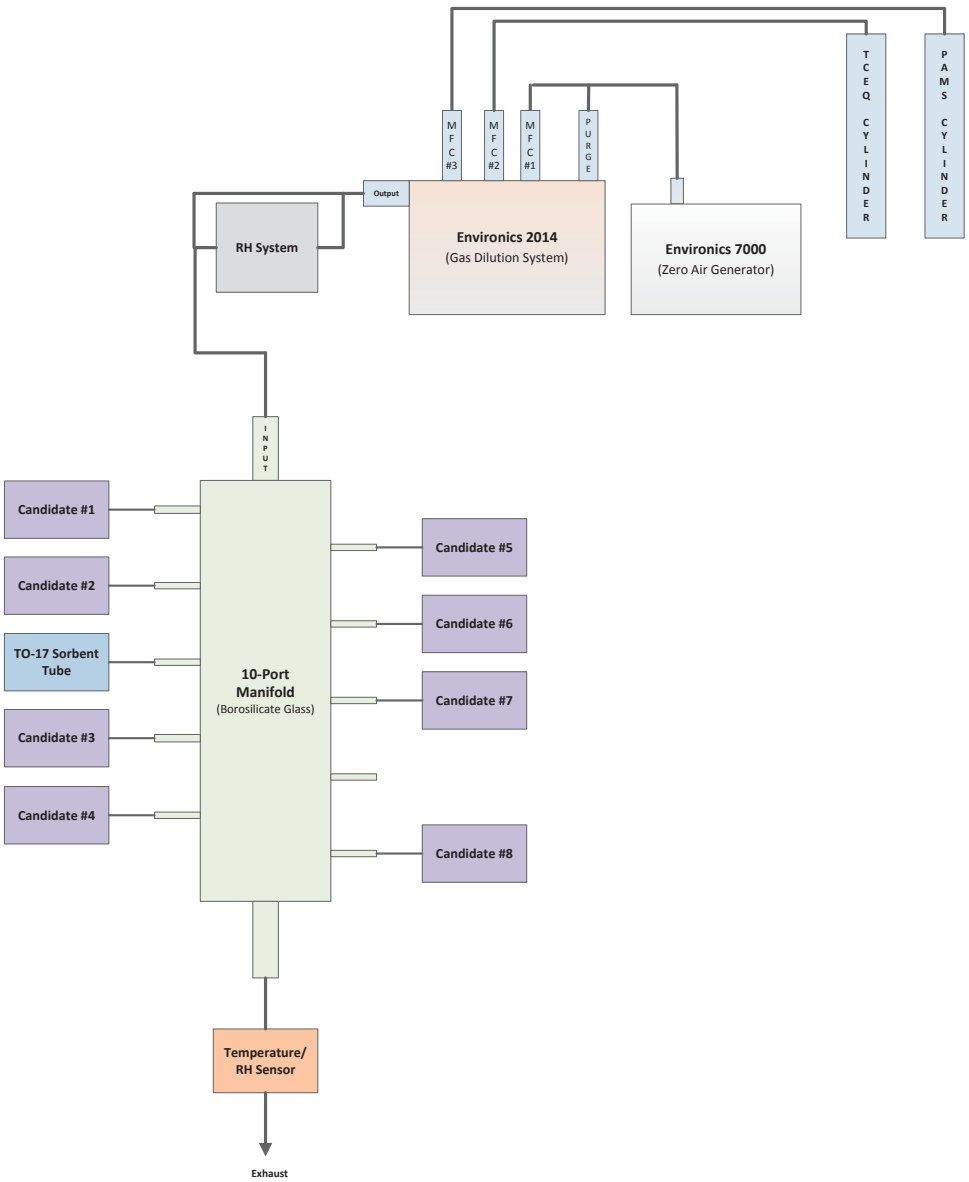


Figure 2-1: Dilution System Overview

The test plan outlined four tests to be completed before the laboratory evaluation phase could begin. These tests ensured the integrity of the system by confirming there were no leaks, verifying there was adequate flow at each sample port, ensuring temperature levels were adjustable and maintainable, ensuring relative humidity (RH) levels were adjustable and maintainable, verifying gas dilution system points were achievable and stable, and data logging occurred and was retrievable. From February 7 through March14, the RTI team conducted the following tests:

1. Ran zero air and confirm no leaks and proper flow rates to the delivery system.
2. Verified the testing system (manifold and in the associated transfer tubing) could maintain the temperature ranges from ambient (20 °C) to 35 °C using zero air at the targeted flow rate of 3 L/min.
3. Verified the testing system (manifold and in the associated transfer tubing) could maintain the RH conditions of 20%, 30%, 50%, and 70% using zero air at the targeted flow rate of 3 L/min.
4. Ran test dilutions to confirm all ports are receiving proper concentrations. Verified the test concentrations by using sorbent tubes under TO-17 Method.

(Test 1) Flow and leak check tests were executed in two phases. The first was a closed system phase where the ends of each line were capped and the flow was measured first at the exhaust port, then at each of the sample ports one at a time. The tests were conducted at flows varying from 3 L/min to 7 L/min. An average loss of less than 1% at each of the sample ports was measured and overall a system loss of <1% was measured at the exhaust line. The second phase was an open line test (at 3 L/min), where small individual pumps were attached to each sample ports to mimic the flow of what the vendor instruments would require under the actual testing. The pumps were set to pull slightly in excess of what each vendor indicated their required flow rate would be, and the total system flow was set to mimic testing conditions. The open line test confirmed an excess flow was present in the exhaust line to ensure adequate sample was available to each candidate instrument during challenge gas testing.

(Test 2 and 3) The temperature system and RH system were tested concurrently at the parameter settings used during the lab testing (20% RH/30°C, 50% RH/25°C, 70% RH/35°C). Based on the system setup, each line was independently set to achieve the desired temperature setting. After the temperature at each port attained the target temperature within ±2°C, the temperature values were recorded, and the settings for each heating coil were noted for future use. All port temperatures were checked using the NIST-traceable Omega thermometer; all post manifold temperatures were recorded using the NIST-traceable Entech 42280 RH/temp datalogger. All temperature targets were achieved prior to any testing. The RH was not independently adjustable, so once the target RH at the datalogger at the end of the manifold was achieved within an absolute value of ±7% (i.e., 70 ±75%), the settings for the bubbler valve flow and rheostat settings were noted for future use. After the RH at the end of the manifold had been established and was stable, the RH/temp datalogger was moved to each of the ports to verify systematic % RH. Each port was within ±3% of the observed post manifold value during this testing, indicating an evenly distributed moisture level through the system.

(Test 4) After test point concentrations were assigned, a spreadsheet was used to confirm all the points could be delivered by the gas dilution system based on the concentration of benzene in the provided NIST-traceable gas mixtures. The gas dilution system was programmed with each target concentration to be used during the study, and was programmed with schedule of events of the study to automatically introduce the gas concentrations at each time point listed in the QAPP/test plan.

The final step in the 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 ninth “candidate” was a viable method to be used for candidate comparison, and
4. There was near equal distribution of challenge gas at each of the ports.

Sorbent tube samples were collected at five of the concentrations and under all the temperature/RH conditions 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% 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 March 24th, and blank zero-air was run through the system for the week leading up to the testing (which was also the vendor setup week).

2.3 Vendor Setup

The vendor candidates sent their auto-GC units and supportive materials and supplies to RTI from March 17 through 20 and vendor setup occurred from March 24 through 28. Each vendor was afforded two weeks of time to ship and install any necessary equipment for the testing in the lab phase of the study. The time taken for instrument installation, instrument footprint, number of personnel for setup, and supplies utilized varied greatly. All candidates demonstrated thorough knowledge of their equipment and vendor staff had sufficient capabilities for installation/setup. A summary of RTI staff observations for each vendor is included below in this section.

During the vendor setup, the RTI team documented some of the activities of the eight vendors. These activities could provide some subjective information to determine the usability and reliability of each auto-GC unit. Any information gathered by RTI is electronically maintained in the Setup Folder for each vendor on RTI's secure server under the Project Folder. Below are some brief points for some of the vendors that pertain to usability of the auto-GC units such as their ability to operate the auto-GC unit remotely; the ability of the auto-GC unit to perform auto calibrations and post automatic data flagging; the space requirement for the auto-GC unit at the field site; the required knowledge of the laboratory analyst or field operator; and the ease of operation, maintenance, and repair of the auto-GC unit. Reliability factors such as the frequency of maintenance, frequency of calibration, and robustness for field use were hard to distinguish during the vendor setup or laboratory evaluation phase, but the time each vendor took for troubleshooting and calibration should provide valuable insight regarding the frequency for maintenance and calibration for each of the auto-GC units.

Observation 1
One Vendor had their equipment shipped and setup a three module system containing an FID, a PID, and a preconcentrator. This auto-GC unit required use of a tank of hydrogen gas and a tank of zero air gas, both of which were arranged for and provided by the vendor. The vendor also brought a cylinder of certified blended VOC gas to use. The install, setup, calibration, and troubleshooting was performed by three staff members over a three days period at approximately six hours per day per person. The estimated footprint of this auto-GC unit was 32" (Depth) by 42" (Length).

Observation 2
A vendor wheeled their complete auto-GC unit in a single transporting cabinet that housed a five module system consisted of a C2-C6 analyzer, a C6-C12 analyzer, a hydrogen generator, a zero air generator, and a calibration system. The system required use of a small vacuum pump. Two staff members were present for two days for approximately six hours per day to troubleshoot and calibrate the auto-GC unit. Three other staff members were present for two days for approximately four hours per day to complete the setup and run initial tests. The estimated footprint of the instrument is 48" (Tall) by 27" (Depth) by 30" (Wide).

Observation 3
Another vendor had a system comprised of a front end sampler unit with a GC/MS bench top unit. The vendor equipment required the use of three support gases: helium and zero air that was provided by RTI and nitrogen which was provided by the vendor. Other equipment included various dryers and purifiers, and a vacuum pump which were brought by the vendor. Four staff members were present for two days for approximately five hours per day, two staff members were present for one day for six hours, and one staff member was present for two days for approximately five hours per day to complete the setup and run initial tests. The estimated footprint of the instrument is 32" (Depth) by 72" (Length).

Observation 4
A vendor had a system comprised of a front end sampler unit and a GC bench top system. The auto-GC unit required the use of hydrogen, helium and zero air provided by RTI and various dryers, purifiers, and columns provided by vendor. Two staff members were present for two days for approximately five hours per day, three staff members were present for an additional three days for approximately six hours per day, one staff member was present for three days for 5 hours per day, and one day a group of four people were present for 6 hours to complete the setup and run initial tests. The estimated footprint of the instrument is 32" (Depth) by 92" (Length).

Observation 5
Another vendor had a system comprised of a GC unit with a front end sampler included. The system required the use of hydrogen, helium and zero air provided by RTI. The vendor also used an air compressor and zero-air generator to provided additional gas flow. Other equipment included various dryers, purifiers, and columns brought by the vendor. Three staff members were present for three days for approximately six hours per day, and one staff member was present for two days for 3 hours per day to complete the setup and run initial tests. The estimated footprint of the instrument is 32" (Depth) by 92" (Length).

Observation 6
One vendor had a system comprised of just a GC unit that did not require ancillary equipment. One staff member was present for three days for approximately five hours per day to complete the setup and run initial tests. The estimated footprint of the instrument is 32" (Depth) by 32" (Length).

Observation 7
Another vendor's system comprised of a GC unit with a front end sampler. The auto-GC unit required the use of only hydrogen that was provided by RTI. Other equipment included a small customized refrigerator for use as a cold trap. One staff member was present for two days for approximately six hours per day to complete the setup and run initial tests. The estimated footprint of the instrument is 32" (Depth) by 54" (Length).

Observation 8
Another vendor had a system comprised of a two module units with a PID and a PID/FID sampler. The vendor equipment required the use of hydrogen and zero air provided by RTI (for part of the testing period a vendor provided zero air generator was utilized), and nitrogen provided by candidate. Other equipment included a dryer tube provided by RTI. Three staff members were present for two days for approximately five hours per day, and two staff members were present for two days for approximately three hours per day to complete the setup and run initial tests. The estimated footprint of the instrument is 27" (Depth) by 58" (Length).

During the vendor setup, some vendors requested that RTI provide calibration gases from the NIST-traceable gas cylinders that RTI planned to use during the laboratory phase. After some discussion with the EPA WAM, it was decided to provide the vendors some gas concentrations for them to use to adjust/calibrate their auto-GC units. The gas concentrations were provided on March 26th, 27th, and 28th as shown below in **Table 2-1**. The design to provide a zero air and three test points was consistent with what the daily activities would be for the laboratory evaluation. The sample time was designed so the vendors could pull two 1-hour samples.

Date	Test Point	Gas Concentration	Time for Sampling
3/26	1	Zero air	1230 to 1420
	2	0.5 ppb benzene from PAMS cylinder	1445 to 1620
	3	1.5 ppb benzene from PAMS cylinder	1645 to 1820
	4	3ppb benzene from PAMS cylinder	1845 to 2020
3/27	1	Zero air	1230 to 1420
	2	0.5 ppb benzene from TCEQ cylinder	1445 to 1620
	3	5.0 ppb benzene from TCEQ cylinder	1645 to 1820
	4	12.0 ppb benzene from TCEQ cylinder	1845 to 2020

3/28	1	Zero air	1230 to 1420
	2	0.5ppb benzene from PAMS cylinder	1445 to 1620
	3	1.5 ppb benzene from PAMS cylinder	1645 to 1820
	4	2 ppb benzene from PAMS cylinder	1845 to 2020

Table 2-1: Gas Concentrations Provided Surfing the Vendor Setup

During the testing listed above, it was determined that Linde Electronic and Specialty Gases provided RTI with the wrong cylinder mixture. Several of the vendors were detecting acetone that was not in the PAMS or TCEQ blends. The blend actually provided by Linde was an USA 112 VOC Standard blend. This resulted in an issue for the laboratory evaluation phase because the USA 112 was missing 20 PAMS compounds from the Exhibit 4 of the QAPP. These missing compounds are listed below:

Cyclopentane	2, 3-Dimethylbutane	2, 3-Dimethylpentane	m-Diethylbenzene
m-Ethyltoluene	3-Methylheptane	2-Methylpentane	2, 3, 4-Trimethylpentane
p-Diethylbenzene	3-Methylhexane	2, 4-Dimethylpentane	1-Hexene
Methylcyclohexane	Methylcyclopentane	2-Methylhexane	3-Methylpentane
2, 2-Dimethlybutane	o-Ethyltoluene	2-Methylheptane	1, 2, 3-Trimethylbenzene

In order for the vendors to know which VOCs needed to be reported during each test point of the laboratory evaluation phase, RTI provided them with **Table 2-2** (displayed below) of the gas blends to be used for each test point. Where TCEQ is listed, it was actually the USA 112 blend. Each vendor was also supplied with the list of compounds in the USA 112 blend so that they could assign peaks (if needed) as interferents.

Day	Test	Gas Blend	Day	Test	Gas Blend	Day	Test	Gas Blend
The Day and Test Number can be found in the test plan (Appendix A of the QAPP).								
Test Conditions: 30˚ C and 20% RH			Test Conditions: 25˚ C and 50% RH			Test Conditions: 35˚ C and 70% RH		
1	1	Zero Air	1	4	Zero Air	1	7	Zero Air
	2	TCEQ	2		TCEQ	2		TCEQ
	3	PAMS	3		PAMS	3		PAMS
	4	TCEQ	4		TCEQ	4		TCEQ
	5	TCEQ	5		TCEQ	5		TCEQ
	6	TCEQ	6		TCEQ	6		TCEQ
2	1	Zero Air	1	5	Zero Air	1	8	Zero Air
	2	TCEQ	2		TCEQ	2		TCEQ
	3	PAMS	3		PAMS	3		PAMS
	4	TCEQ	4		TCEQ	4		TCEQ
	5	TCEQ	5		TCEQ	5		TCEQ
	6	TCEQ	6		TCEQ	6		TCEQ
3	1	Zero Air	1	6	Zero Air	1	9	Zero Air
	2	TCEQ	2		TCEQ	2		TCEQ
	3	PAMS	3		PAMS	3		PAMS
	4	PAMS	4		PAMS	4		PAMS
	5	TCEQ	5		TCEQ	5		TCEQ
	6	PAMS	6		PAMS	6		PAMS

Table 2-2: Gas Blends Used During the Laboratory Evaluation Phase

2.4 Laboratory Evaluation

The laboratory evaluation was conducted from March 31, 2014 to April 10, 2014. Prior to the initiation of testing, the EPA technical team visited the laboratory to verify the testing system was adequate to proceed with testing.

At the start and end of each test day the temperature and relative humidity readings for the testing system were recorded using the NIST-traceable Extech datalogger. During the testing, the temperature and RH readings were observed and adjusted as needed. The excess flow coming from the exhaust line of the manifold was also

recorded each morning. The average temperature and RH information for each of the test days (as recorded by the Extech datalogger) is displayed in the **Table 2-3**. For each of the days, all temperature readings were within the acceptance limits stated in the QAPP (±2°C and ±7% RH) and there was excess flow present at the exhaust.

Day	Target Temperature	Target Relative Humidity	Measured Temperature		Measured Relative Humidity	
			Average	Standard Deviation	Average	Standard Deviation
1	30˚ C	20 %	30.3˚ C	1.5˚ C	24.1 %	4.0 %
2	30˚ C	20 %	28.6˚ C	1.1˚ C	23.8 %	4.4 %
3	30˚ C	20 %	30.7˚ C	0.55˚ C	19.8 %	3.6 %
4	25˚ C	50 %	25.8˚ C	0.32˚ C	51.6 %	3.8 %
5	25˚ C	50 %	25.8˚ C	0.25˚ C	49.3 %	3.5 %
6	25˚ C	50 %	25.6˚ C	0.17˚ C	51.2 %	4.0 %
7	35˚ C	70 %	34.5˚ C	1.1˚ C	72.1 %	3.7 %
8	35˚ C	70 %	34.0˚ C	0.60˚ C	73.5 %	3.1 %
9	35˚ C	70 %	33.6˚ C	0.66˚ C	72.9 %	3.2 %

Table 2-3: Gas Blends Used During the Laboratory Evaluation Phase

Over the nine days of testing, a majority of the testing was executed according to plans. Using benzene as the target VOC, **Table 2-4** displays the target concentration of benzene in ppb for each of the six test points collected over the 9-day evaluation.

Day	1	2	3	4	5	6	7	8	9
Test	Target ppb Benzene								
1	0	0	0	0	0	0	0	0	0
2	2	2	2	2	2	2	2	2	2
3	1.25	0.5	0.25	1.25	0.5	0.25	1.25	0.5	0.25
4	6	3	1.35	6	3	1.35	6	3	1.35
5	12	7	5	12	7	5	12	7	5
6	9	4	1	9	4	1	9	4	1

Table 2-4: Target Concentration for Benzene (ppb) for the Laboratory Evaluation Phase

During the laboratory evaluation phase, there were a few issues that occurred and were documented. Those issues are:

- March 31 (Day 1), Test Point A (overnight stability point), the Environics gas dilution system shut itself off at midnight – which is assumed to be caused by a bug in the system when the month switched from March to April. No other evening issues were observed. Data from midnight (0:00) to 04:00 for March 31/April 1 were not used during the evaluation.
- On April 2 (Day 3), the initially designed Test Point 4 (1.5 ppb benzene) could not be maintained with the mass flow controllers in the Environics 2014 using the automated sequencer. The concentration of this test point was changed to 1.35 ppb benzene. For the laboratory evaluation phase, the concentrations (benzene), Schedule Day, and Test Numbers are listed in the Table 2-4. It is not anticipated there were any issues with the delivery time as the issue was discovered immediately as the gas concentration was changed, allowing for almost the total scheduled manifold flush time prior to collection.
- Day 7 was scheduled to be run on Monday April 7th, but due to large amounts of rain the air handlers of the building became unstable leading to RH instability in the test system. The testing was rescheduled to April 8th and all events were subsequently pushed back one day. No data were affected by this change of schedule.

2.5 Vendor Unit Removal

After the completion of the lab testing, each vendor was required to disassemble their unit and arrange for shipping off the RTI campus. The disassembly work was completed very quickly with most vendors accomplishing the breakdown of their unit within a few hours. Three of the vendors packaged their equipment

and made arrangements to take everything with them. One vendor made arrangements with RTI staff to package their equipment and send back to their home office using pre-labeled shipping boxes. Most of the other vendors were well prepared with only minor shipping label issues. Another vendor had difficulty arranging their schedule with RTI staff, so that part of their equipment was left at RTI for an additional week after testing had been completed. No damage was done to any part of the laboratory from any of the equipment removal and the laboratory was restored to its original order.

3.0 List of Candidates Involved

From the literature search, the EPA WAM selected eight vendors to participate in the laboratory evaluation phase. **Table 3-1** displays the vendor candidates and contact information. For the laboratory evaluation phase, these vendors were assigned a Vendor ID Number (1 through 8). For the course of the GC study and this report, these vendor candidates were identified by their Vendor ID Number.

For the laboratory evaluation, the vendor candidates were responsible for:

- Shipping the auto-GC unit and all necessary supportive equipment to RTI,
- Providing a laboratory operator and/or personnel contact information,
- Providing RTI an itemized list of equipment, materials, and supplies for the auto-GC unit,
- Installing the auto-GC unit in the RTI laboratory,
- Conducting all necessary quality assurance (QA)/quality control (QC) activities,
- Operating the auto-GC unit during the laboratory evaluation phase,
- Providing hard copy or electronic data for all test points evaluated, and
- Troubleshooting and repairing units as required.

Candidate Vendor	Contact Information
Markes International and Agilent	Dr. Nicola Watson (+44 (0) 1443 230935; nwatson@markes.com) Dr. David Wevill (866-483-5684; dwevill@markes.com) Michael W. Cox (866-793-4961: michael_g_cox@agilent.com) Kelly Beard (970-310-0324: kelly.beard@agilent.com)
American Ecotech/Baseline/CDS Analytical	Brian Bischof (303-823-6661; brian.bischof@baselineindustries.com) Steve Grantham (303-823-6661: steve.grantham@baselineindustried.com) Ben Kahn (303-823-6661; ben.kahn@baselineindustries.com) Norm Davis (cell: 404-996-7858; norm.davis@baselineindustries.com) Stephen Wesson (610-932-3636: swesson@cdsanalytical.com)
CAS/Chromatotech	Christina Cloran (513-542-1200; ccloran@cas-en.com) Terrence Kizer (513-542-1200: tkizer@cas-en.com) Sylvain Barataud (+33 5 5794 0629: sylvain.barataud@chromatotec.com) Michel Robert (+33 5 5794 0475; michel.robert@chromatotec.com)
Defiant Technologies	John Kiegel (505-999-5880 Extension 25; jkiegel@defiant-tech.com) Doug Adkins (505-999-5880; adkins@defiant-tech.com) Patrick Lewis (505-307-3576; prlewis@defiant-tech.com)
Perkin Elmer	Heidi Grecsek (203-922-2403; heidi.Grecsek@perkinelmer.com) Lee Marotta (914-954-1779; lee.Marotta@perkinelmer.com) Cory Whipp (225-747-7707; cory.whipp@perkinelmer.com) Rick Brooks (774-222-2138; rick.brooks@perkinelmer.com) Miles Snow (miles.snow@perkinelmer.com)
SRI Instruments, Inc.	Hugh Goldsmith (310-214-5092; hugh@srigc.com) Greg Benedict (310-214-5092: techsupport@srigc.com)
Synspec	John Wilbur (603-880-7100; johnw@jjwilbur.com) Michael Wilbur (603-880-7100; michaelw@jjwilbur.com) Thomas Wilbur (603-880-7100; thomasw@jjwilbur.com) Michael Rijpkema (+11 31 50 5266454; m.rijpkema@synspec.nl) Titia Meuwese (+11 31 50 5266454; t.meuwese@synspec.nl) Wouter Lautenbach (w.lautenbach@synspec.nl)

Thermo Scientific and Markes International	Terry Jeffers (904-248-8204; terry.jeffers@thermofisher.com) Suresh Seethapathy (301-803-0896; suresh.seethapathy@thermofisher.com) Nick Hubbard (919-414-7497; Nicholas.Hubbard@thermofisher.com) Nicola Watson (+44 (0) 1443 230935; nwatson@markes.com) Jerry Sainsbury (866-483-5684; jsainsbury@markes.com)

Table 3-1: Candidate Vendors for the Laboratory Evaluation Phase

4.0 Acquisition and Compilation of Candidate Raw Data

4.1 Vendor Results Processing and Analysis Dataset Construction

Results were received from each vendor generally in a timely manner (typically daily), although in some cases multiple deliveries from some vendors were received for a particular day's evaluation based on the vendor's decision to reprocess their own data. All data received from the vendor was transferred from email attachments to specifically-designated folders under the Project Folder on the RTI server corresponding to each vendor and evaluation day (as described in the approved QAPP). Result files which were superseded by more current deliveries of the same day's results were moved to the "Boneyard" folders in the same folder path to ensure only the correct information was used.

At the request of the project data manager and statistician, vendor results were received in one of two basic formats:

1) one result record per day, test, and analyte (i.e. Day 1, Test 4, compound benzene) or
2) one result record per day and test with all analytes presented as independent columns on that record (i.e. Day 1, Test 4, all 58 compounds).

All data was received in MS Excel format and processed with SAS (v9.3). Individual SAS data import and processing routines were written and fully-documented to accommodate the somewhat different data nuances between vendors. Each vendor's data was checked by RTI for completeness, and then returned to the vendor for them to confirm it was an accurate representation of their day's results. The finalized primary raw dataset was created as a composite of all test days and all vendors. This intentional, stepwise process was followed to provide a pathway along which data integrity evaluations could be traced. A Vendor ID Number was assigned to all results from a given vendor to support 'blind' data analyses and reporting.

Although standardized compound names had been provided to each vendor, they were not universally employed. Compound names were harmonized across vendors and compound numbers (using EPA AQS/AIRS parameter ids.), and were assigned to each compound to facilitate more reliable data analyses. For vendors who reported m-xylene and p-xylene separately, their results were summed to yield a calculated result for m, p-xylene in order to maintain harmonization with data comparisons. Sampling dates and times for each vendor record were processed into a common format and expressed in SAS; this data and time format requires the programmer's knowledge to facilitate any additional processing at a later date.

A 'frame' of all possible combinations of vendor, day, test number, and analyte was constructed and subsequently populated with the complete vendor results to reveal where data was present or absent. Within this data frame, new variables, NDIND and NRIND, were created with the following values:

- Raw vendor measurements of <missing> or -999 (requested to indicate 'not reported') were converted to missing and were assigned as NRIND=1;
- All other negative raw vendor measurements or zeros were set to zero and assigned as NDIND=1;
- If neither NDIND=1 or NRIND=1 then NDIND=0 and NRIND=0 was assigned for each measurement.

Finally, a complete 'challenge concentrations' database of all analyte concentrations, temperatures and relative humidities delivered to the manifold, by day and test number, was created and merged onto the compiled vendor raw data to yield a suitable analysis-level SAS dataset.

4.2 Data Review

All reported vendor data, including those considered to be extreme measurement values, were reviewed. If the values were in fact part of the vendor delivered data (and not an effect of possible data migration issues), the data was retained in the SAS dataset for use in calculations.

The distributions of the statistical metrics for precision and accuracy (i.e. %RSD and bias, respectively) were thoroughly investigated for all vendors and analytes, using test number 6 or above for precision and the Test Number 3 through 6 for accuracy. If the calculated precision and/or accuracy in the SAS dataset revealed extreme values, the vendor-provided raw data was re-investigated for all tests, analytes, concentrations, days, and temperatures and relative humidities, to ensure that the vendor-provided data were accurately reflected in the SAS dataset. Detailed information is provided below on selected extreme values identified from the diagnostic statistics and extensive data examination.

- Vendor 1: 2,3-Dimethylbutane of test 14 and 15 on Day 6 show a couple of values that are 2 times greater (1.75 and 1.76 ppbV) compared to the rest (0.63-0.65 ppbV).

- Vendor 2: 2,2-Dimethylbutane reported at a significantly higher value (2.83 ppbV) on Day 8 from Test 10 when compared to Day 8 Tests 6-9 (which had reported values of 0.015-0.060 ppbV). All reported concentrations in Tests 6 and above should be the same as they are all measurements on the same sample.

- Vendor 6: 3-Methylhexane reported at a significantly higher value (2.83 ppbV) on Day 6 from Test 6 compared to reported values for Day 6 Tests 7-10 (0.015-0.060 ppbV); n-Undecane of Test 6 on Day 2 shows some measurements near 2 ppbV and others near 6.7 ppbV; m,p-Xylene of Test 6 on Day 4 show a value that is 2 times greater (33.23 ppbV) than the other values (16-17) in the Test series. All reported values in Tests 6 and above should be comparable as they are all measurements on the same sample.

- Vendor 7: 3-Methylpentane of Test 9 and 10 on Day 3, has two measurements: one is 3.64, and the other is 0.83; Methycyclopentane of Test 14 on Day 5 shows a significantly higher value (5.15) than the others (<1) among Test 6 and above; n-Pentane of Test 11 on Day 4 shows a significantly higher value (246.63) than the others (<15) among Test 6 and above. Again, all reported values in Tests 6 and above should be comparable as they are all measurements on the same sample taken at different time points.

- Vendor 8: some analytes showed much greater RSD (>100%) than other analytes. For example, 3-Methylheptane reported on Days 1 and 7 from Tests 6 and 7 showed high %RSDs compared with the rest of days/tests.

4.3 Issues and Problems Resolution

- Data certification and processing
  - Raw data were reported in different formats by some vendors, despite a general guideline being provided.
  - Raw data had been revised and resubmitted multiple times by some vendors. This delayed data assembly, processing, certification, and subsequent data analysis.
  - "Not Reported" values were indistinguishable from "Not Detected" for some vendors because "0" was reported where no result was possible due to instrumental capabilities/failures. In these cases, vendors were contacted to obtain additional information which would facilitate resolution of these ambiguities in the final dataset.

- Reporting differences for m-Xylene and p-Xylene
  - Due to the fact that some vendors were able to chromatographically resolve m- and p- Xylene and some were not, careful data processing was needed to sum the reported measurements for the individual xylene isomers when they were reported independently. In cases where m-xylene and p-xylene were reported separately, the results were appropriately summed within the constraints of evaluation day and test number to yield an accurate calculated result for "m, p-Xylene".

5.0 Qualitative and Quantitative Statistical Evaluations

5.1 VOCs Measured by Vendors

Target analytes were selected by EPA and were divided into 'Priority' and "Optional', reflecting their level of importance in the evaluation. **Table 5-1** lists the chemical compounds employed in the laboratory evaluation 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 not on the priority or optional list were acquired (and possibly reported), these compounds were excluded from any statistical evaluation.

Priority Compounds	Optional Compounds
Acetone	1,3,5-Trimethylbenzene
1,2,3-Trimethylbenzene	1-Pentene
1,2,4-Trimethylbenzene	2,2-Dimethylbutane
1-Butene	2,3,4-Trimethylpentane
2,2,4-Trimethylpentane	2,3-Dimethylbutane
Benzene	2,3-Dimethylpentane
cis-2-Butene	2,4-Dimethylpentane
Ethane	2-Methylheptane
Ethylbenzene	2-Methylhexane
Ethylene	2-Methylpentane
Isobutane	3-Methylheptane
Isopentane	3-Methylhexane
Isoprene	3-Methylpentane
m/p Xylene	Acetylene
m-Ethyltoluene	cis-2-Pentene
n-Butane	Cyclohexane
n-Hexane	Cyclopentane
n-Pentane	Isopropylbenzene
o-Ethyltoluene	M-Diethylbenzene
o-Xylene	Methylcyclohexane
p-Ethyltoluene	Methylcyclopentane
Propane	n-Decane
Propylene	n-Heptane
Styrene	n-Nonane
Toluene	n-Octane
trans-2-Butene	n-Propylbenzene
	n-Undecane
	p-Diethylbenzene
	trans-2-Pentene

Table 5-1: Chemical Compounds Employed in the Laboratory Evaluation

5.2 RTI Measurements by EPA Method TO-17

The reliability of the RTI method for analyzing test atmospheres was demonstrated during the evaluation of the dilution system (Section 2.2). As previously stated, the primary intention of the pre-evaluation testing was to demonstrate equivalency between ports, and to verify gas dilution system settings required to generate the target analyte concentrations could be achieved. This was to be accomplished by generating test atmospheres under a variety of conditions of analyte concentration, humidity, and temperature, and measuring the analyte

concentrations at each port. At each set of conditions, the calibration port and all ten manifold ports were sampled using glass thermal desorption tubes packed with Carbopack B®, coupled to AirChek® 2000 pumps (SKC Inc.). Sample collection flow rates were targeted at a sample flow 100 mL/min, with a collection time of either 30 minutes or 60 minutes depending on the concentration of delivery gas to the system. It is important to note, the tubes enabled collection and analysis of selected analytes from the challenge mixtures in the manifold for the purpose of assessing system performance and were not intended as "reference standards" for the subsequent laboratory evaluation phase. Thermal desorption tubes were conditioned in batches prior to use, and one sample per batch was analyzed to verify cleanliness. Sampler flow rates were checked using a Gilibrator-II flowmeter (Gilian Inc.) immediately prior to sampling and recorded manually. Samples were analyzed by thermal desorption and gas chromatography with mass selective detection (GC/MS) based on EPA Air Toxics Method TO-17, using a Perkin-Elmer Turbomatrix autosampler and an Agilent 6890/5973 GC/MS operated in selected ion monitoring mode. Thermal desorption tubes were loaded with 100 ng toluene-d8 as a reference compound prior to analysis, using an ATIS™ loader (Supelco, Inc.). Based on the limitation of the collection materials in the tubes, the GC/MS analysis was limited to the analytes listed in **Table 5-2**. The analytes selected are a representative cross-section of structure, chemical class, and carbon number for all compounds. Due to time constraints, we did not perform a determination of the method detection limit (MDL). However, based on the blank data, we believe that a reasonable upper limit of the MDL for most analytes, and therefore an upper constraint on the system background, is about 0.05 ppb for a 60 minute sampling time at typical sampling rates.

We considered the generation, distribution, and analytical systems as a single method to evaluate linearity and precision. For each concentration tested in the setup, RTI determined the average relative response for each analyte in the sample from each port (as peak area [normalized for sample volume] divided by toluene-d8 peak area), and calculated the average and relative standard deviation (RSD) of the relative response across all ports, for each calculated analyte value was averaged. Sensitivity profiles with bracketing error bars are plotted across test concentrations for representative analytes in **Figure 5-1**. Linear regressions on all PAMS analytes with >5 carbons yielded $r^2 > 0.99$. Precision across all ports was consistently acceptable for most analytes with RSDs typically in the range of 4% to 9%. Both 3-methyl-1-butene and 1-pentene had RSDs > 10%, which we attribute to inconsistent retention of those highly volatile analytes by Carbopack B®. RSDs for n-decane were also high, likely due to transient adsorption of that analyte by the distribution system, caused by its lower volatility relative to other analytes.

Although the precision calculations show that the distribution system is delivering a consistent concentration to all ports, it does not identify low-level bias. To determine this, the RTI team calculated the port bias for each analyte listed in Table 5-2, at each concentration, by dividing the relative response of the analyte at each port by the average relative response for that analyte at all ports. RTI averaged the port bias and then averaged the bias again across all analytes, at each concentration. A "global" port bias was obtained by averaging across all concentrations. For the inter port evaluations, the experimental conditions were 30 °C/20% RH. The results, in **Table 5-3**, indicate that for any given experiment, the concentration delivered at any given port is likely to be within 5% of the average across all ports.

3-methyl-1-butene	Chlorobenzene
1-Pentene	Ethylbenzene
Freon-113	m/p-Xylene
n-Hexane	o-Xylene
Chloroform	Styrene
Benzene	1,1,2,2-Tetrachloroethane
Dibromomethane	Isopropylbenzene
Methylcyclohexane	2-Chlorotoluene
Toluene	1,3,5-Trimethylbenzene
1,1,2-Trichloroethane	n-Decane
Tetrachloroethylene	

Table 5-2: Analytes Included in RTI Method

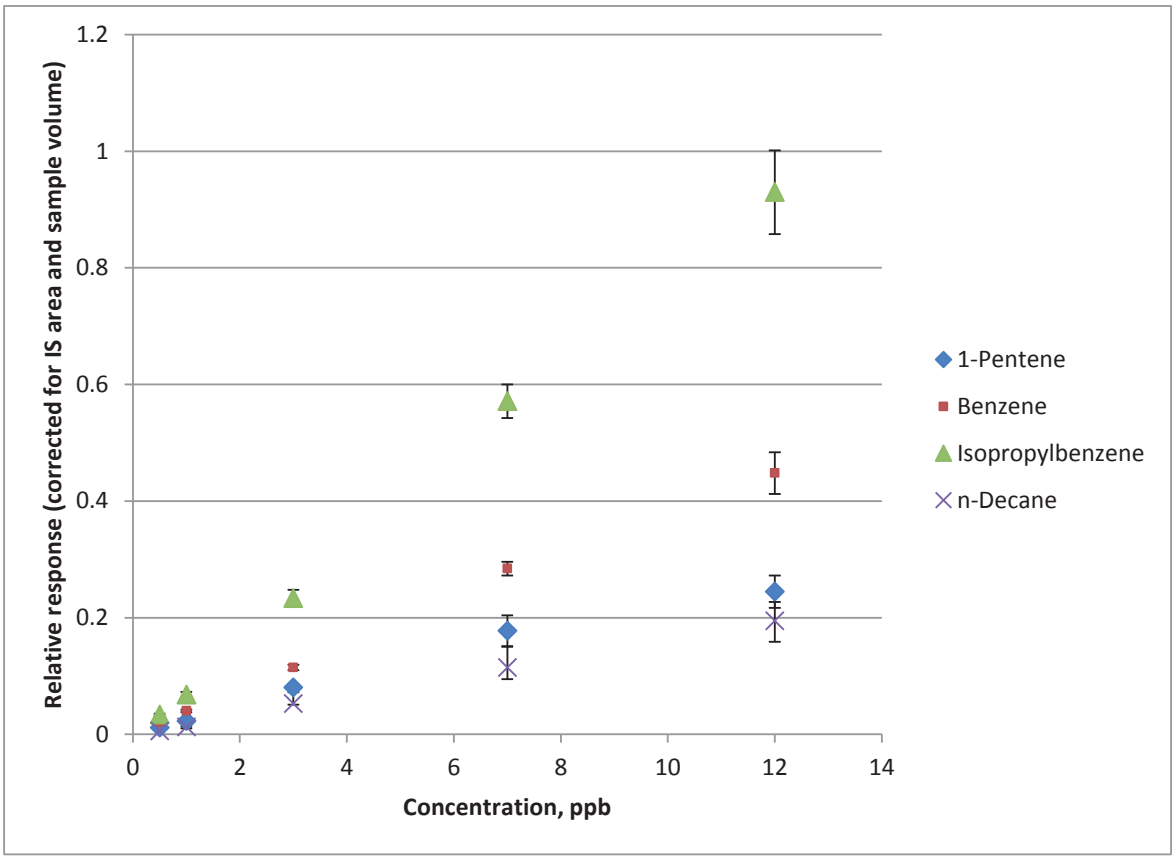


Figure 5-1: Sensitivity Profiles for Select PAMS analytes

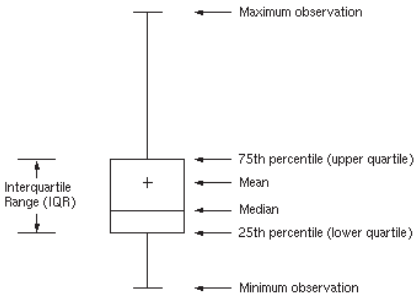
	PORT									
	C	1	2	3	4	5	6	7	8	9
0.5 ppb	0.94	1.04	1.07	0.94	1.01	0.93	0.98	1.04	1.00	1.05
1.0 ppb	1.09	1.09	1.04	0.94	0.94	0.99	1.01	0.96	0.95	1.00
3.0 ppb	0.89	1.01	1.13	1.03	0.95	1.01	0.99	1.04	1.01	0.95
7.0 ppb	1.09	1.09	1.04	0.94	0.94	0.99	1.01	0.96	0.95	1.00
12.0 ppb	1.08	1.06	0.98	0.93	*-	0.83	1.01	1.03	1.00	*-
Overall, net	1.5%	6.1%	5.2%	-4.5%	-4.1%	-5.1%	0.0%	0.5%	-2.0%	-0.3%

* The missing values for 12.0 ppb for Ports 4 and 9 are attributable to a pump malfunction and a subsequent lack of sampled sorbent tube for analysis.

Table 5-3: Port-by-Port Bias Port Mean Relative Response across Analytes, Normalized to Average for All Ports

6.0 Statistical Results

Statistical analyses for the laboratory report encompassed all priority and optional (Table 5.1) target compounds and all three temperature/ relative humidity combinations employed in the laboratory evaluation phase: 30 °C/20% RH, 25 °C/50% RH, and 35 °C/70% RH. The results provided by the eight vendor candidates and from RTI's TO-17 analyses are included. To facilitate some of the visual comparisons between vendors or analytes, distributions for the various statistical metrics are presented as box and whisker plots. A key to the features of these plots has been excerpted from SAS documentation and is provided below.



The lower fence is located at the minimum observation or 1.5*IQR below the 25th percentile; the upper fence is located at the maximum observation or 1.5*IQR above the 75th percentile. Values of the distribution outside 1.5*IQR are identified with the special symbol "o".

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

Precision was computed for sample tests numbered 6 and greater by each individual analyte, across vendors and challenge concentrations and also by analyte group (priority, optional) according to:

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

%RSD results were summarized as tabular descriptive statistics (**Appendix A, Table A1**) and in box and whisker plots (**Figure 6-1, Figure 6-3, and Figure A-57 in Appendix A**) by analyte, across vendors and as the corresponding scatter plots in **Figure 6-2** and **Figure 6-4**. **Appendix A, Table A.2** contains the summaries of %RSD for each analyte, by vendor, with box and whisker plots displayed in Figures A-1 through A-53.

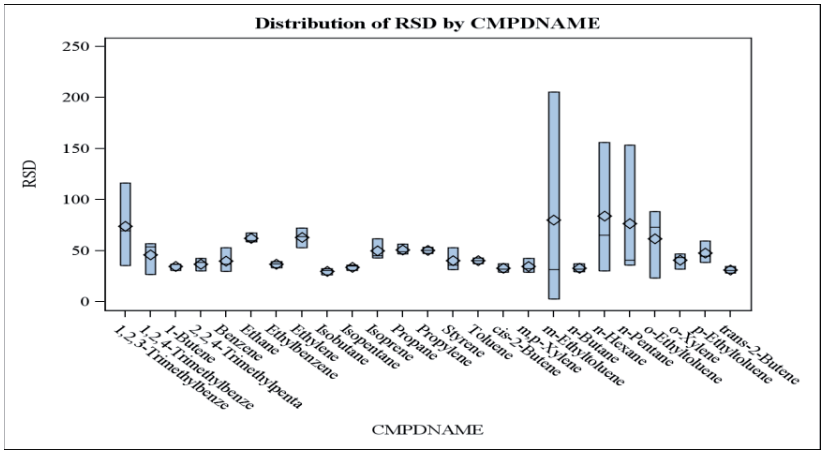


Figure 6-1: Distribution of %RSD by Target Analyte across all Vendors – Priority Analytes

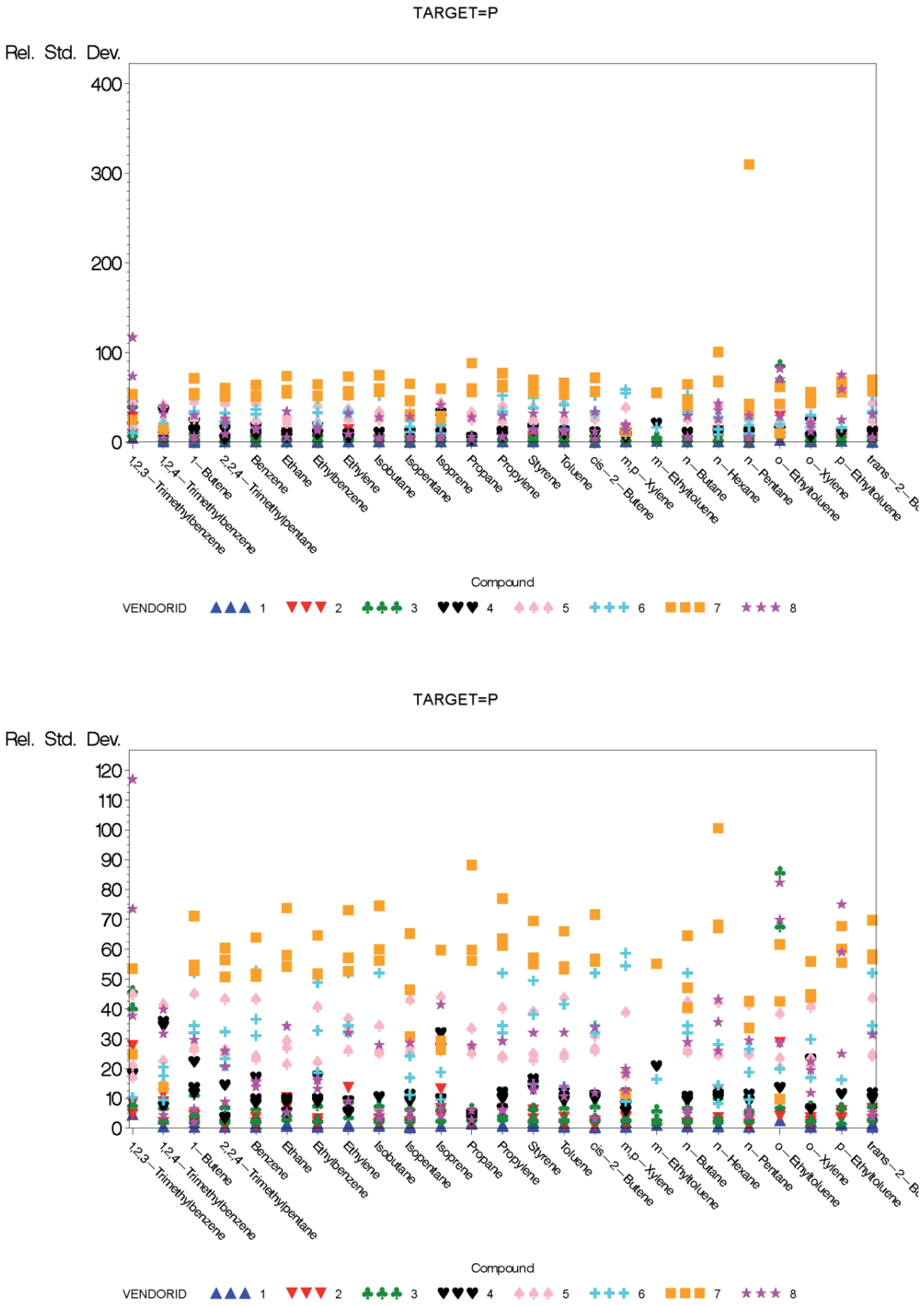


Figure 6-2: Distribution of %RSD among Vendors by Target Analyte – Priority Analytes (Full scale and expanded scale)

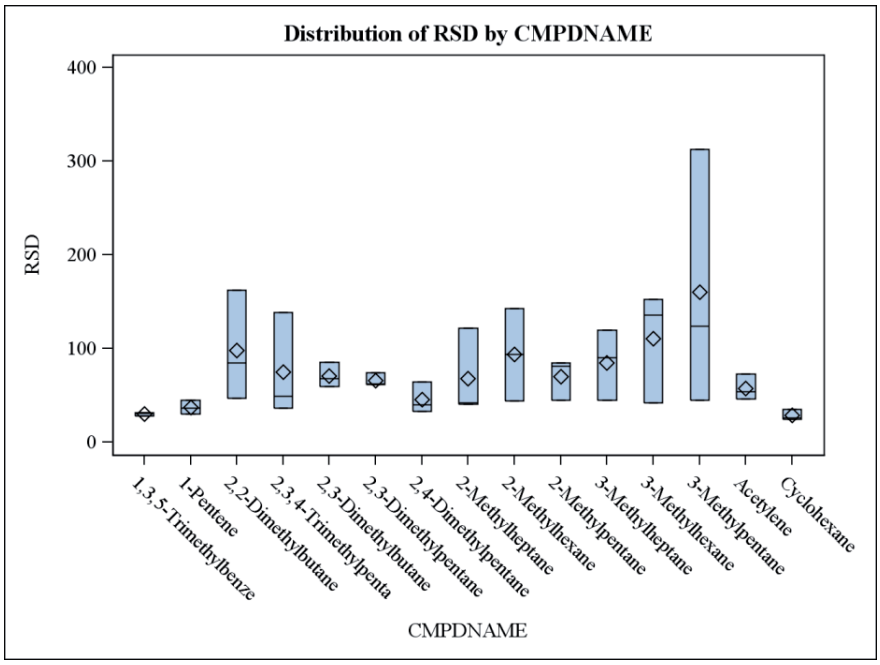


Figure 6-3: Distribution of %RSD by Target Analyte across all Vendors – Optional Analytes

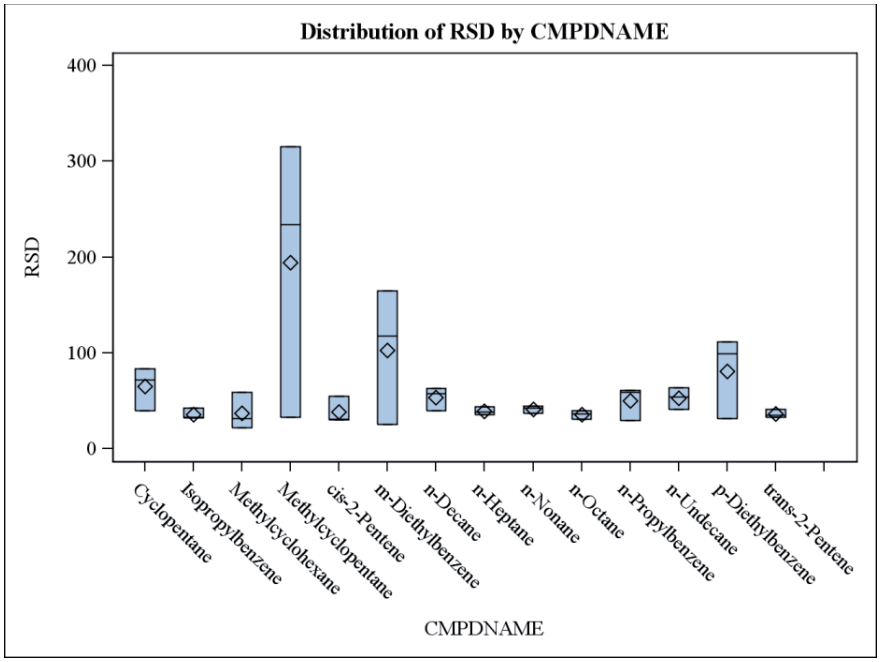


Figure 6-3 (continued).

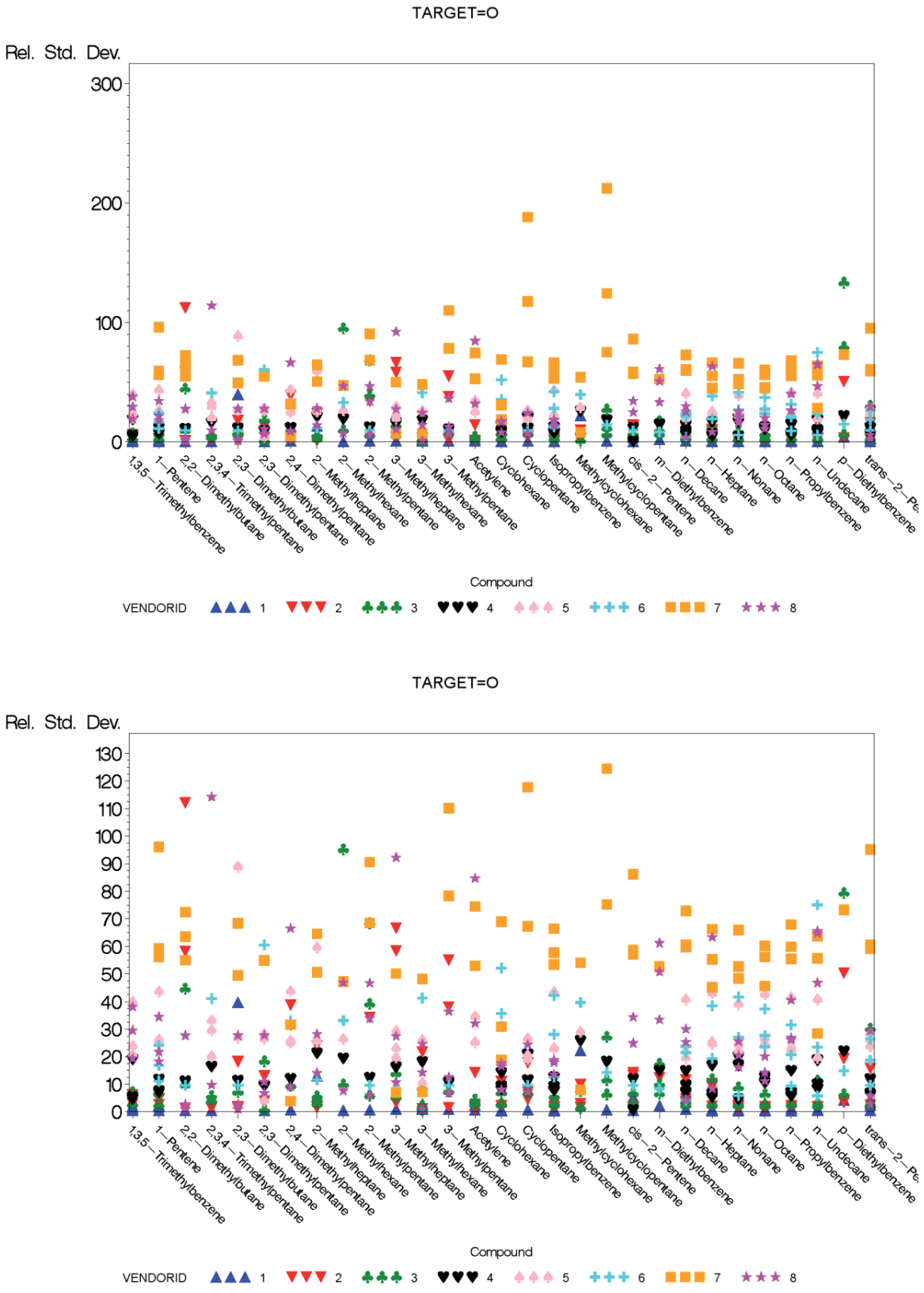


Figure 6-4: Distribution of RSD among Vendors by Target Analyte – Optional Analytes (Full scale and expanded scale)

Comparison of %RSD among all vendors and across all analytes and experimental conditions, shown in **Figure 6-5**, reveals substantial differences in precision, %RSD, results. When the effect of the experimental conditions on %RSD is considered, differences attributable to temperature (**Figure 6-6**) and/or relative humidity (**Figure 6-7**) are apparent both within vendor and among vendors. Mean %RSD is shown independently for (P)riority and (O)ptional analytes. The height of the bars in the charts, augmented with error bars illustrating the 95% confidence interval, show the mean percent relative standard deviation (i.e., relative precision). In this sense, shorter bars indicate 'good' precision and taller bars indicate 'poorer' precision. The additional information derived from the variations in temperature and relative humidity still follows the same general trends among vendors seen overall in Figure 6-5. %RSD for Figure 6-5 represents the average of the ratio of standard deviation to the mean of measurements across all target analytes and experimental conditions. These average %RSD are predictably and appreciably larger than those revealed in Figures 6-6 and 6-7 because the latter figures include only a subset of experimental conditions (i.e., a particular temperature or relative humidity) among which the variability (i.e., the standard deviation) would likely be smaller. The mean %RSD values for priority analytes from Figure 6-5 were used to determine the ranking of vendors for precision.

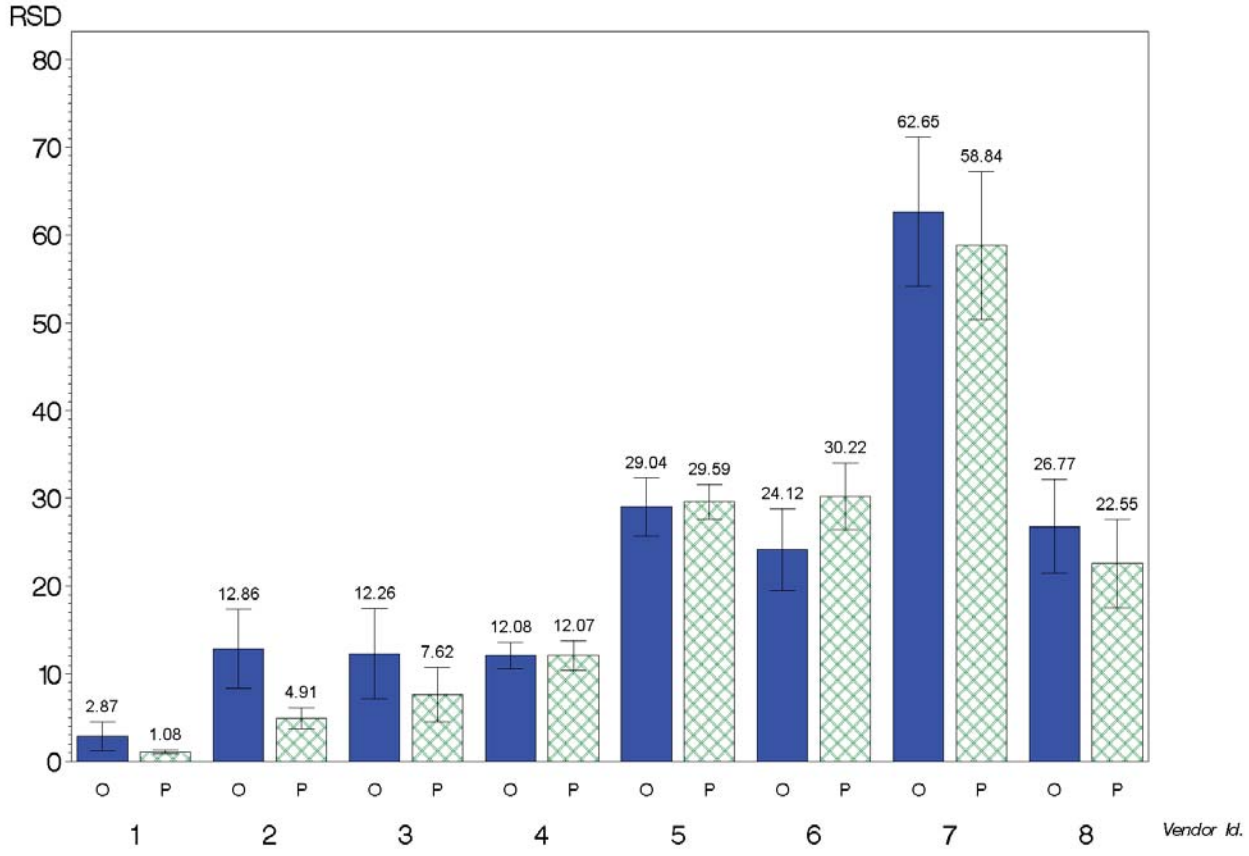


Figure 6-5: Comparison of %RSD among vendors, all analytes (95% confidence intervals; mean values in annotation)

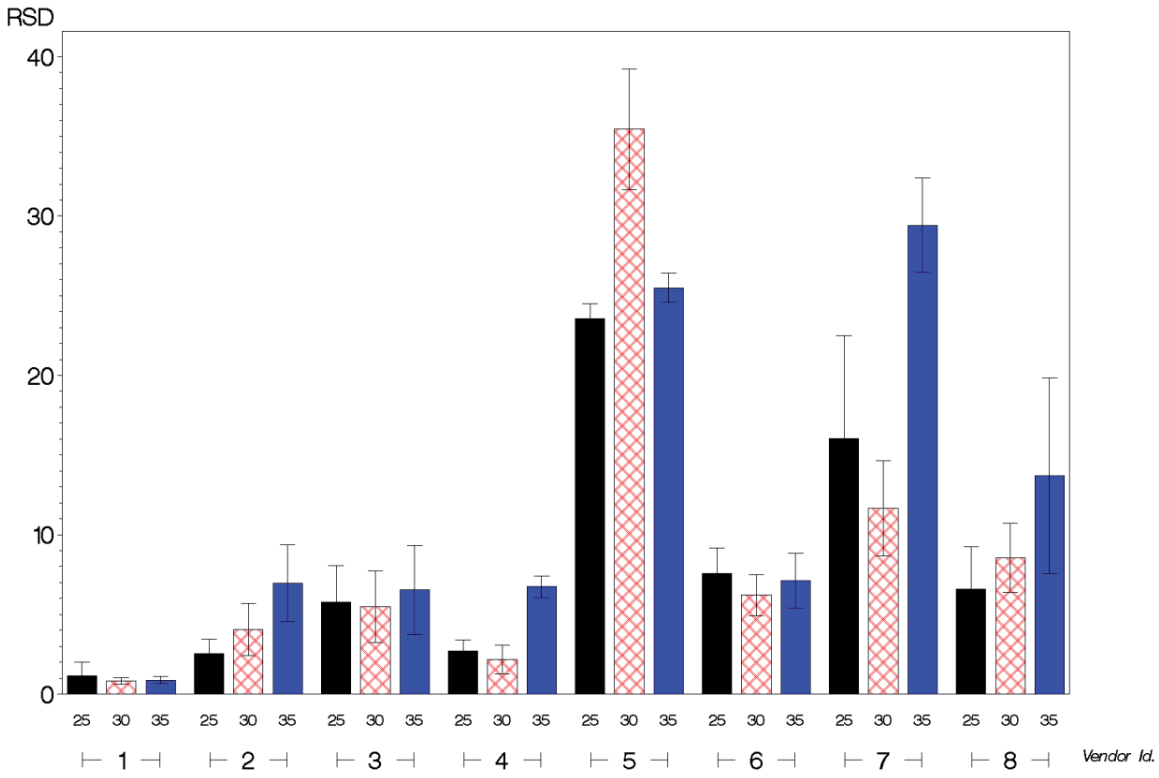


Figure 6-6: Effect of Temperature on %RSD by vendor (95% confidence intervals)

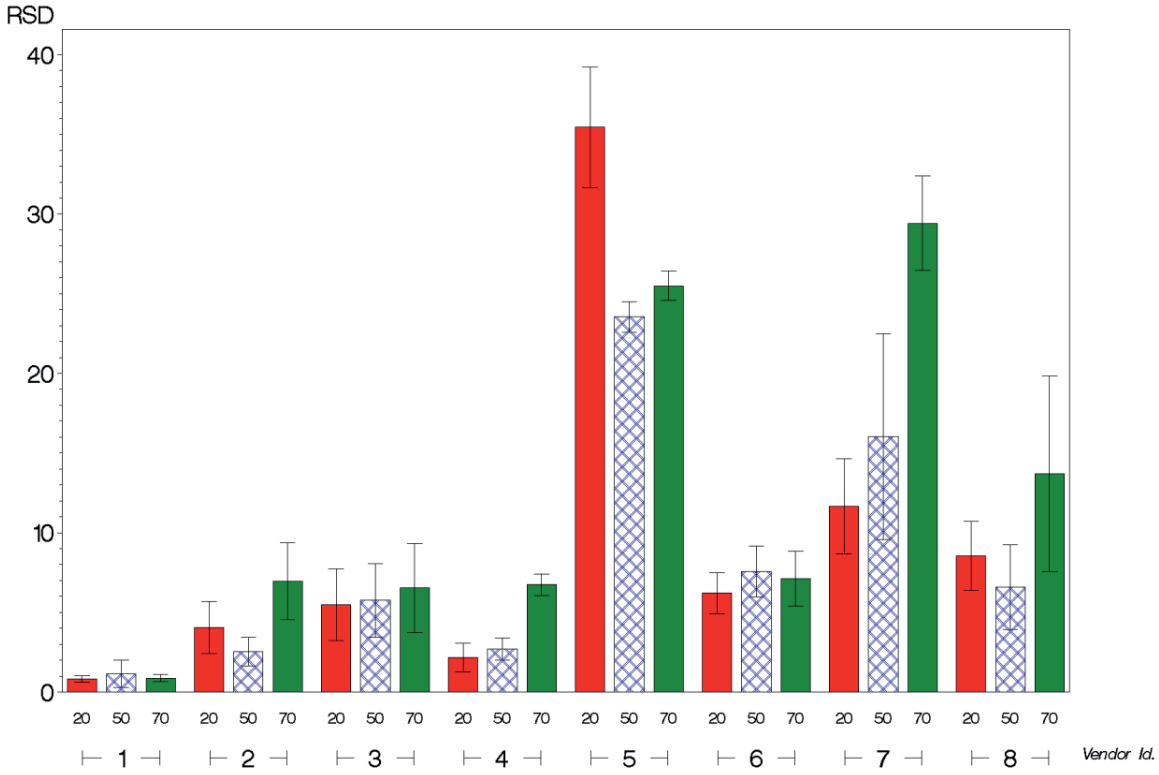


Figure 6-7: Effect of % Relative Humidity on %RSD by vendor (95% confidence intervals)

6.2 Bias (Quantitative Difference between Reference Method Measurement and Each Instrumental Measurement)

Bias was computed at all challenge concentrations, based on benzene concentration from a certified VOC standard concentration and exclusive of blank test points, among Test Numbers 3, 4, 5, and 6 were evaluated according to:

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

Essentially, bias is defined in this section as the calculated difference between observed value and delivered concentration. The bias results are summarized by analyte, across all vendors and challenge concentrations in **Appendix B, Table B1**. The box and whisker displays are illustrated below in **Figures 6-8** and **6-10**. The scatter plots of individual bias values are shown in **Figures 6-9** and **6-11**, for these figures each candidate will have up to 36 points (4 tests x 9 days) for each compound. To improve discernment of differences among vendors, the bias values contributing to the scatter plots have been limited to an absolute value of 20. Bias results are further summarized by analyte and Vendor ID Number in Appendix B, Table B2 and in the Figures B-1 through B-54.

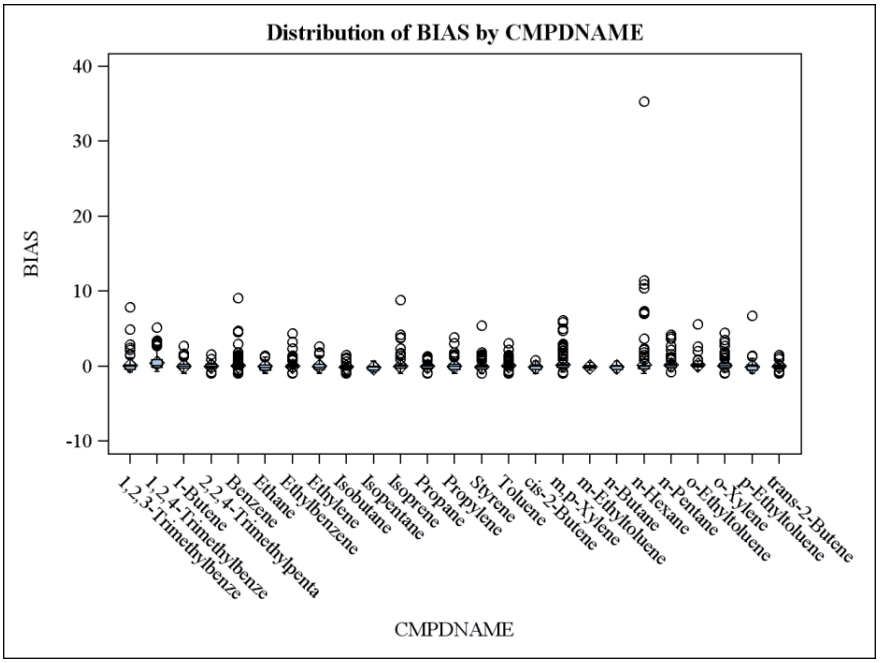


Figure 6-8: Distribution of Bias by Target Analyte across all Vendors – Priority Analytes.

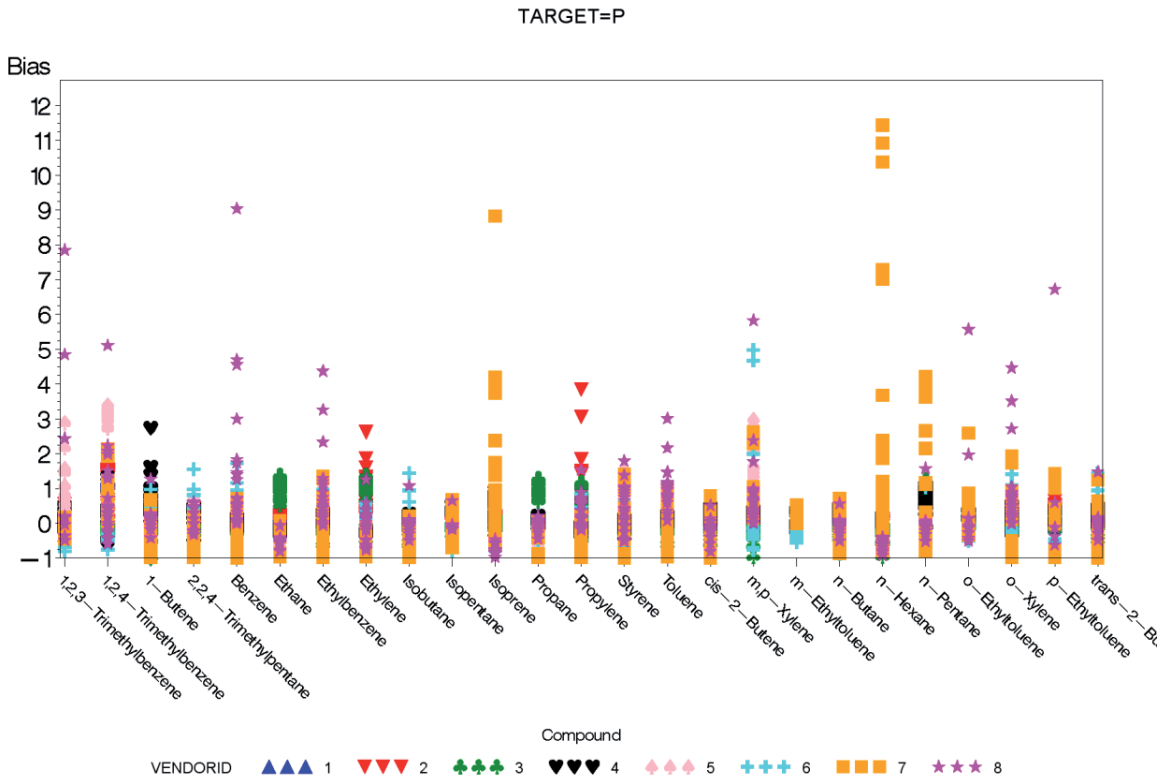


Figure 6-9: Distribution of Bias among Vendors by Target Analyte – Priority Analytes

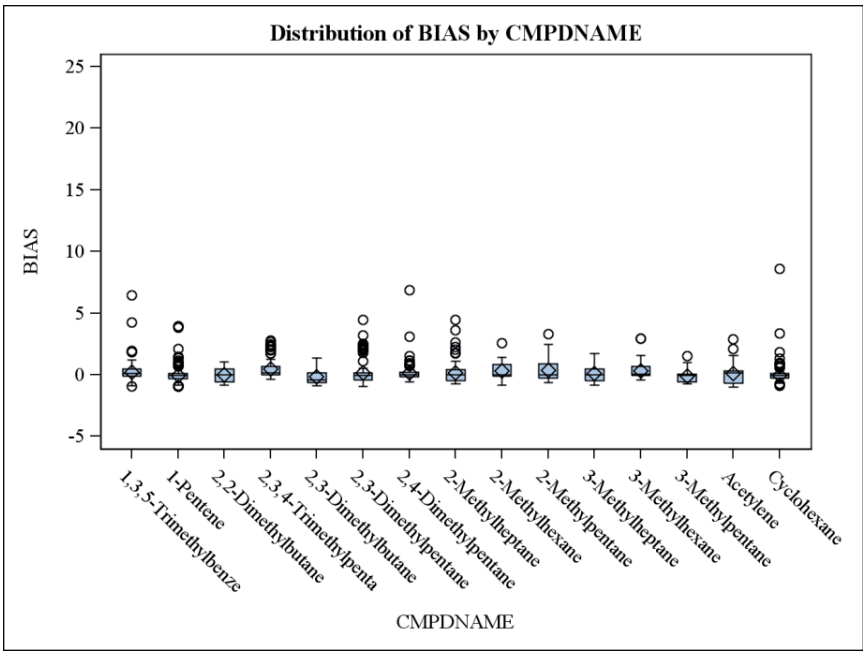


Figure 6-10: Distribution of Bias by Target Analyte across all Vendors – Optional Analytes

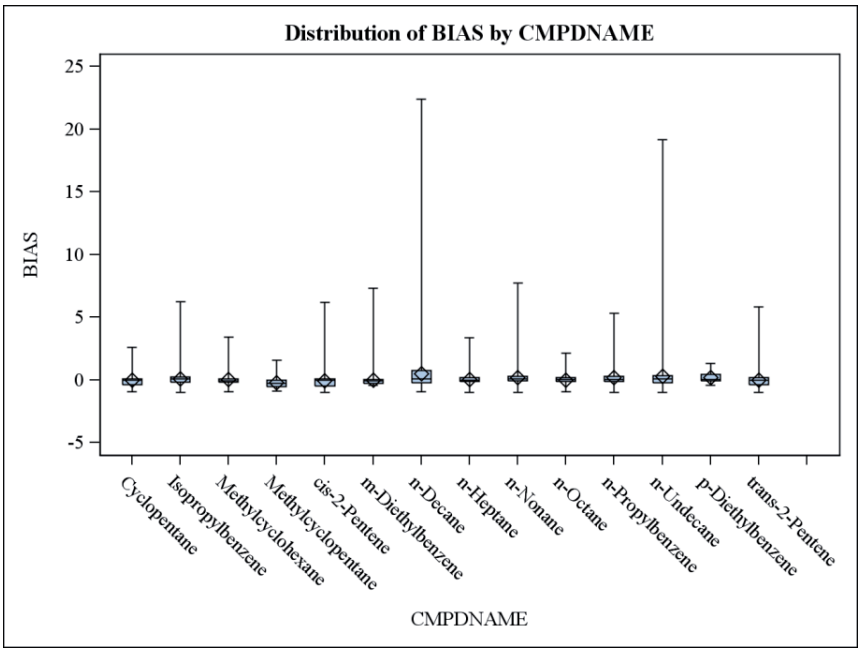


Figure 6-10 (continued).

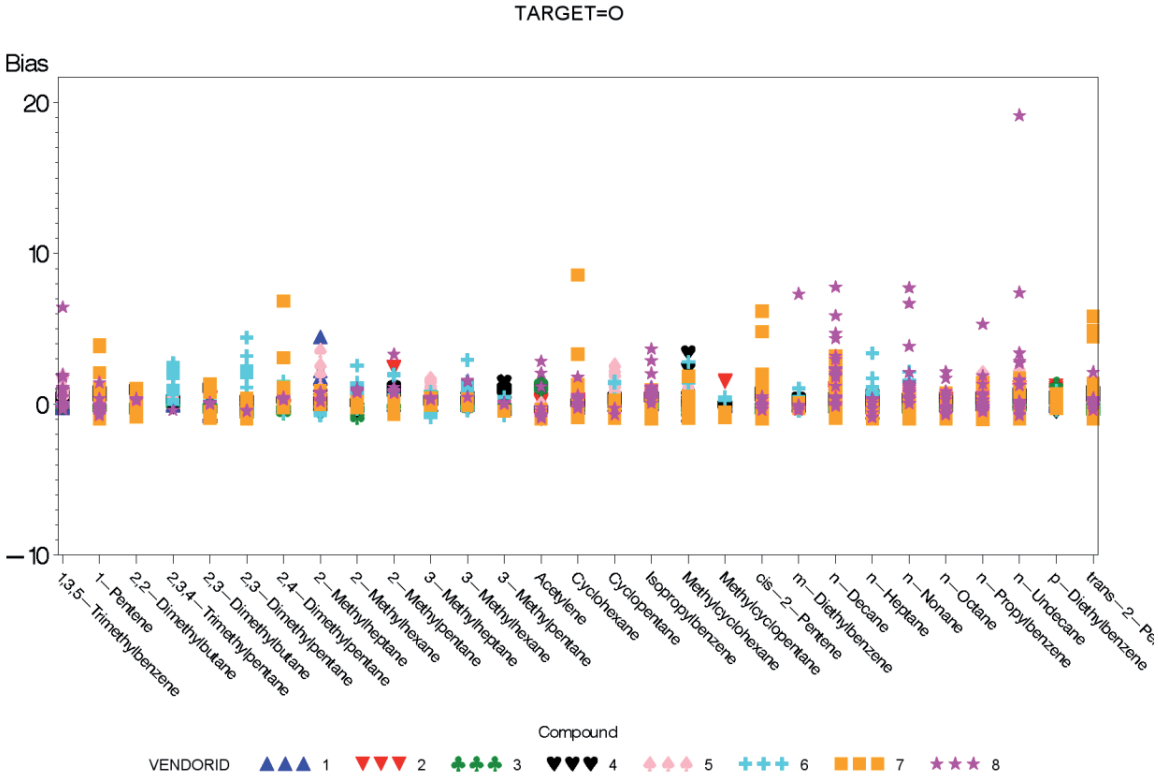


Figure 6-11: Distribution of Bias among Vendors by Target Analyte – Optional Analytes

Bias, both signed and absolute values, encompassing all priority and optional analytes, are presented grouped by vendor in **Figures 6-12** and **6-13**. The 95% confidence intervals are displayed to reflect the spread in the bias for each vendor and analyte category. Substantial differences in instrument performance are seen between signed bias (Figure 6-12) and absolute value of bias (Figure 6-13); it is proposed that the absolute bias is a better representation of performance due to the fact that a large positive value for one analyte will not be cancelled out by an equally large negative value for another analyte. Figure 6-12 shows the tendency of bias to be positive or

negative but can be slightly misleading in that large positive biases can be nullified by large negative biases. Figure 6-13 shows the magnitude of this metric without consideration of whether it is positive or negative. Vendor performance ranking for bias, presented in Section 8.1, was computed from the absolute value. Mean bias is shown independently for (P)riority and (O)ptional analytes. The height of the bars in the charts, augmented with error bars illustrating the 95% confidence interval, show the mean bias, either signed or absolute value. In this sense, shorter bars indicate 'small' bias and taller bars indicate 'larger' bias. The effect of the experimental conditions on bias is presented quantitatively in Section 8.

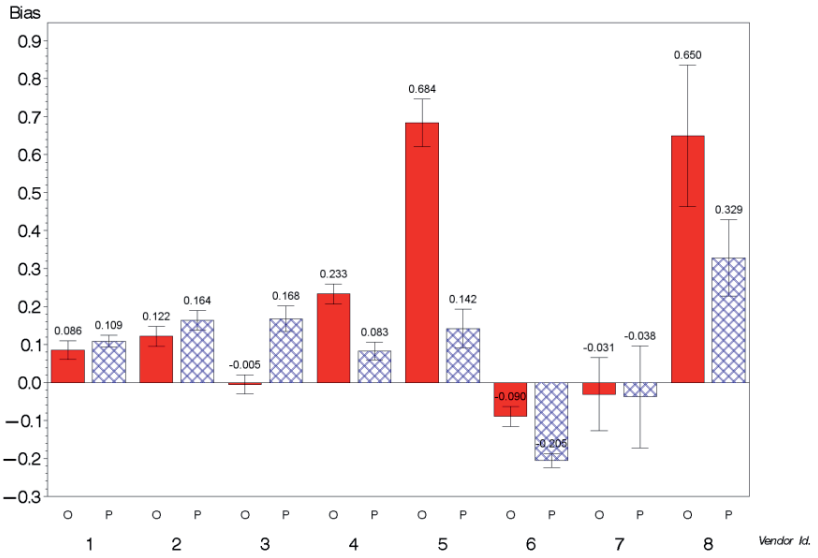


Figure 6-12: Comparison of Bias (signed) among Vendors, all Analytes (mean values in annotation)

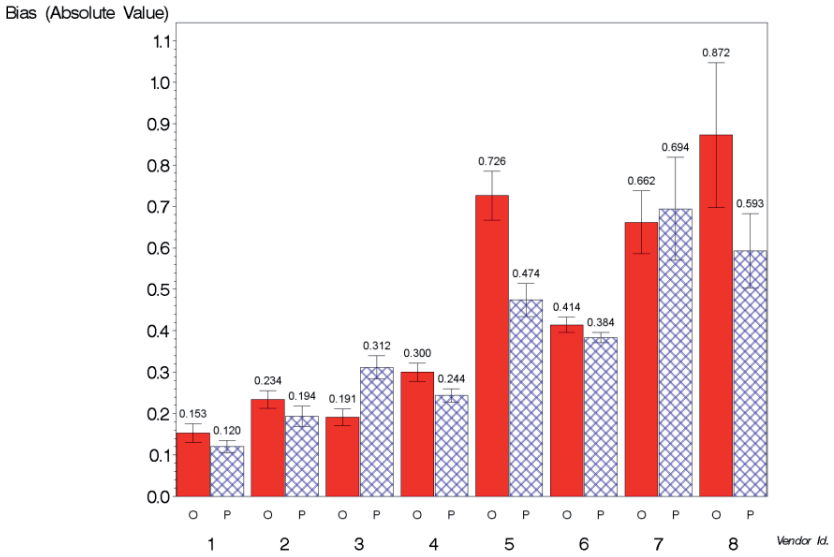


Figure 6-13: Comparison of Bias (absolute value) among all Vendors, all Analytes (mean values in annotation)

6.3 Chromatographic Performance (Number of Individual Compounds Resolved Chromatographically)

As part of the selection criteria for participation in the study, each vendor indicated their instrumentation had the ability to chromatographically resolve all of the priority and optional compounds. Since only numeric results were collected by RTI, this section of the evaluation criterion cannot be addressed at this time. The field study portion of this work should better lend itself to drawing useful conclusions on this subject.

6.4 Completeness (Proportion of All Targets Reported (Detected and Not Detected) across All Test Days and Tests)

Completeness was computed as the proportion of all targets reported across all days, at all challenge concentrations (Test Points 3, 4, 5, and 6), based off the CoA for benzene. All reported blank and calibration check points (Days 1-9; Test Point 2) were excluded from calculations.

The completeness results are summarized individually for priority and optional target analyte, test condition (temperature and relative humidity), and challenge concentration by Vendor ID Number in the horizontal bar charts in **Figures 6-14, 6-15, 6-16, 6-17** and **6-18**. Overall, most vendors reported most analytes but substantial differences in completeness are seen for several vendors (Figure 6-14). The length of the bars in the charts, augmented with error bars illustrating the 95% confidence interval, show the mean proportion of Priority and Optional analytes reported. In this sense, longer bars indicate higher percent completeness and shorter bars indicate lower percent completeness. Vendor performance ranking for completeness, presented in Section 8.1, was computed from the values displayed in Figure 6-14. Comparable charts show the effect of experimental conditions independent of concentrations (Figures 6-15 and 6-16). For a concentration dependent evaluation, expressed as the benzene level, Figures 6-17 and 6-18 are used to illustrate differences in vendor completeness for four out of twelve selected concentrations (Figure 6-17 include priority compounds and Figure 6-18 include optional compounds, both are independent of temperature and RH). Low completeness values for Vendor 8 in certain of the figures reflect instrument problems on specific days of the evaluation (discussed further in Section 6.9).

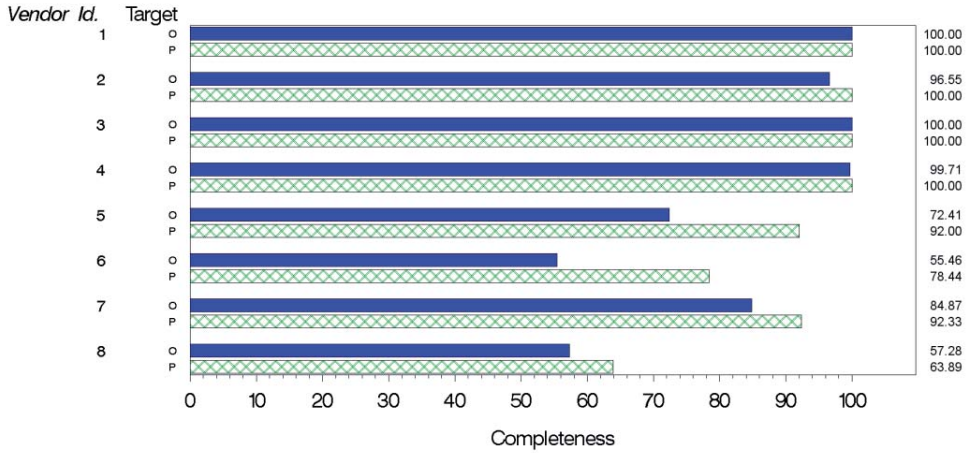


Figure 6-14: Distribution of Completeness by Target Analyte across all Vendors and Experimental Conditions (mean values in annotation)

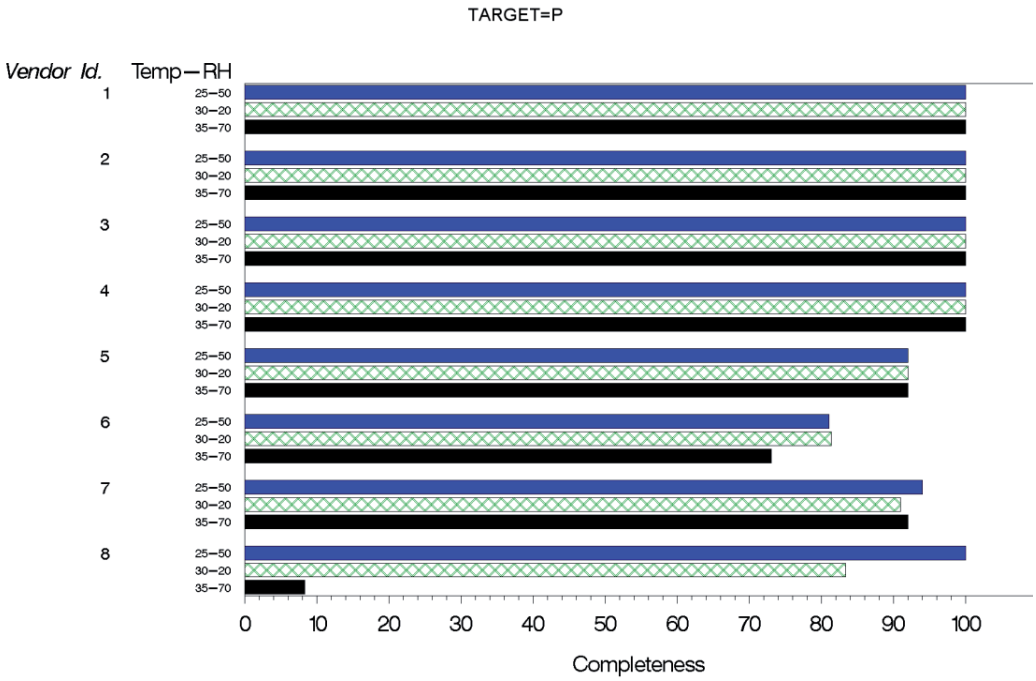


Figure 6-15: Distribution of Completeness by Temperature and Relative Humidity Condition for all Vendors – Priority Analytes

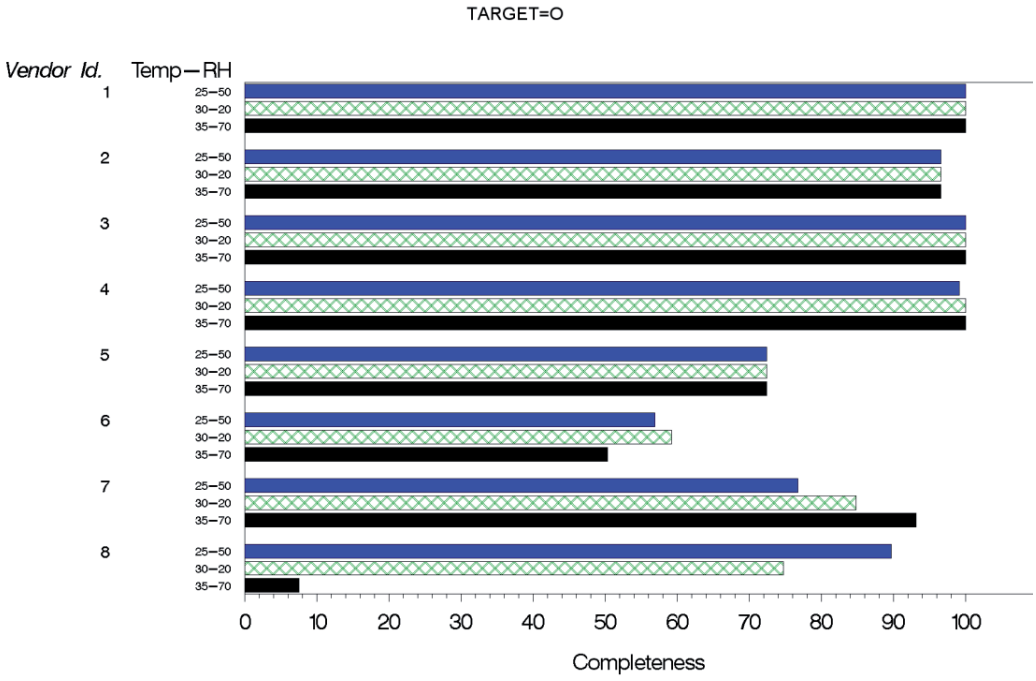


Figure 6-16: Distribution of Completeness by Temperature and Relative Humidity Condition for all Vendors – Optional Analytes.

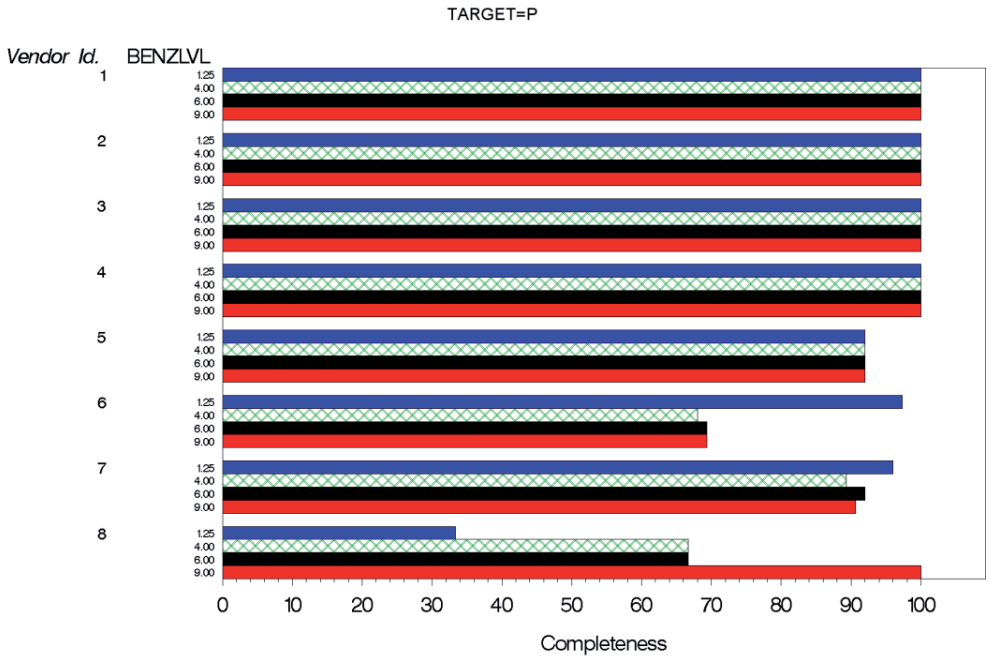


Figure 6-17: Distribution of Completeness by Challenge Concentration for all Vendors – Priority Analytes (BENZLVL=benzene concentration in the challenge mixture)

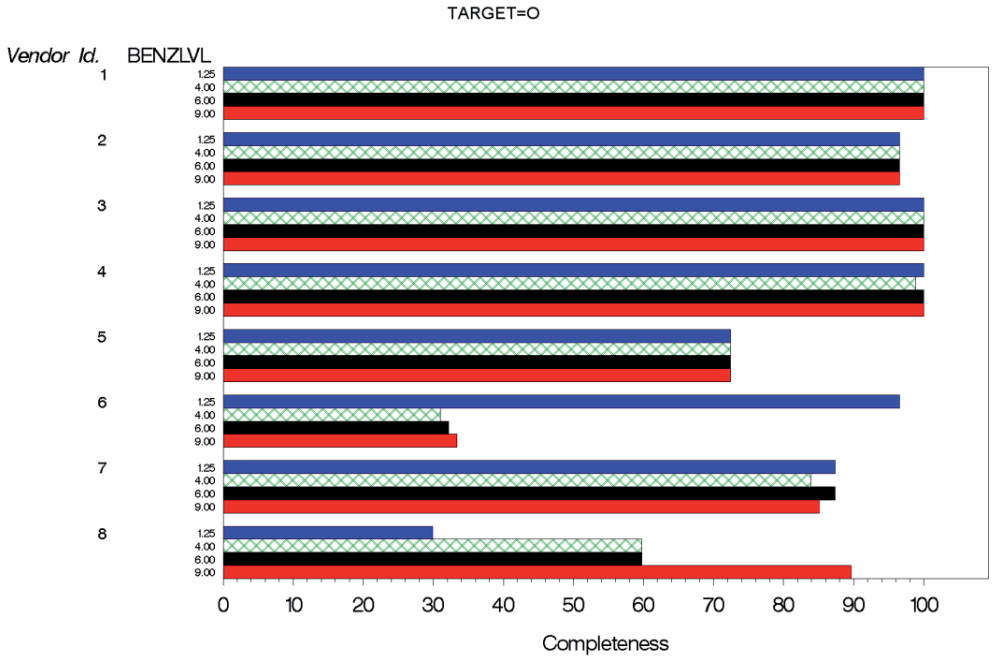


Figure 6-18: Distribution of Completeness by Challenge Concentration for all Vendors – Optional Analytes (BENZLVL=benzene concentration in the challenge mixture)

6.5 Method Detection Limit (Quantitative Determination of the Lowest Measurement Which can be Distinguished from Zero)

The method detection limit (MDL) is defined as the lowest sample concentration which 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 the

laboratory evaluation phase, formal method detection limits are not calculable because the actual instrumental limits of detection (LOD) were different among vendors and a common challenge concentration for determination of vendor precision near the LOD was impossible. In lieu of a formal MDL computation, the following qualifying conditions and criteria were applied to provide comparable "Relative Measurement Thresholds" (RMT) between vendors:

- Only the vendor-reported measurements for Test 6 on Days 3, 6, and 9 were used. The PAMS mixture was supplied to the manifold for these time points and the benzene concentration was 4 ppbV. This was the lowest concentration for which replicate measurements were available.
- Only priority and optional analytes whose challenge concentration was less than 0.8 ppbV were included.
- A consistent 99% confidence interval t-statistic for 7 degrees of freedom was used, regardless of the number of replicate measurements reported by a given vendor.

Relative Measurement Thresholds were computed for selected target analytes according to the expression:

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

where:

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

s = standard deviation of 8 replicate measurements (d.f.=7) where the challenge concentration was ≤0.8 ppbV.

Relative measurement threshold (RMT), as a surrogate for the method detection limit (MDL), is basically a measure of precision at low challenge concentrations. Lower values of relative measurement threshold reflect better instrument performance and, hence, improved analyte detectability. **Figures 6-19** and **6-20** reveal the differences not only among selected priority and optional analytes but also discernable trends among vendors. When RMT is computed across all analytes present below 0.8 ppbV, the results presented in **Figures 6-21** and **6-22** are revealed. Differences in RMT in these charts directly reflect differences in measurement precision among both specific analytes and vendors. The overall vendor ranking for relative measurement threshold across analytes was extracted from Figure 6-21 for Table 8.1.

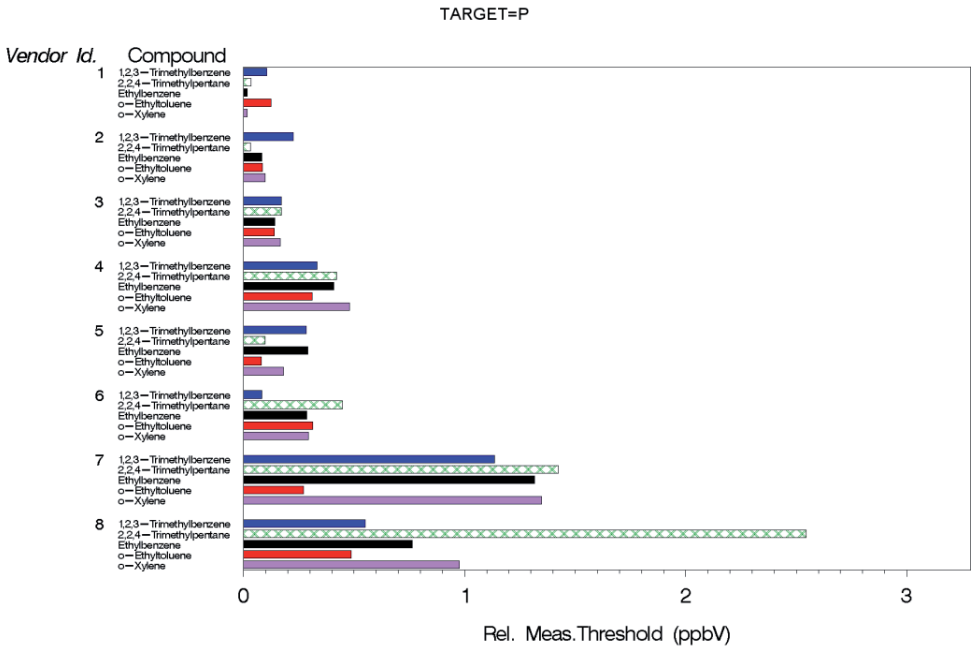


Figure 6-19: Comparison of Relative Measurement Thresholds among Vendors, Selected Priority Analytes at <0.8 ppbV

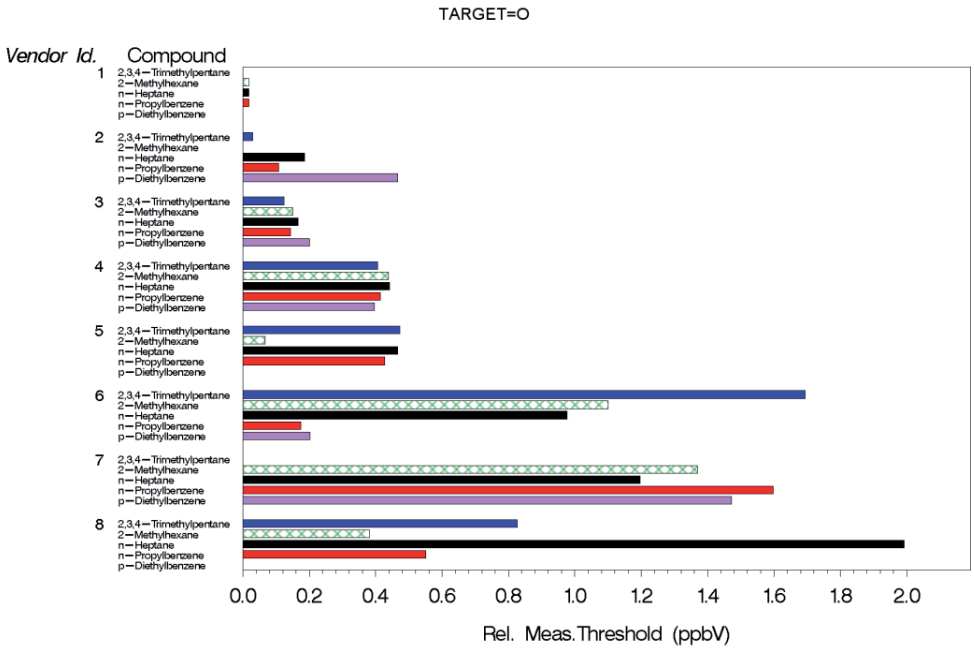


Figure 6-20: Comparison of Relative Measurement Thresholds among Vendors, Selected Priority Analytes at <0.8 ppbV

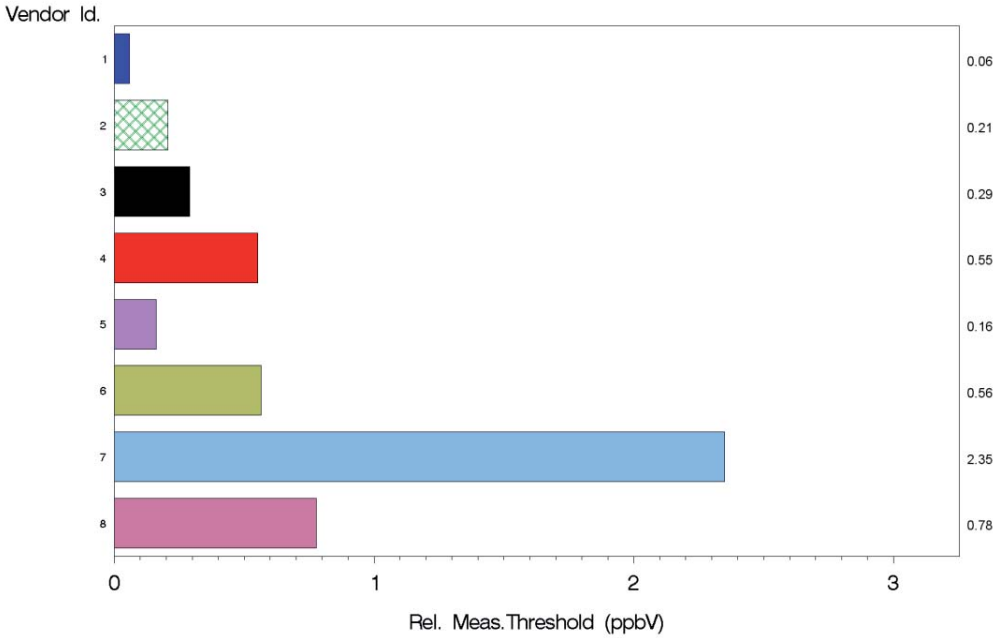


Figure 6-21: Comparison of Relative Measurement Thresholds among Vendors all Priority Analytes at <0.8 ppbV (mean values in annotation)

6.6 Effect of Temperature and Relative Humidity of the Gas Stream (Temperatures Ranging from 25-35 ºC and 20-70 % RH)

Linear models were constructed with bias as the dependent (outcome) variable and Vendor ID, temperature, and relative humidity as the independent (predictor) variables. While in our experimental design, temperature and relative humidity are not strictly independent, they are not likely correlated because they were not varied in the direction (i.e., increasing temperature was not associated with either increasing or decreasing relative humidity). Therefore for completeness in this draft final report, both predictors were included in the model with bias as the outcome to determine if a linear association with either temperature or relative humidity might exist. Subsequent to EPA's review of the draft report, a categorical variable "TEMP_RH" will be created and employed in all models and graphical displays to elucidate any effect of experimental conditions. All priority and optional analytes were included. After further model examination, it was determined that transforming the bias variable by taking its log (base 10) of the absolute (i.e., unsigned) bias and utilizing it as the model outcome provided a clearer output result. With this reasonable modification, the results reported in **Table 6-1** were obtained.

Model Predictor	Deg. freedom	p-value
Vendor ID	8	<.0001
Temperature (ºC)	1	<.0001
% Rel. Humidity	1	0.0107

Table 6-1: Effect of Vendor ID, Temperature, and Relative Humidity on Bias

The interpretation of the p-values is that for Vendor ID, temperature, and relative humidity there are <0.01, <0.01, and ~1% probabilities, respectively, indicating the predictor has no effect on the outcome. Since these are extremely small probabilities, RTI may reasonably conclude that it is likely all three independent variables are important in accounting for the variability in bias and that the graphically-observed differences in bias among vendors are likely reflective of real differences. The parameter estimates for temperature (0.0117) and

relative humidity (0.0007) are both positive, which correlates with an increase in either result causes an increase in bias (i.e., as temperature or relative humidity rise, the absolute value of bias increases).

Table 6-2 shows the difference in mean bias for parameter estimates of all vendors where the difference was significant. For example, the mean bias (all priority and optional analytes) for Vendor 5 is significantly higher than the mean bias for Vendor 2 by 0.219 bias units. Similarly, the mean bias (all priority and optional analytes) for Vendor 7 is significantly lower than the mean bias for Vendor 3 by 0.122 bias units.

Vendor ID	1	2	3	4	5	6	7	8	9
1		---	---	---	0.2660	-0.251	-0.133	0.362	---
2			---	---	0.219	-0.297	-0.18051	0.316	-0.150
3				---	0.277	-0.240	-0.122	0.373	---
4					-0.212	-0.304	-0.1870	0.308	-0.157
5						-0.516	-0.399	---	-0.3694
6							0.1179	0.613	0.1476
7								0.495	---
8									-0.466
9									

Table 6-2: Comparison of Mean Bias between Vendors (difference is "column" minus "row")

Temperature and relative humidity were always varied together in the experimental design so the quantitative effect of temperature alone on bias was examined with simple, one-predictor, linear models on the $\log_{10}$ of the bias metric. **Table 6-3** shows that temperature accounted for a significant proportion of the variability in bias for Vendors 4, 6, and 7. The effect for Vendors 6 and 7 was positive (i.e., as temperature increased, bias increased) and was negative for Vendor 4 (i.e., as temperature increased, bias decreased). It is important to note that as temperature increased from 25 to 30 to 35 ºC, humidity was simultaneously changing from 50 to 20 to 70% RH. Therefore, the effect of temperature, where significant, might actually have been due to relative humidity. Ideally, temperature and relative humidity would have been varied independently in the experimental design but were not because of limitations in the time allowed for the laboratory evaluation. Nevertheless, we may conclude from these results that temperature and relative humidity are significant influences on bias for three of the eight vendors.

Vendor ID		p-Value[a]
1		0.4343
2		0.7125
3		0.8873
4	-	<0.0001[c]
5		0.8519
6	+	<0.0001[b]
7	+	<0.0001[b]
8		0.1497

[a] Probability that temperature/relative humidity have no effect on bias
[b] Highly significant in a positive direction
[c] Highly significant in a negative direction

Table 6-3: Effect of Experimental Conditions on Bias, by Vendor

A comparable approach could not be applied to RSD because this statistic is a measure of dispersion and, therefore, violates traditional linear model assumptions. The graphical display in Figure 6.5 shows appreciable differences in RSD among vendors.

6.7 Intrinsic Data Processing Capabilities (Assessment of Internal Peak Detection and Data Processing Algorithms and File Export Procedures; Peak Identification)

Insufficient information is available to assess this capability. All auto-GC units had means to collect, process, and store electronic data. During this study, all vendors converted their electronic printout to an Excel spreadsheet for RTI to review and compile for this laboratory evaluation report.

6.8 Representativeness of Hourly Concentration (Proportion of a One Hour Sample (i.e., Consistency of Historical 1-hr PAMS Sample))

Participation in the laboratory evaluation phase required that each vendor have the capability of collecting and analyzing all priority and optional compounds within an hour of gas introduction to the sampling system. All vendors demonstrated this capability. **Table 6-4** displays the sample, analysis, and total duration for each vendor **during the evaluation phase** and if the unit is capable of sampling and analyzing at the same time. These conditions were designed to maximize performance. The sample duration for the vendors ranged from 1.25 minutes to 45 minutes.

Vendor	Sample Duration, (minutes)	Analysis Duration, (minutes)	Total Duration, (minutes)	Sampling/Analyzing can occurs simultaneously
1	20	40	40	Yes
2	9 (C2-C6) 22.5 (C6-C12)	16.8 (C2-C5) 23.75 (C6-C12)	30 (C2-C5) 30 (C6-C12)	Yes (C2-C5) No (C6-C12)
3	10	43.15	53.15	Yes
4	40	43	83	Yes
5	10	30	60	Yes
6	1.25	17	22	No
7	60	53	113	Yes
8	45	45	90	Yes

Table 6-4: Sample Duration for Represented 1-Hour Sample

Vendor-specific observations are presented below based on our observations or direct conversations with vendors:

- Three of the vendors adjusted their sampling times to optimize chromatographic separation of compounds and detection. At least one of the vendors indicated that they were able to collect two samples per sample event and use the data from either or the average of the two sample runs to report their final result.

- One vendor required at least 45 minutes of time to collect and analyze a single sample. This posed a problem with Sample Test Number 2 (optional instrument calibration), in that Test 2 was only scheduled for a 30 minute collection time. For this reason, RTI staff agreed to provide the mixture of Sample Test 2 for two hours on and off to allow the vendor to run the verification point on their instrument. It is not known if the vendor's instrument has the capability to run more quickly or if it needs the full 45 minutes per sample by default.

- One vendor was able to run a sample in a 15 to 20 minute window. This allowed the vendor to take multiple readings for each test point. Only one data point for each test was provided to RTI for evaluation.

- There were no reported issues with the other two vendors with regard to difficulty in sample collection in the one hour time frame.

6.9 Unattended operation (Assessment of Duration of Unattended Operation without Compromise in Data Integrity Including the Level of Operator Knowledge Required to Maintain Instrument Operation)

Information provided in this section is based on observations made by RTI staff during the laboratory testing phase only, and will not include time or effort involved in set-up or take down of the actual instrumentation. Overall, it was observed that most of the candidates were able to achieve a reasonable level of unattended operation. The following specific observations were made:

- One vendor appeared to have the most difficulty with the automation of their instrumentation due to unforeseen mechanical issues which arose during the testing. A dozen or so hours were spent fixing issues by multiple instrument technicians over the course of the two week lab phase. While each operator either appeared to have the necessary knowledge of how to fix the issue or knew who to contact for ideas on strategies for fixing equipment, the duration of time spent working on the equipment would not be feasible in a field setting. Problems with instrumentation for the vendor may be reflected in missing data and in bias and precision results.

- Three of the vendors spent little amounts of time in the lab at their instruments. After set-up, each of the three vendors left soon after testing started and were able to operate with what appeared to be minimal interruptions in data collection. One of the three vendors had an issue towards the end of the study when an operating system update was installed and the laptop computer connected to the instrument restarted itself causing a connection loss and data not to be collected. The remedy to the issue was simply that a representative from company came to the lab, re-connected the instrument and made a minor sample line adjustment. The second of the three vendors had two representatives on-site available for troubleshooting. Typically they would arrive in the morning to ensure the instrument was still operating, and then leave for the day after an hour or so. As the study went on, instrument checks from this vendor became less and less frequent. The only observed hands-on maintenance performed by this vendor's staff involved switching a gas cylinder sometime in the middle of the testing. The third of three vendors in this section had no representatives on site for the majority of the testing and had full remote capability. The only observed issue was a drop in remote network connectivity on one of the days, which likely could have been avoided if the instrument was connected by the supplied CAT-5 cable instead of a Wi-Fi signal.

- Four of the vendors were in the lab either every day, or almost every day of the testing. It is difficult to determine if any on-the-fly adjustments were made to the instrumentation during the testing because each of the vendors spent significant time near their instruments. No significant instrument maintenance was performed while testing was executed. One of the four had at least one representative at their instrumentation from around 9 am to 6 pm each of the first six testing days, and one representative at their instrumentation for approximately half of the day on the last three days; maintenance for this vendor included one instance where a small amount of moisture was observed in the sample line and was quickly flushed out. The second vendor of four had a rotation of representatives on site over the course of the study. It appeared each representative checked their instrument at the start of every sample event (during business hours); however no system changes were reported to RTI staff. The third vendor of four made a trip to the lab for what is estimated to be six of the nine sampling days for an estimated one to four hours each time. Instrument adjustments were not observed by RTI lab staff during the visits, however the vendor did have an issue with the equipped zero-air generator in the middle of the study and had to switch to house zero-air provided by RTI (RTI also provided silica desiccant to dry the air to a sufficient level). The fourth vendor in this subsection had either one or two representatives on site for the entirety of the testing. Representatives only checked the instruments periodically each day, and it appeared they were accessing the instrument remotely

from a room across the hall from the lab on an as needed basis; the only instrument maintenance observed by RTI staff from was the exchange of a gas cylinder after approximately six days of running.

Overall and based on our observations, only one vendor's instrument may present significant difficulties and maintenance needs to a field analyst. Three of the vendors appeared to each have a high level of unattended operation. It is suspected that three of the vendors likely have sufficient unattended operation capabilities, however; since they were present throughout the laboratory evaluation, this cannot be determined accurately. A vendor had problems related to their zero-air generator which is likely an atypical event; they likely have the necessary unattended operation capabilities for field deployment.

Two other issues are important to address:

1) due to the fact that the testing period was too short for instrument failures to have occurred, it is not possible to accurately assess the level of operator knowledge needed to maintain their instruments. Based on conversations with representatives, there appeared to be excellent knowledge of equipment, VOC analysis requirements, and potential troubleshooting activities from all of the vendors.

2) the extent of post-processing of data needed cannot be accurately determined from a laboratory evaluation, so overall labor effort involved in instrument operation cannot be accurately determined. The field phase testing will provide a much clearer picture of actual data processing effort, since RTI representatives will be directly involved in data collection.

6.10 Internal Standard Calibration (Capability for Independent Internal Standard Introduction)

Insufficient information is available to assess this capability.

6.11 QC (Capability for Introduction of QC Samples)

The introduction of quality control samples (e.g., gas of known analyte concentrations) to any given instrument would likely involve the instrument's ability to draw from a pressurized gas mixture similar to the calibration gas. In a field application, this might be accomplished by any one of several mechanisms, none of which were evaluated during the lab phase, although the following observations were made:

- One vendor had a second inlet port for the introduction of a QC gas, and utilized a QC gas (which they provided for themselves) over the course of the study. RTI is not aware of the frequency, amount, concentration, or components of the gas which was introduced into the system, though it was observed that the bag gradually lost volume over time indicating it was utilized.

- One vendor also had a second inlet port for the introduction of a QC gas, and had a tank of compound mixtures connected over the course of the study. RTI is not aware of any automated activity from the compound gas over the course of the study, and it is likely that the secondary tank of compound mixtures were introduced manually at the start of the start of the study for instrument calibration.

- Two of the vendors had readily accessible secondary and tertiary sample input lines. This would allow for not only a QC sample to be introduced to the instruments, but also for dilution with zero-air prior to analysis, facilitating the control of concentrations delivered to the system. The presence of a second available input line would reduce the chances of contamination introduced by the field analyst by eliminating the need to physically switch the lines, and would reduce wear on any ferrules and threaded nuts causing less need for maintenance. These vendors also told RTI staff that the instrument had the capability to automatically introduce the gas at programmable times.

- Two of the vendors had visible connections for alternative sample inlet sources, but neither seemed as easily accessible as those in the previous section. The presence of the second inlet should allow the introduction of a QC gas to the instrument automatically. During the lab testing one of these two vendors utilized both inlet ports to supply the instrument with the needed flow; if this configuration was implemented in the field, a source of QC gas could not be introduced without a line change.

- One of the vendors appeared to have a second inlet port with the capability of an automated QC sample introduction system, however this information was not disclosed to RTI staff, nor was there a second source line connected at any point during the study.

- A vendor did not appear to have a system capable of automatic QC introduction. Based on the appearance and size of the unit, there would likely have to be a physical switching of the lines (or valve switching mechanism somewhere upstream of the sample inlet) in order to achieve desired QC introduction.

7.0 General Findings

7.1 Auto-GC Unit Performance

Below are some significant events encountered during the laboratory testing which had an affect specific auto-GC unit's performance and scoring.

- One auto-GC unit had a catastrophic failure and was unable to complete approximately 30% of the actual laboratory evaluation. Based on information provided during and after the lab phase testing, the issue was a mechanical failure of a single part in an ancillary pump for which a replacement part was unattainable before the completion of the study.

- One auto-GC unit had a failure which severely impacted the ability to measure under conditions of high humidity.

- Three auto-GC units had difficulty creating the simple output format required for reporting of results to RTI. Two vendors, in particular, had great difficulty in providing a consistent output format.

- Four vendors reprocessed their results, two of them multiple times, after being provided with their original data deliveries for certification.

- One vendor had difficulty collecting a representative sample because their sample volume was small compared to the volume of the transfer tubing between their instrument and the manifold.

- One vendor had an issue with their zero-air generator, which had to be replaced. This change was suspected to have caused a slight shift in peak retention times due to a slight difference of moisture between the two zero air sources.

- Chromatographic performance during the laboratory phase was difficult to evaluate objectively because vendors could optimize their systems based on knowledge of the compounds of interest. However, even with this optimization, some vendors were able to resolve m- and p-xylene and some were not.

7.2 Usability

Although RTI had no hands-on time with any of the units, information provided in this section is based solely on observations and is not intended provide a complete picture of usability. This will be more thoroughly addressed in the Field Phase Report at the conclusion of the study. Our general observations included:

- Instrumentation for three vendors was controlled exclusively by a portable computer. Each vendor's instruments utilized custom developed software for their instrument which controlled all necessary functions (chromatographic times, temperature steps, data collection, etc.) for sample analysis. All three vendors had a typical user interface which appeared to be straight forward for simple user commands.

- Instrumentation for two of the vendors had a computer integrated into one of the modules of the unit. All functions, including remote operation were controlled through the unit. The interface, which was a GUI operating system, appeared to be straight forward for simple user commands, and likely had the capability for more user entered commands if needed.

- Instrumentation for one of the vendors contained both an on-board computer and a second portable computer. Based on observations, it appeared the control of the instrument was conducted by the on-board computer which likely contained the necessary functions for sample

analysis. The secondary computer appeared to be used exclusively for data transfer and likely was where some automated post-processing of data was conducted.

- Instrumentation for two vendors each had an onboard touch screen computer and a second portable computer. The control of the instrument could be conducted by either the touch screen or the connected computer and both likely could control necessary functions for sample analysis. The secondary computer appeared to be used the primary data transfer tool, and likely was where some automated post-processing of data was conducted.

All the instruments in the study appeared to be user friendly and with some training and technical guidance, a field operator should be able perform the basic operations and maintenance. For repairs and troubleshooting of the auto-GC units, advanced knowledge and understanding of the unit's operation would be a task the field operator would need to develop. All vendor candidates offer technical support when a unit is purchased, but this support comes at a financial cost.

7.3 Reliability

Insufficient information is available to assess this capability.

7.4 Cost

While the performance, usability, and reliability of each vendor's equipment tested are all important factors, the evaluation of the cost of each unit, ancillary equipment, and add-ons is essential to ascertain a complete picture of not only total overall performance but also feasibility of the inclusion of equipment in both new and established monitoring networks. RTI requested that each vendor supply a total cost estimate to RTI for EPA use, not only in an evaluation capacity but also as a purchase price if the unit qualifies for the field testing portion of the study. It is also important to note that all cost estimates are a reflection of the complete system tested during the lab phase. There should be no additional equipment parts or upgrades as either part of the quote or utilized during the testing which is not included in the quote.

The evaluation of the cost criteria will only include core equipment, unit ancillary equipment (i.e., computers, hydrogen or air generators, software packages, instrument drivers, gas purifiers, and air compressors), and add-on parts (i.e., vacuum pumps, dryer, fitting kits, repair kits, and flowmeters). Though the complete price quotes from some vendors include other relevant information such as training, setup costs, operating costs, technical support costs, etc. – all these "extras" will be excluded from this report evaluation. Justification for excluding the "extras" is two-fold, first utilizing only the price for the equipment will compare essentially the minimum cost point which may be all that would be required to start analysis in certain instances. Second since not all vendors provided the same extent of information in the "extras", no vendor will be graded more harshly for their candor of total potential costs.

Due to the sensitive nature and confidentiality of vendor price points, the provided costs will not be included in this report but will be supplied to the EPA as a secondary document. Each price quote in its entirety will be supplied to the EPA in order to give a complete picture of potential costs. The overall evaluation performance ratings matrix will include a cost section, but any cost justifications for ratings will not be included as part of this document.

8.0 Summary

8.1 Scale (ranking) Vendors from High to Low for Each Category

A decision matrix was developed by EPA that resulted in four categories and weighted scoring for each category. The categories and weighted scoring for each are displayed in **Table 8-1**. For each category, a list of evaluation criterion was developed. For example, Category 1 is related to the performance of the auto-GC unit during the laboratory evaluation phase. The evaluation criterion for Category 1is: bias, precision, completeness, relative measurement threshold, effect of temperature/relative humidity, and representativeness of hourly concentration. The evaluation criterion listed in the Table 8-1include both quantitative and subjective data. For all quantitative criterions, RTI was able to review the data from the laboratory evaluation and develop a ranking based on the performance of the vendor's auto-GC unit. This vendor ranking is discussed below and displayed in the following tables. The subjective information gathered during the laboratory phase by RTI staff was documented and placed on RTI's server under the Project Folder. In order to maintain anonymity, RTI will provide the subjective information for Category 2 and 3 directly to the EPA WAM and no details will be described in this report. Some of the evaluation criterion for Categories 2 and 3 could not be accessed during the laboratory evaluation phase. Based on critical evaluation limitations, the rating for these evaluation criterions will be "Y" for acceptable, "N" for unacceptable, or "U" for unknown or unable to determine. Category 4 information is confidential and will also be provided in a separate report to the EPA WAM.

	Category	Weighting
1	Performance ▪ Precision ▪ Bias ▪ Representation of hourly concentration ▪ Completeness ▪ Relative Measurement Threshold ▪ Influence of humidity and temperature	**50%**
2	Usability ▪ Ability to operate remotely ▪ Auto calibration capability ▪ Automatic data flagging ▪ Output format (AQS or cvs) ▪ Space requirement at field site ▪ Operator knowledge capability ▪ Ease of operation, maintenance, and repair	**20%**
3	Reliability ▪ Frequency of maintenance ▪ Frequency of calibration ▪ Robustness for field use	**15%**
4	Cost ▪ Capital cost ▪ Add-ons ▪ Replacement parts ▪ Setup at field site ▪ Training ▪ Service or technical support ▪ Annual operating cost	**15%**

Table 8-1: Decision Matrix for the Results of Laboratory Evaluation Phase

Vendor ranking for each of the quantitative evaluation criteria, shown below in **Table 8-2**, were derived from the graphical presentation of the criteria across all priority analytes. The contribution (weighting) of each criterion is presented in **Table 8-3**. The statistical calculations and determinations for the evaluation criterion in Tables 8-2 and 8-3 are discussed in Section 6.

Evaluation Criterion	Vendor ID Ranking (High → Low)
Bias	1 > 3 > 2 >4 >6 > 7 > 5 > 8
Precision	1 > 4 > 3 > 2 > 6 > 8 > 5 > 7
Completeness	1 = 4 = 3 > 2 > 7 > 5 > 8 > 6
Relative Measurement Threshold	1 > 5 > 2 > 3 > 4 > 6 > 8 > 7
Effect of Temperature/Relative Humidity	8 = 2 = 1 = 5 = 3 > 6 = 4 = 7
Representativeness of Hourly Concentrations	Not evaluated quantitatively

Table 8-2: Vendor Ranking for Quantitative Evaluation Criteria across Vendors

Evaluation Criterion	Percent of Total Ranking
Bias	10
Precision	10
Completeness	10
Relative Measurement Threshold	5
Effect of Temperature/Relative Humidity	10
Representativenesss of Hourly Concentrations	5

Table 8-3: Percent Contribution for Each Quantitative Evaluation Criterion

Table 8-4 and **Figure 8-1** show the contribution of scores for each evaluation criterion and the overall vendor score for each vendor using the weights shown in Table 8-3 to each of the performance metrics. A score of 8 is assigned to the highest ranking vendor in each category, 7 to the next highest, and to 1 which is the lowest ranking vendor. Since Vendors 1, 4, and 3 ranked equally in completeness, all three vendors were assigned the average ranking of 7 (the average of 8, 7, and 6). Similarly, since temperature/relative humidity was significant only for Vendors 6, 4, and 7, these vendors were assigned a score of 2 (i.e., the average of scores 3, 2, and 1) while Vendors 1, 2, 3, 5, and 8 were assigned the score of 6 (i.e., the average of 8, 7, 6, 5, and 4). The overall score for each vendor was the arithmetic sum of the scores in each of the five evaluation criterions (bias, precision, completeness, relative measurement threshold, effect of temperature/relative humidity, and representativeness of hourly concentration).

	VENDOR SCORE[a]								
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**% of Total**
Bias	8	6	7	5	2	4	3	1	22
Precision	8	5	6	7	2	4	1	3	22
Completeness	7	5	7	7	3	1	4	2	22
Relative Measurement Threshold	8	6	5	4	7	3	1	2	11
Effect of Temperature/Relative Humidity	6	6	6	2	6	2	2	6	22
Overall[b]	**33**	**25**	**28.5**	**23**	**16.5**	**12.5**	**10.5**	**13**	

[a] 1=poorest score, 8= best score.
[b] Weighted overall score

Table 8-4: Overall Scoring for Quantitative Evaluation Criteria across Vendors

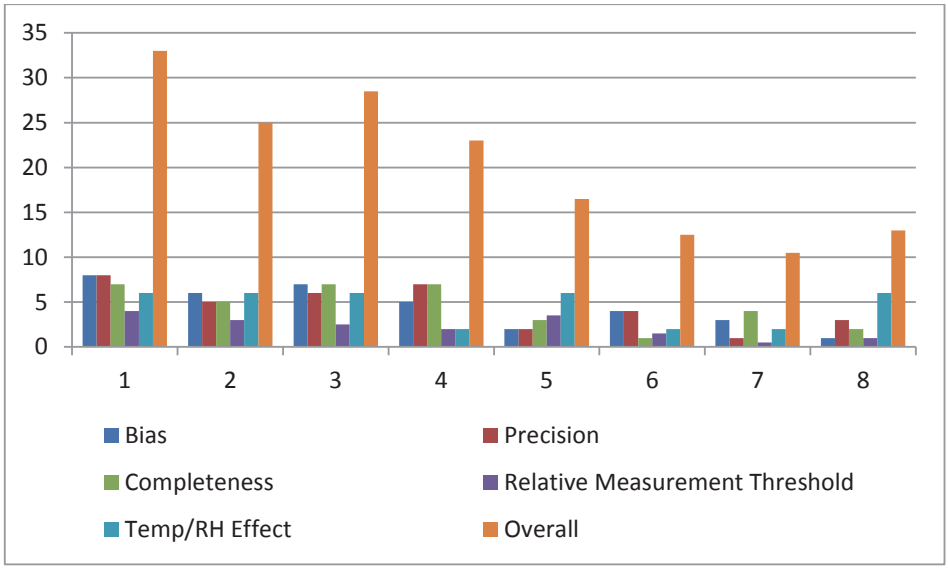


Figure 8-1: Distribution of Vendor Scores across Quantitative Evaluation Criteria

From **Table 8-4**, the overall ranking of vendors for the five quantitative evaluation criteria for auto-GC unit performance in Table 8-1 is calculated as:

1 > 3 > 2 > 4 > 5 > 8 > 6 > 7

8.2 Base Discussion on Decision Matrix

The scoring matrix for ranking of vendor instruments is provided below in **Table 8-5** and includes evaluation criteria. Percent contribution to the overall evaluation score is provided as "Weight" for each category or evaluation criterions. Vendor scores and subjective capability assessments are provided to the EPA to facilitate their selection of vendor instrument to be included in the field evaluation phase.

Definitive information for some of the evaluation criteria could not be determined during the laboratory evaluation phase. This information will be acquired during instrument operation in the field phase for vendors which EPA selects for that phase.

			Vendor ID							
	Category	**% Weight**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
1	Performance	**50**								
	Bias[a]	10	8	6	7	5	3	4	3	1
	Precision[a]	10	8	5	6	7	2	4	1	3
	Completeness[a]	10	7	5	7	7	3	1	4	2
	Relative Measurement Threshold[a]	5	8	6	5	4	7	3	1	2
	Influence of humidity and temperature[a]	10	6	6	6	2	6	2	2	6
	Representativeness of hourly concentration	5	Y[b]	Y	Y	Y	Y	Y	Y	Y
	Overall Quantitative Score[c]		**33**	**25**	**28.5**	**23**	**16.5**	**12.5**	**10.5**	**13**
2	Usability	**20**								
	Ability to operate remotely		Y	Y	Y	Y	Y	Y	Y	Y
	Auto calibration capability		Y	Y	N[d]	Y	Y	U[e]	Y	Y
	Automatic data flagging		U	Y	U	Y	Y	U	U	Y
	Output format (AQS, CVS, Excel)		Y	Y	Y	Y	Y	Y	Y	Y
	Space requirements in field		6	5	8	1	3	4	7	2
	Operator knowledge required		U	U	U	U	U	U	U	U
	Ease of operation, maintenance, repair		U	U	U	U	U	U	U	U
3	Reliability	**15**								
	Maintenance frequency		U	U	U	U	U	U	U	U
	Calibration frequency		U	U	U	U	U	U	U	U
	Robustness for field use		U	U	U	U	U	U	U	U
4	Cost ($)	**15**								
	Capital cost		This information is confidential and will be delivered to the EPA WAM in a separate document.							
	Add-ons									
	Replacement parts									
	Field setup									
	Training									
	Service/technical support									
	Annual operating cost									

[a] Values for each vendor are ranked scores (1=lowest score, 8=highest score).
[b] "Y", vendor's auto-GC unit has this capability
[c] Overall weighted score across bias, precision, completeness, relative measurement threshold, and influence of humidity and temperature.
[d] "N", vendor's auto-GC unit does not have this capability.
[e] "U", the information is currently not available and will be collected during the Field evaluation.

Table 8-5: Scoring Matrix for the Results of Laboratory Evaluation Phase

9.0 References

Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air, Second Edition, Compendium Method TO-17 Determination of Volatile Organic Compounds in Ambient Air Using Active Sampling Onto Sorbent Tubes. Center for Environmental Research Information, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH. EPA/625/R-96/010b, January 1999.

RTI International and EC/R Incorporated, 2014, Gas Chromatograph (GC) Evaluation Study Quality Assurance Project Plan (QA Level III). Approved by EPA on March 11, 2014 and submitted to vendor candidates on March 11, 2014.

RTI International and EC/R Incorporated, 2014, Evaluation Test Plan for Field Deployable Automated-Gas Chromatographs in Controlled Laboratory and Uncontrolled Field Environments. Approved by EPA on March 11, 2014 and submitted to vendor candidates on March 11, 2014.

SAS Documentation, Version 9.3, Statistical Graphics Procedures Guide, SAS Institute Inc., Cary, NC, 2010.

Appendices

Appendix A Box and Whisker Comparison of Precision Estimates Across Vendors for Individual Target Analytes.

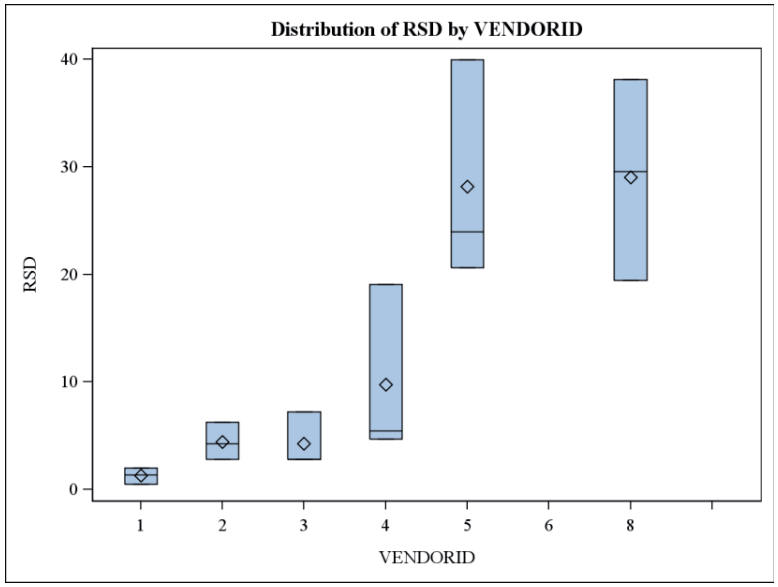


Figure A-1: Distribution of RSD for optional target 1,3,5-Trimethylbenzene

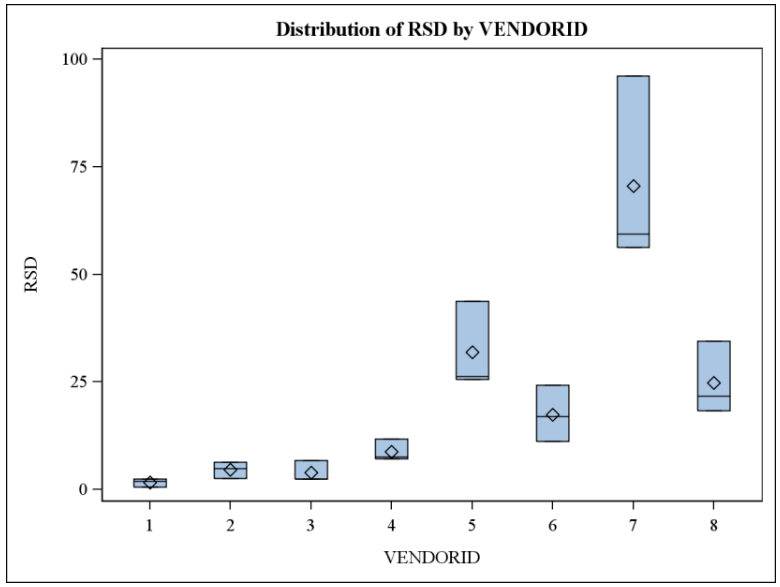


Figure A-2: Distribution of RSD for optional target 1-Pentene

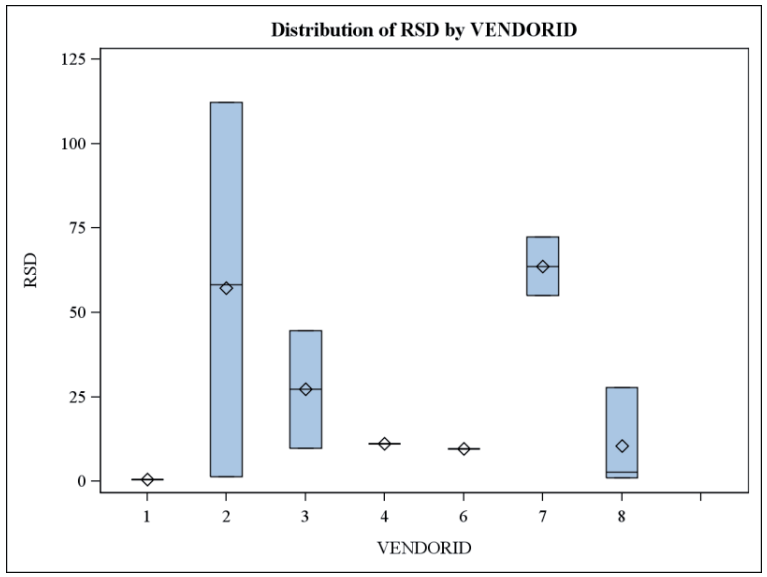


Figure A-3: Distribution of RSD for optional target 2,2-Dimethylbutane

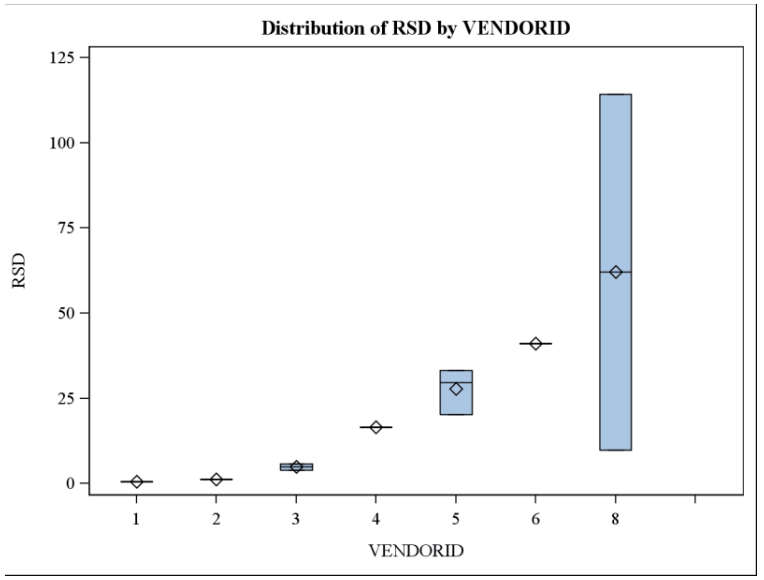


Figure A-4: Distribution of RSD for optional target 2,3,4-Trimethylpentane

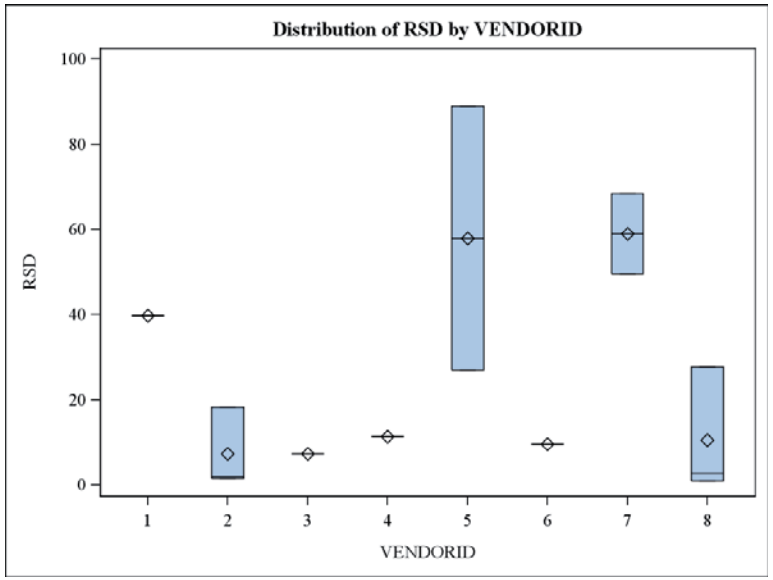


Figure A-5: Distribution of RSD for optional target 2.3-Dimethylbutane

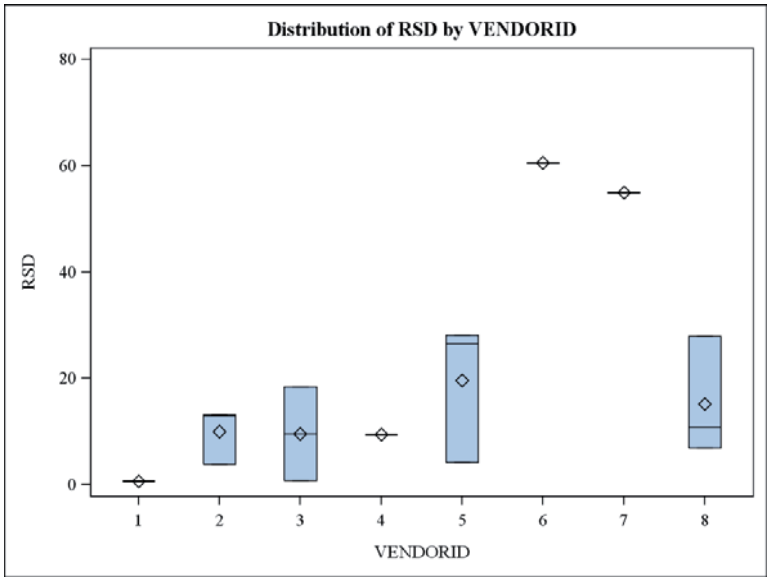


Figure A-6: Distribution of RSD for optional target 2.3-Dimethylpentane

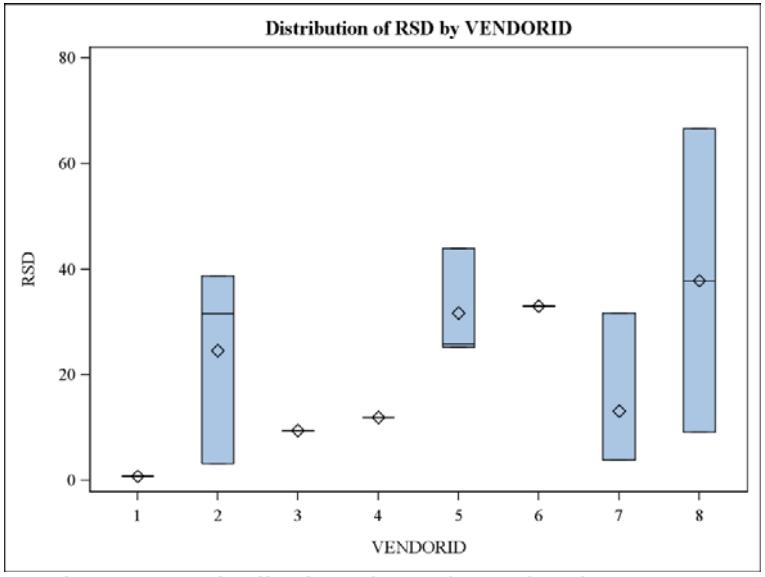


Figure A-7: Distribution of RSD for optional target 2.4-Dimethylpentane

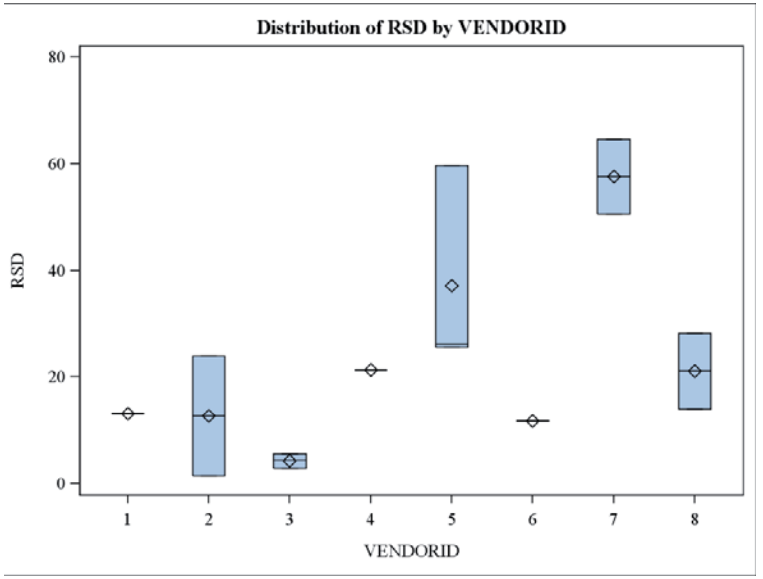


Figure A-8: Distribution of RSD for optional target 2-Methylheptane

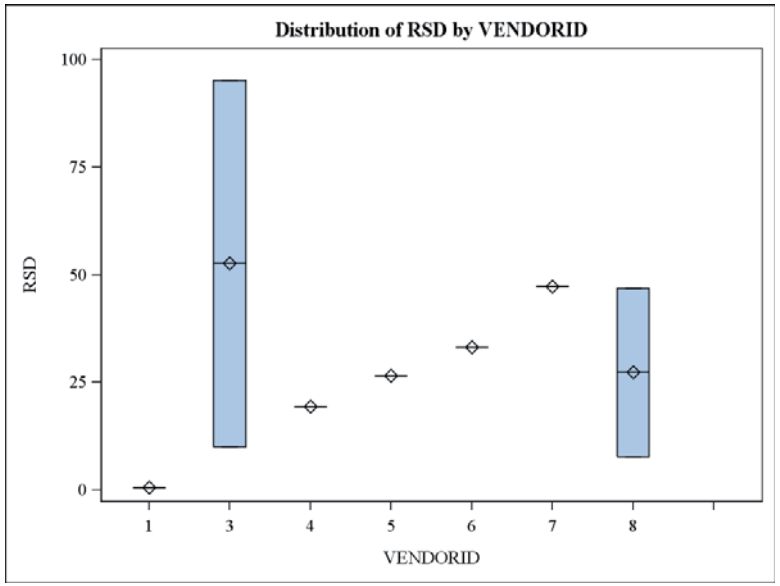


Figure A-9: Distribution of bias for optional target 2-Methylhexane

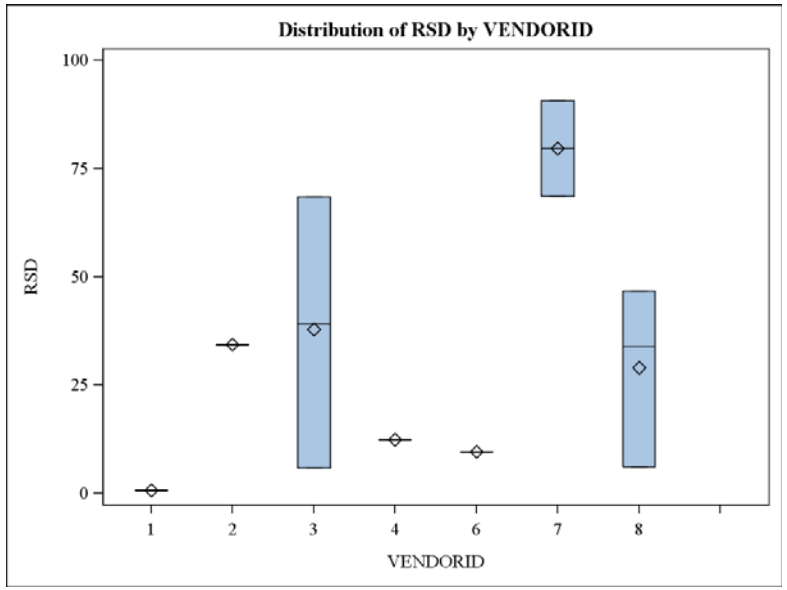


Figure A-10: Distribution of bias for optional target 2-Methylpentane

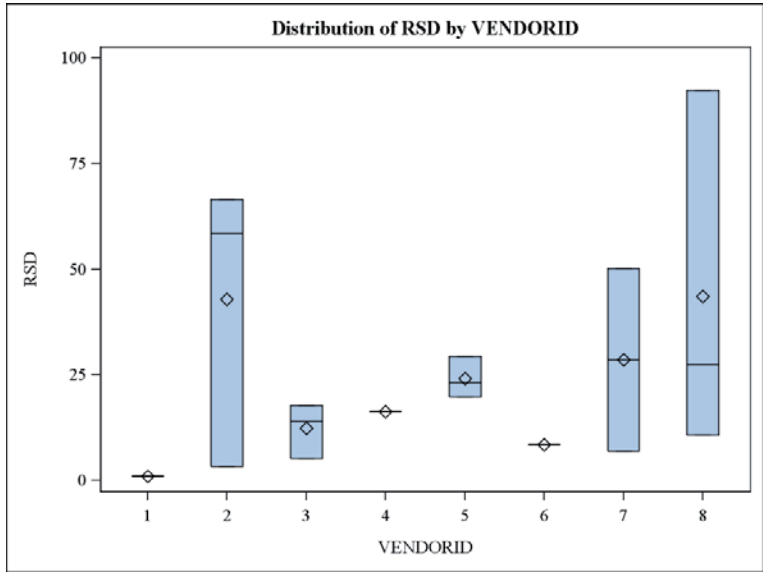


Figure A-11: Distribution of RSD for optional target 3-Methylheptane

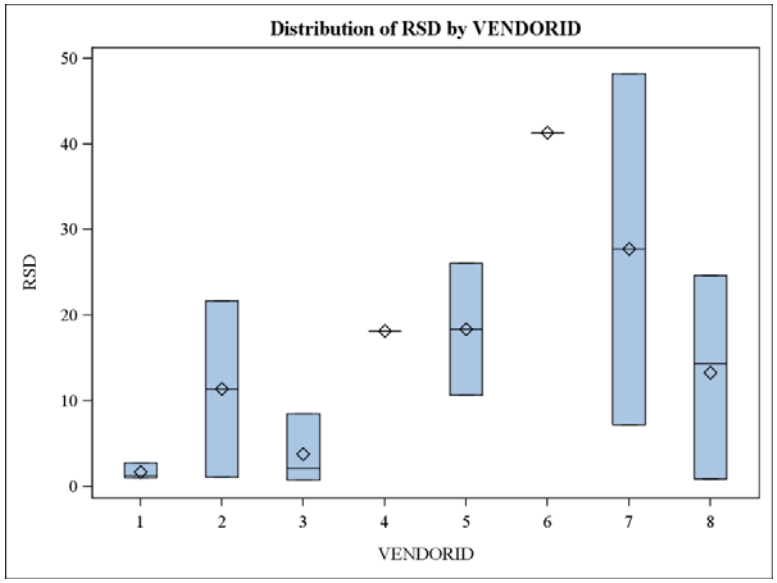


Figure A-12: Distribution of RSD for target 3-Methylhexane

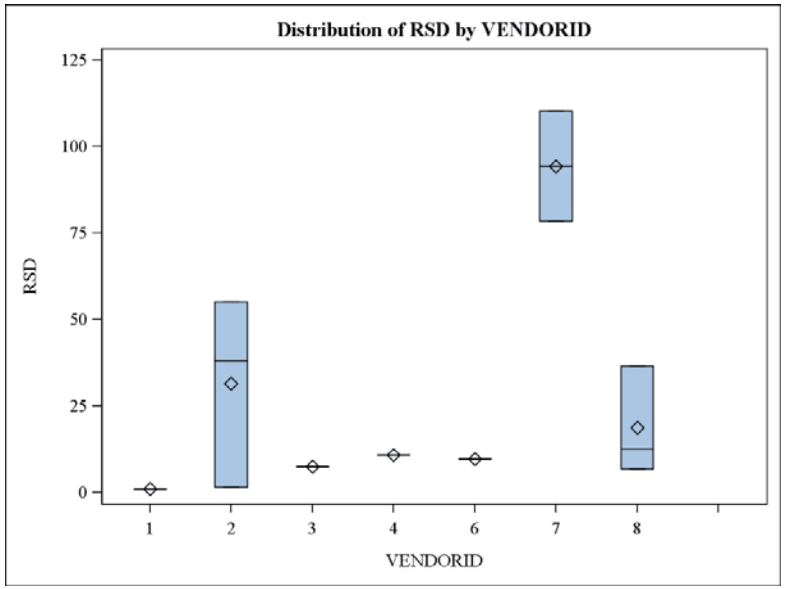


Figure A-13: Distribution of RSD for optional target 3-Methylpentane

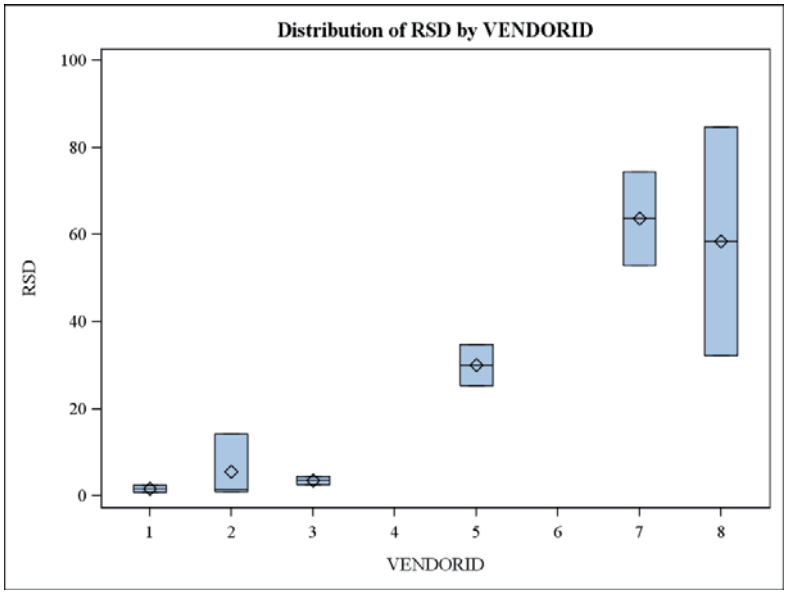


Figure A-14: Distribution of RSD for optional target Acetylene

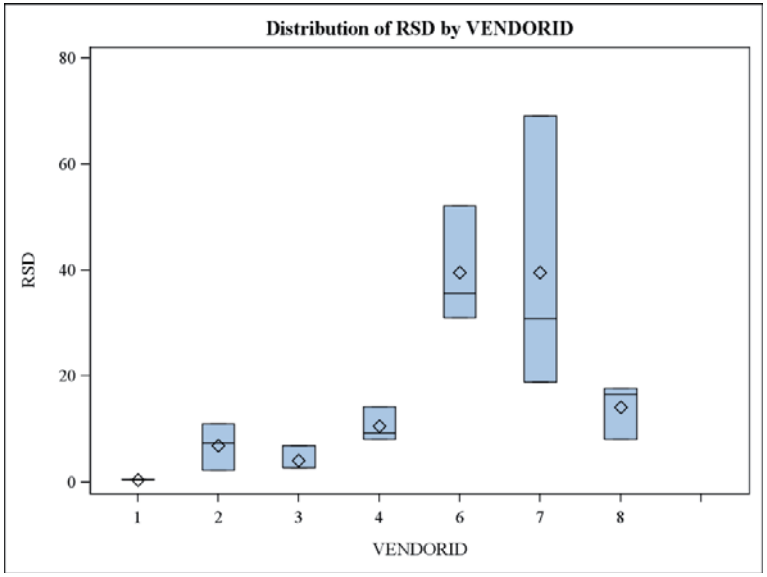


Figure A-15: Distribution of RSD for optional Cyclohexane

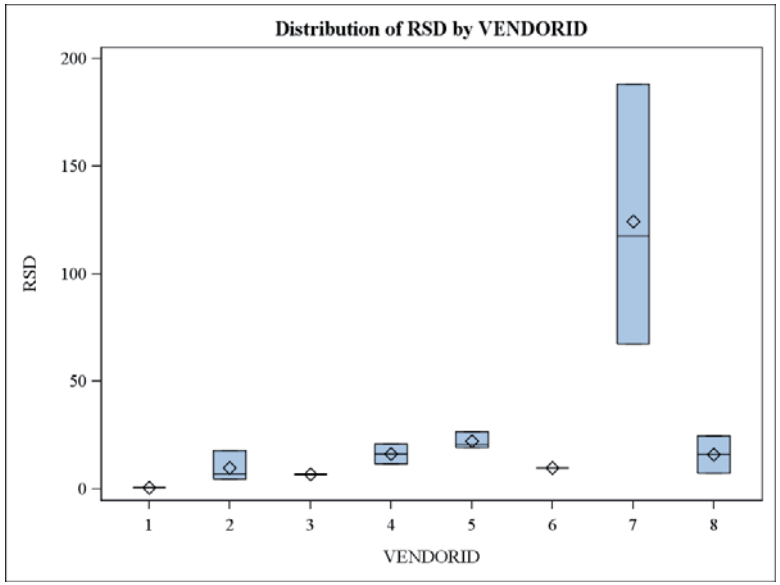


Figure A-16: Distribution of RSD for target Cyclopentane

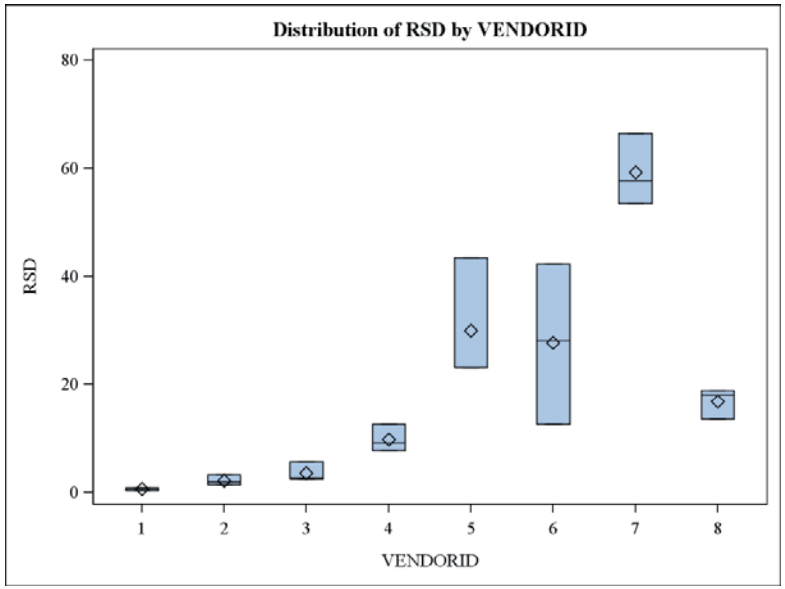


Figure A-17: Distribution of RSD for optional target Isopropylbenzene

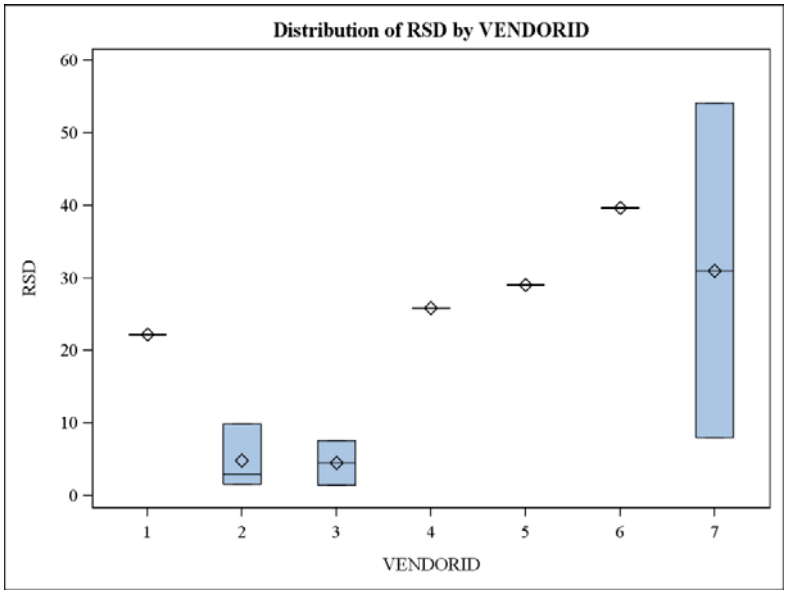


Figure A-18: Distribution of RSD for optional target Methylcyclohexane

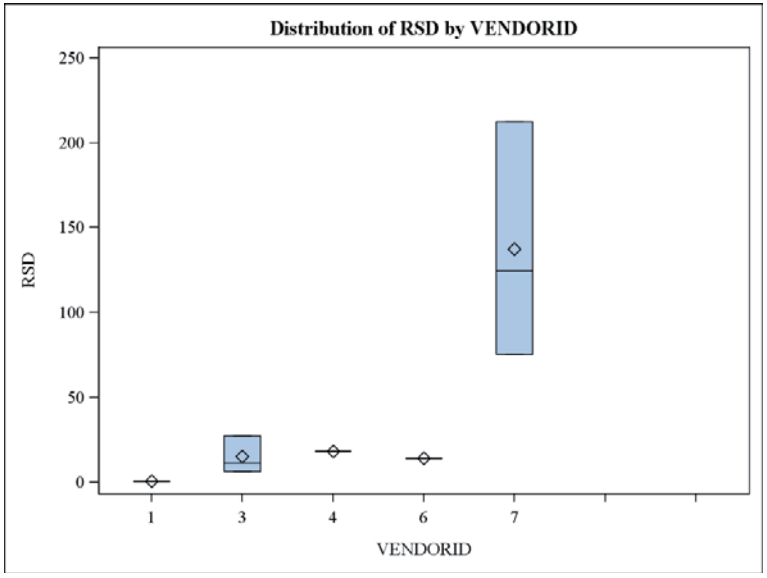


Figure A-19: Distribution of RSD for optional target Methylcyclopentane

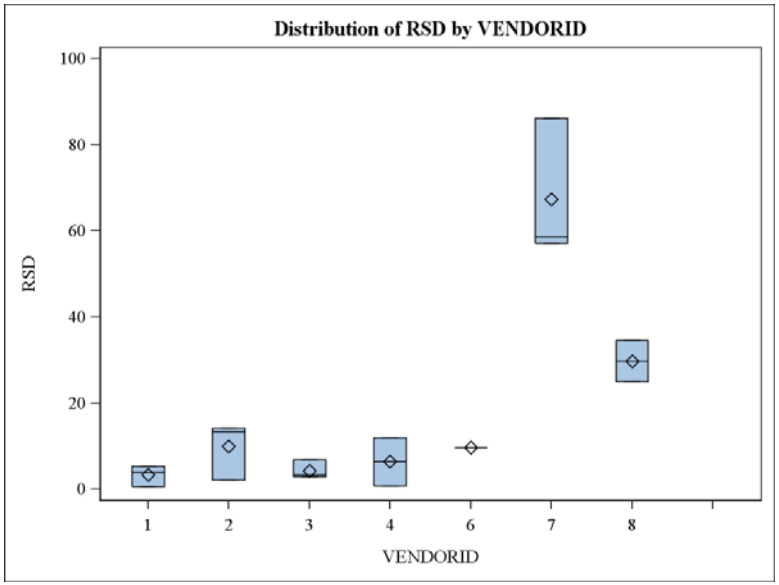


Figure A-20: Distribution of RSD for optional target cis-2-Pentane

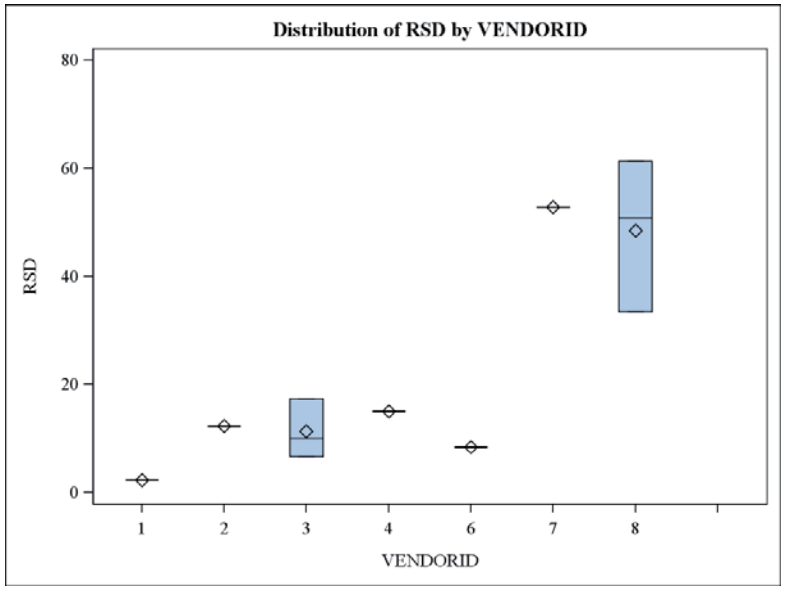


Figure A-21: Distribution of RSD for optional target m-Diethylbenzene

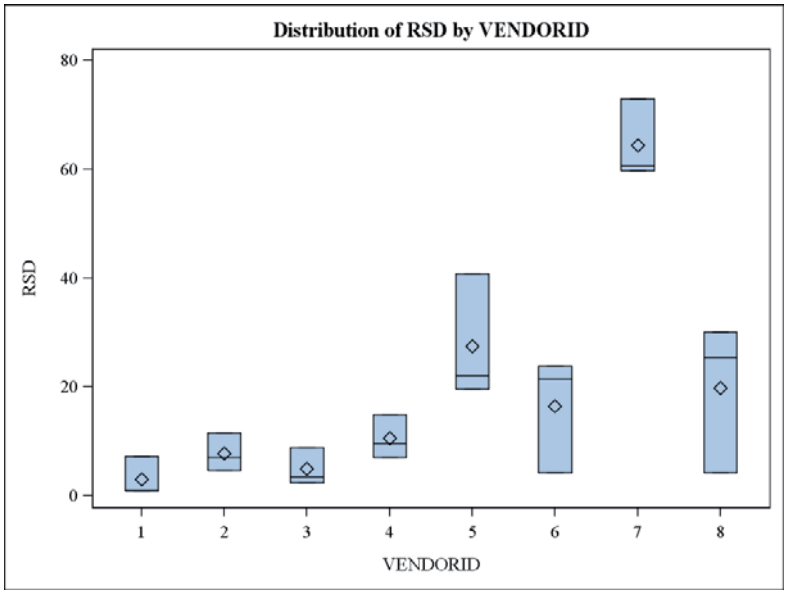


Figure A-22: Distribution of RSD for optional target n-Decane

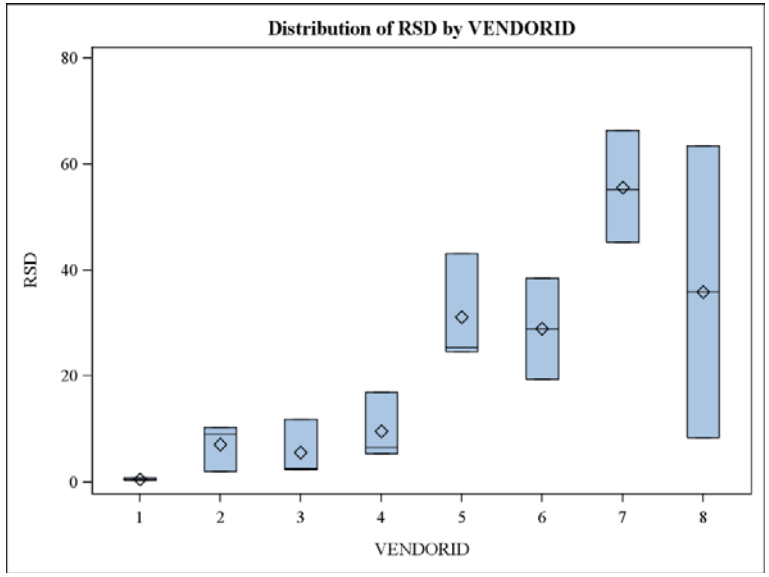


Figure A-23: Distribution of RSD for optional target n-Heptane

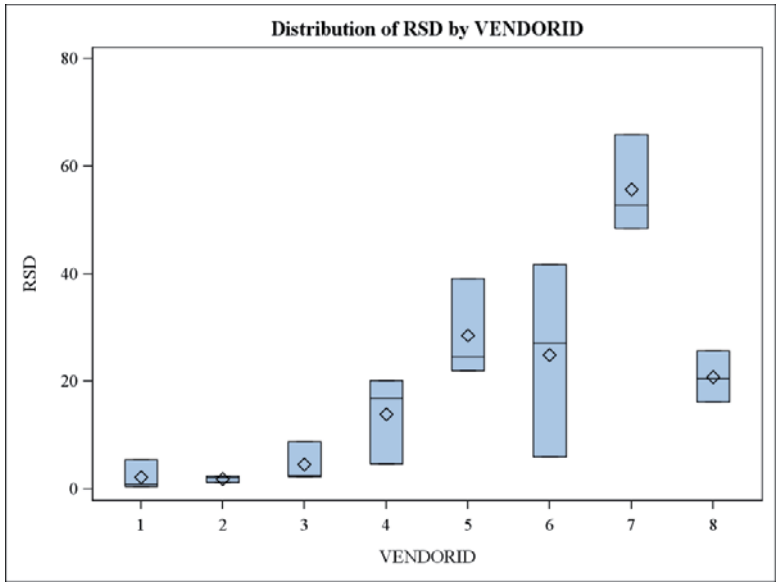


Figure A-24: Distribution of RSD for optional target n-Nonane

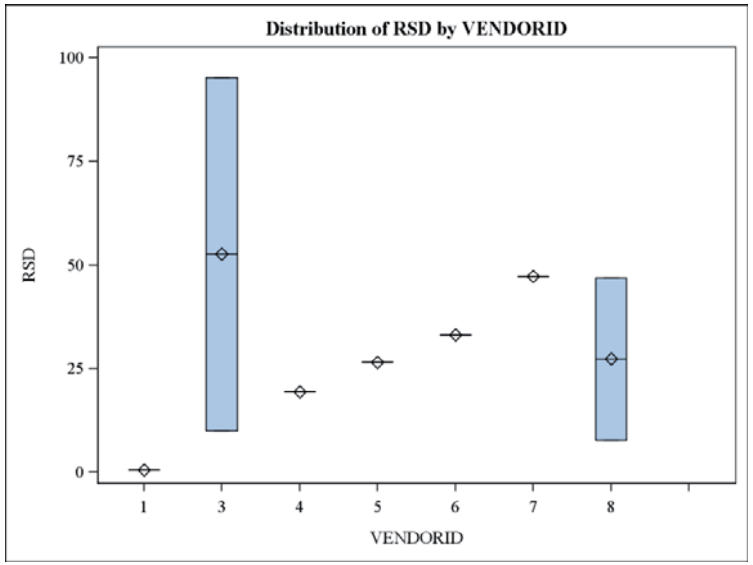


Figure A-25: Distribution of RSD for optional target n-Octane

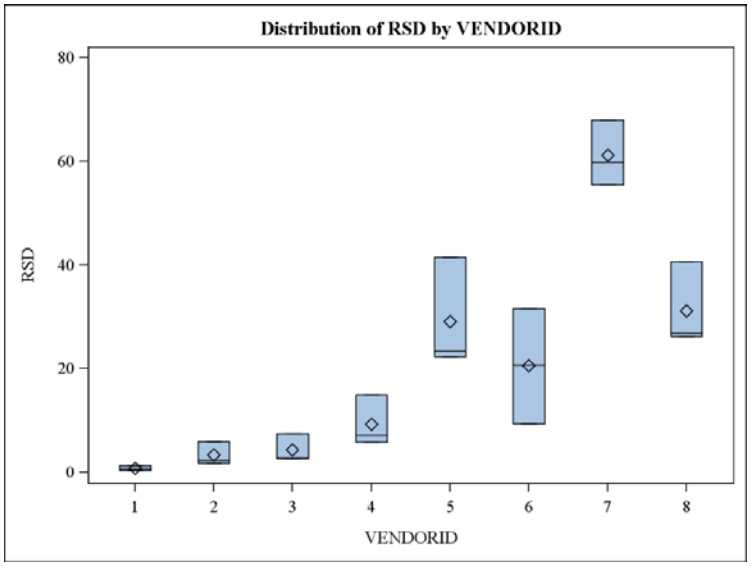


Figure A-26: Distribution of RSD for optional target n-Propylbenzene

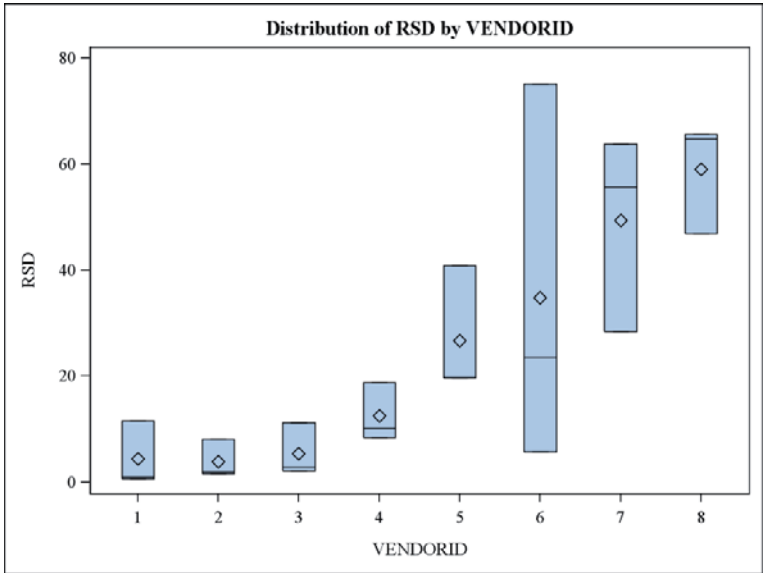


Figure A-27: Distribution of RSD for optional target n-Undecane

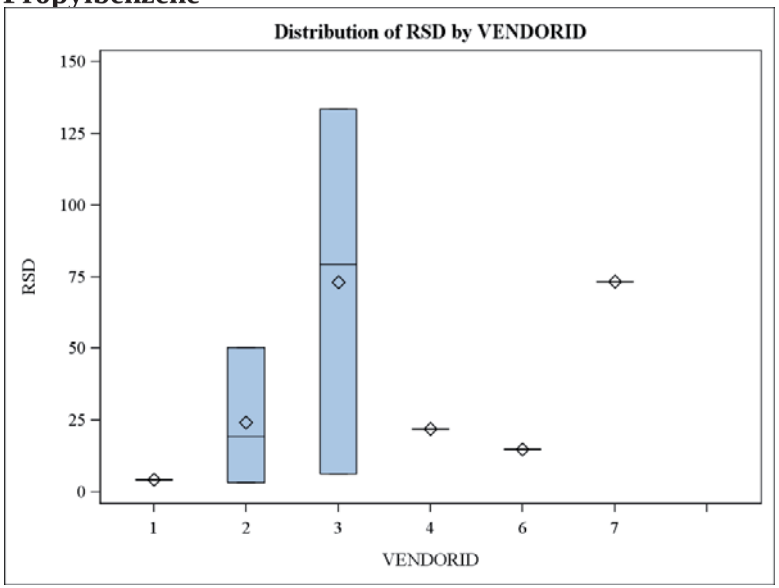


Figure A-28: Distribution of RSD for target p-Diethylbenzene

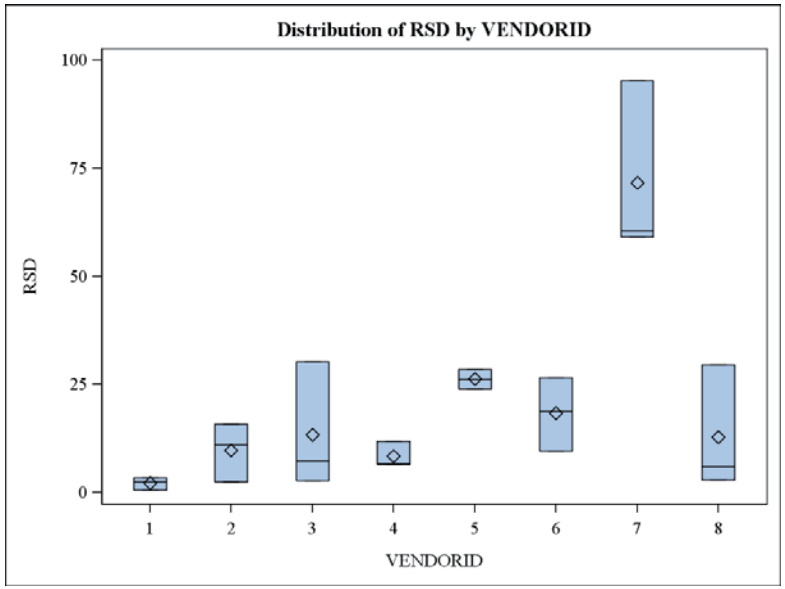


Figure A-29: Distribution of RSD for optional target trans-2-Pentene

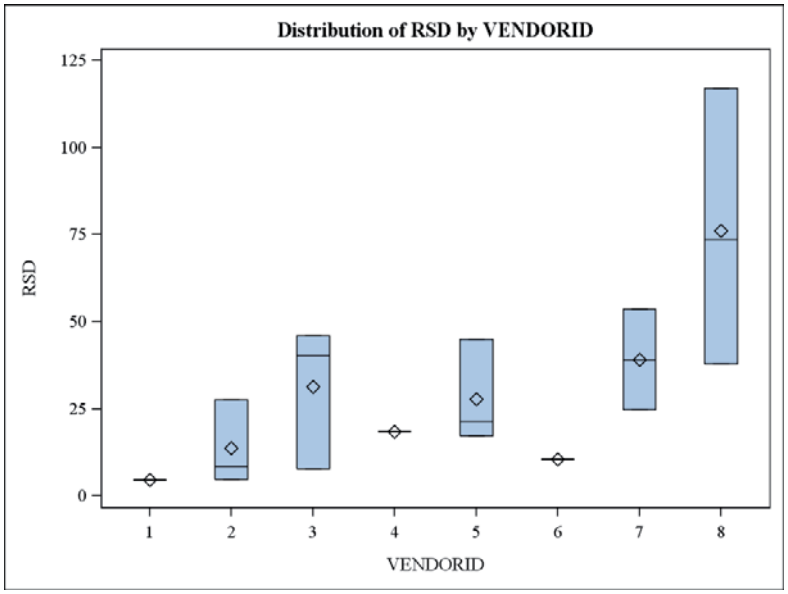


Figure A-30: Distribution of RSD for priority target 1,2,3-Trimethylbenzene

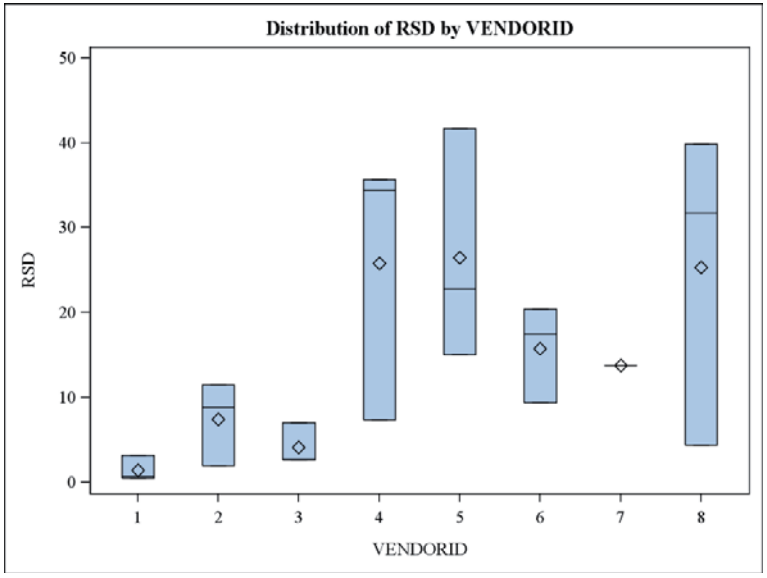


Figure A-31: Distribution of RSD for priority target 1,2,4-Trimethylbenzene

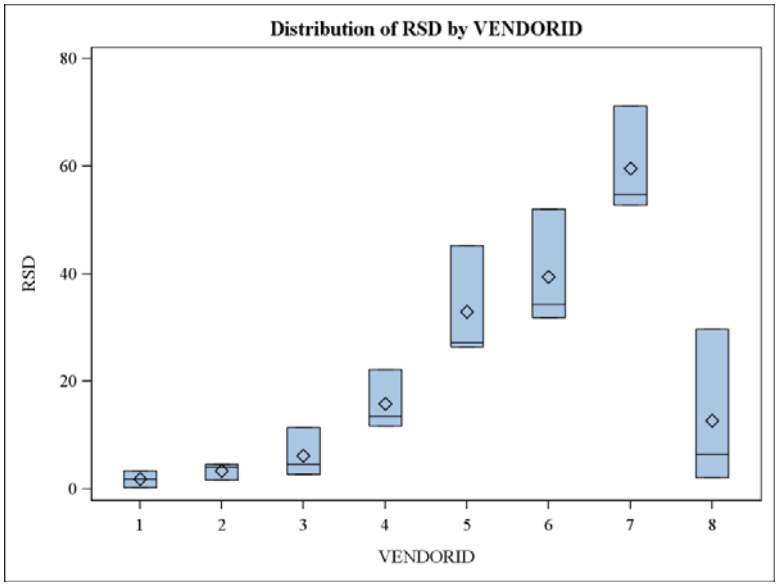


Figure A-32: Distribution of RSD for priority target 1-Butene

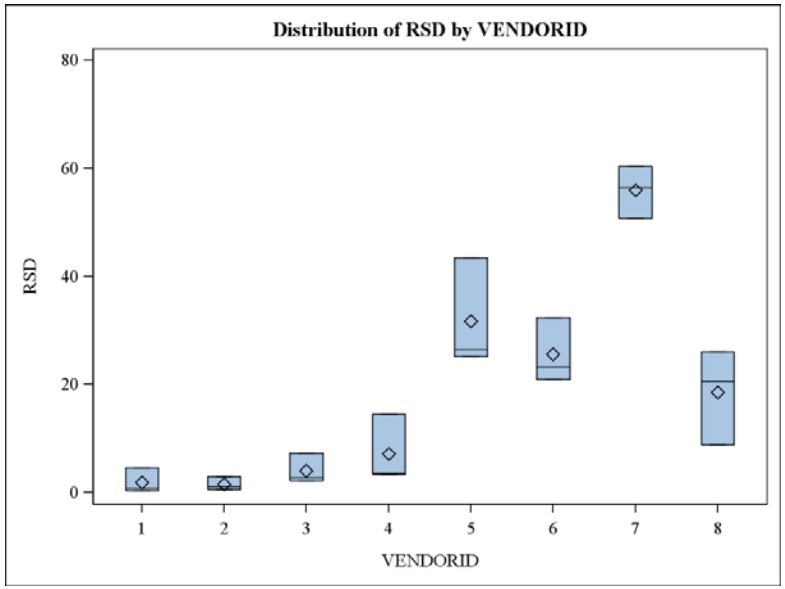


Figure A-33: Distribution of RSD for priority target 2,2,4-Trimethlpentane

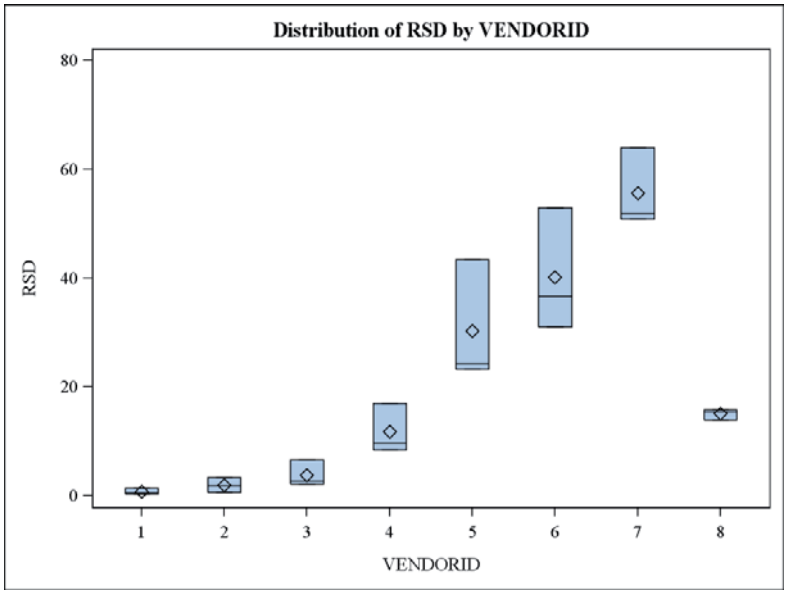


Figure A-34: Distribution of RSD for priority target Benzene

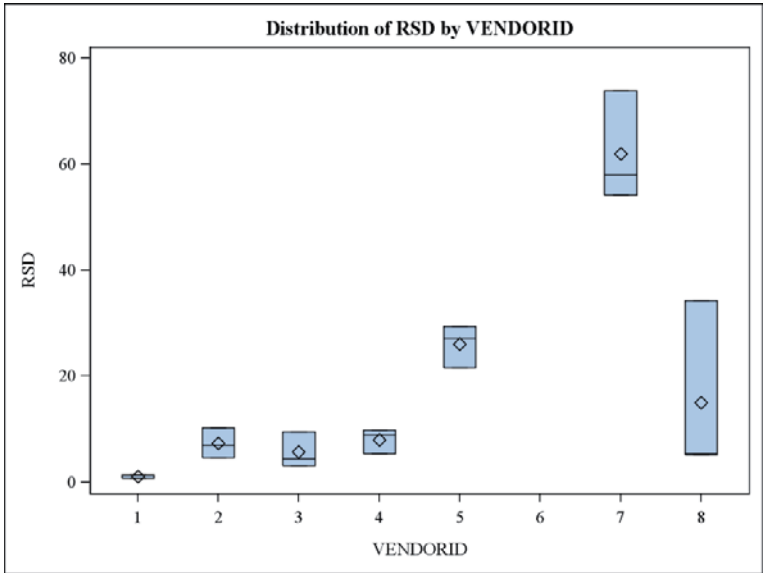


Figure A-35: Distribution of RSD for priority target Ethane

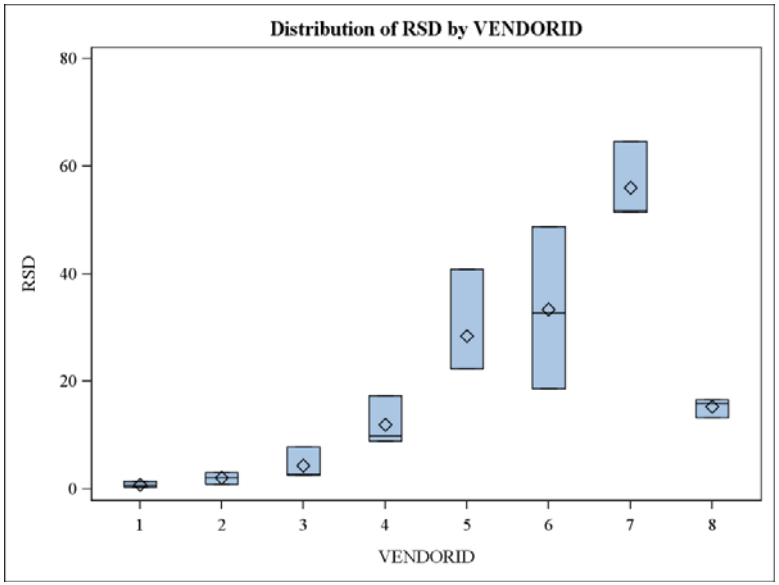


Figure A-36: Distribution of RSD for priority target Ethylbenzene

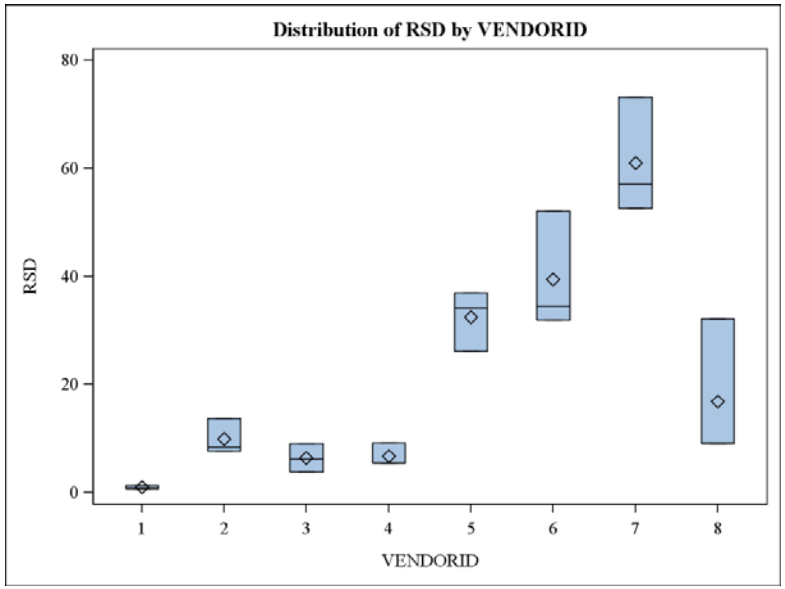


Figure A-37: Distribution of RSD for priority target Ethylene

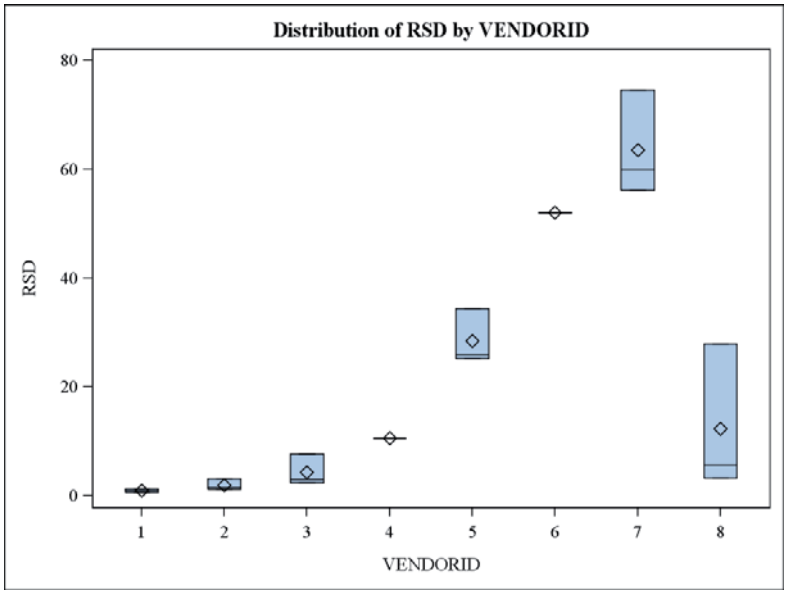


Figure A-38: Distribution of RSD for priority target Isobutane

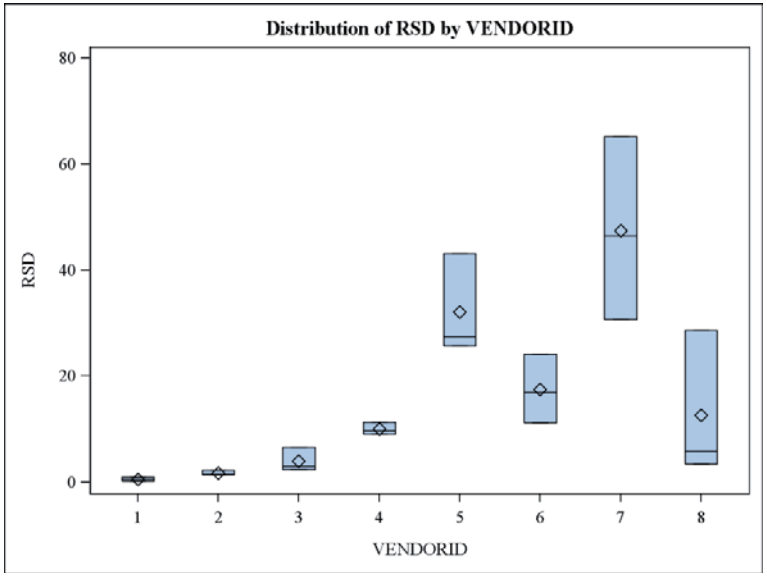


Figure A-39: Distribution of RSD for priority target Isopentane

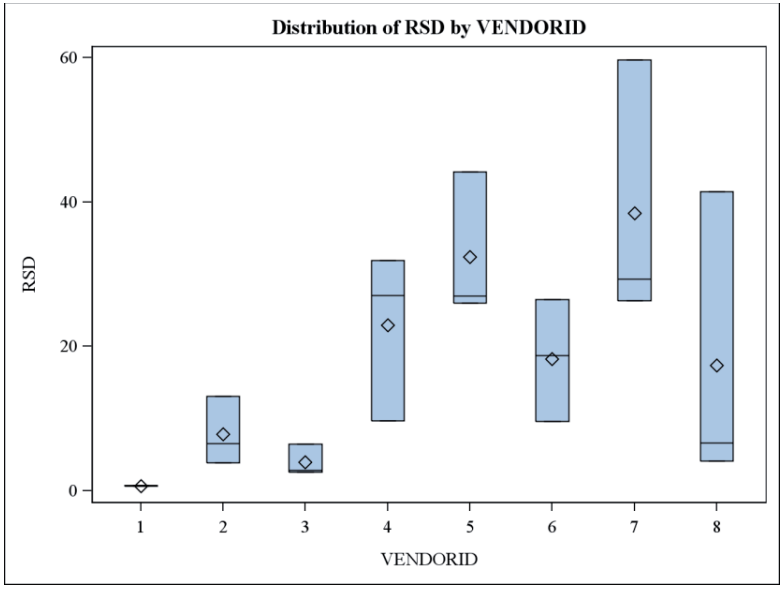


Figure A-40: Distribution of RSD for priority target Isoprene

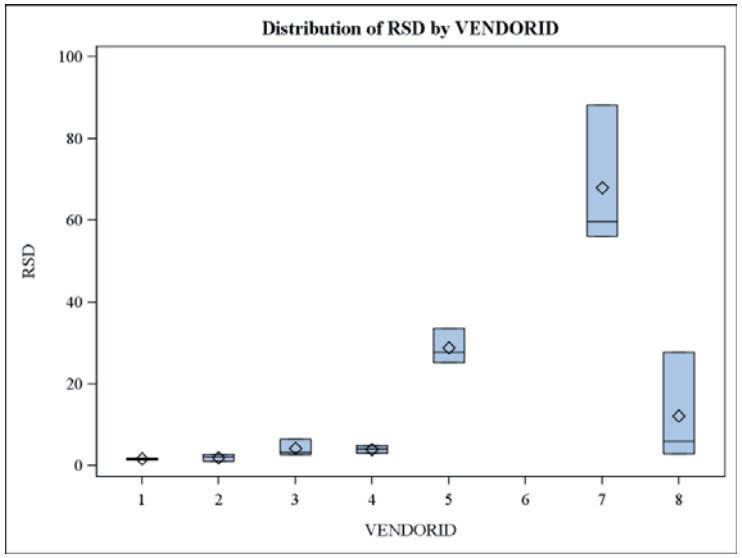


Figure A-41: Distribution of RSD for priority target Propane

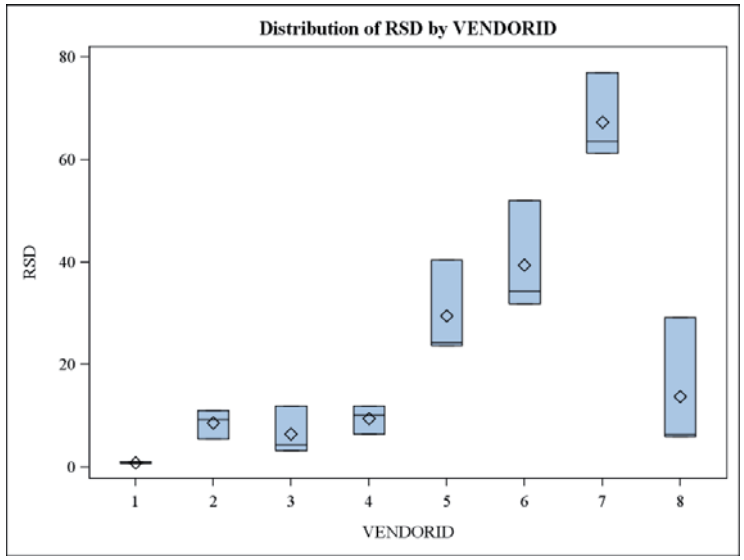


Figure A-42: Distribution of RSD for priority target Propylene

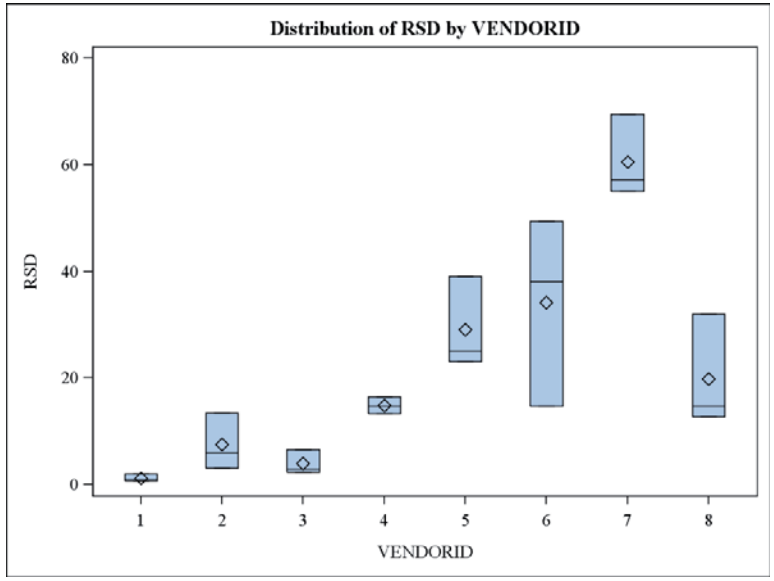


Figure A-43: Distribution of RSD for priority target Styrene

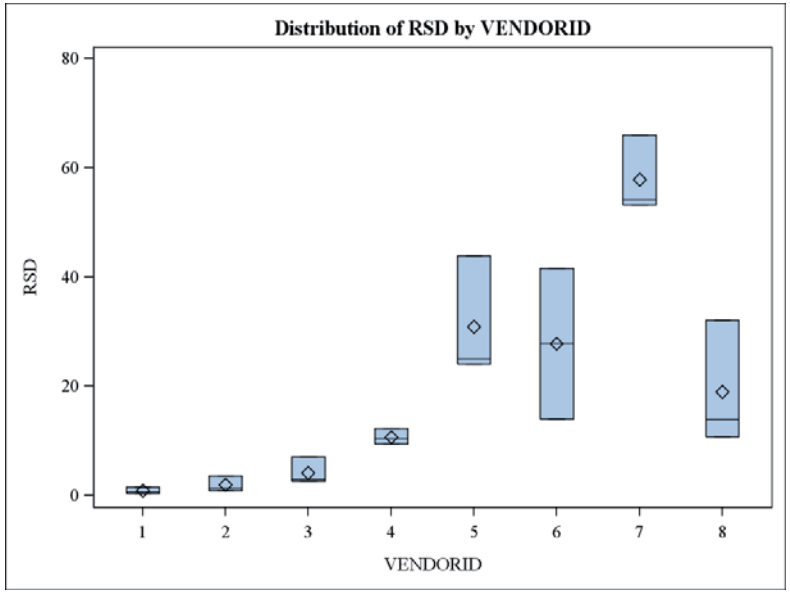


Figure A-44: Distribution of RSD for priority target Toluene

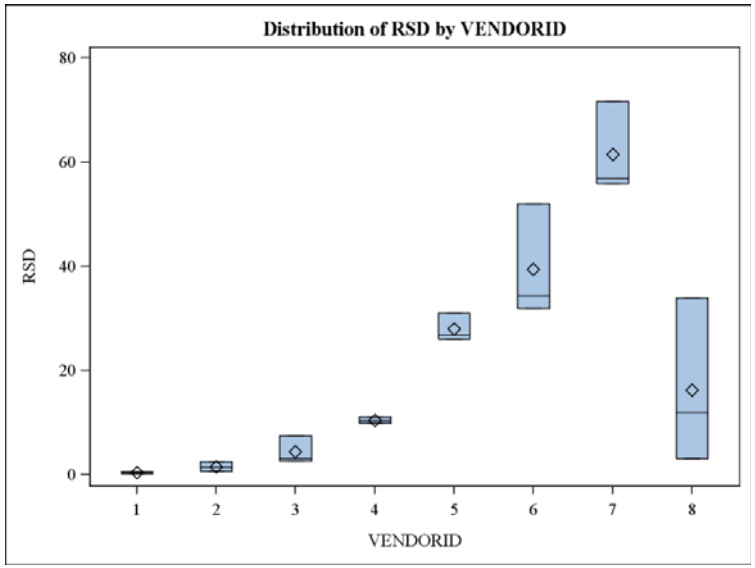


Figure A-45: Distribution of RSD for priority target cis-2-Butene

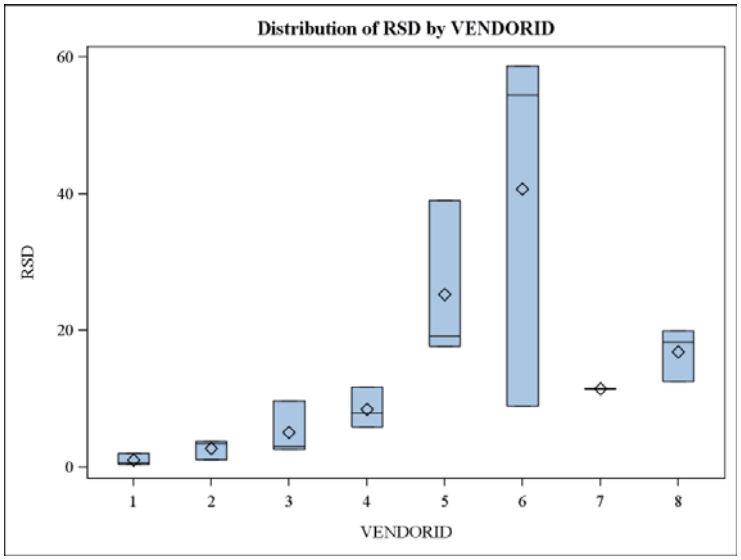


Figure A-46: Distribution of RSD for priority target m,p-Xylene

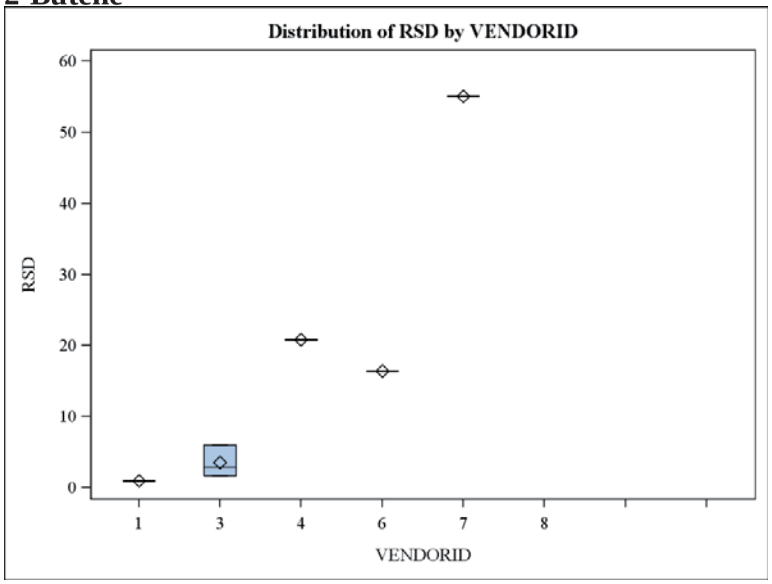


Figure A-47: Distribution of RSD for priority target m-Ethyltoluene

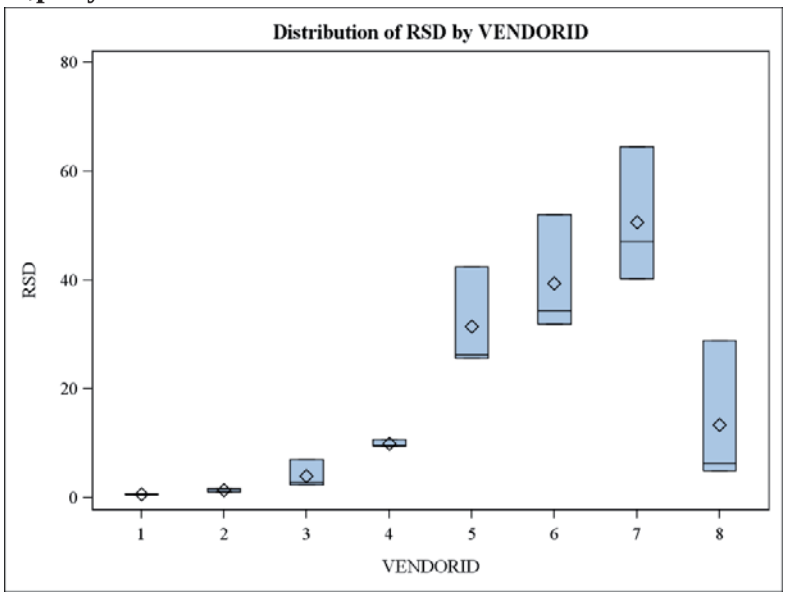


Figure A-48: Distribution of RSD for priority target n-Butane

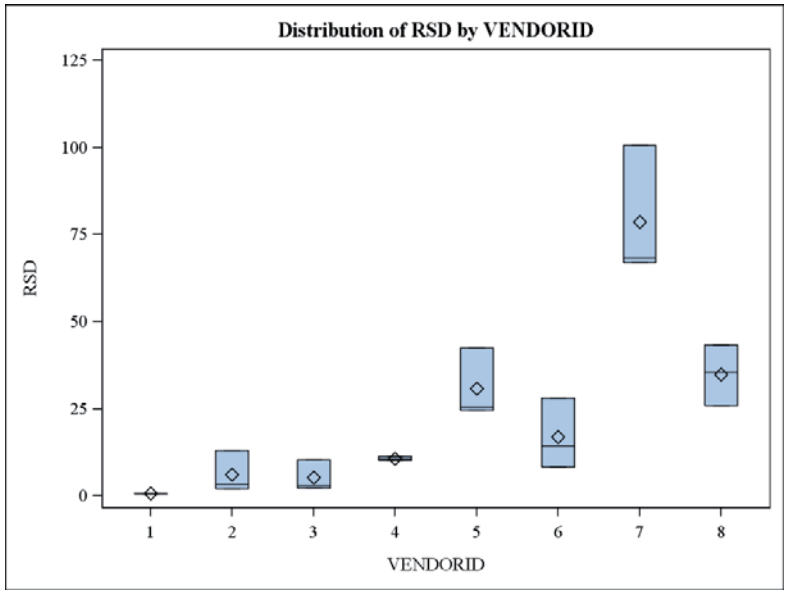


Figure A-49: Distribution of RSD for priority target n-Hexane

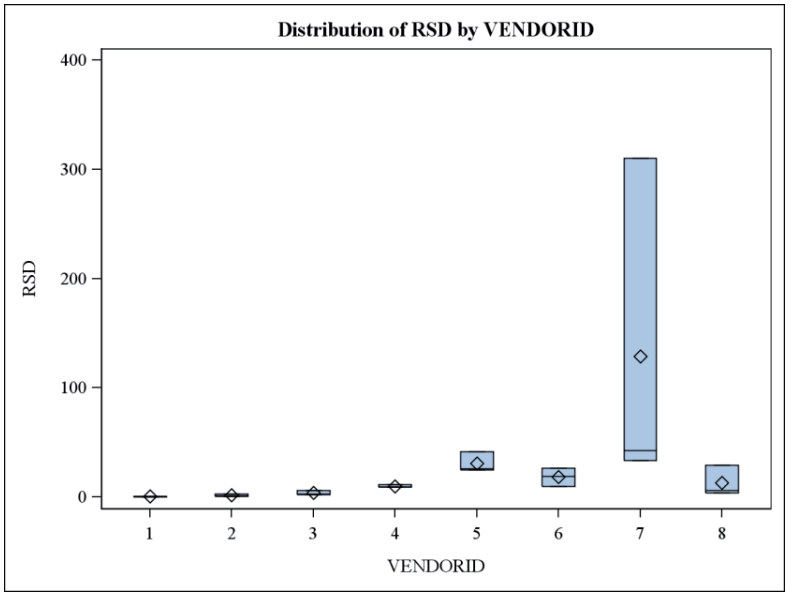


Figure A-50: Distribution of RSD for priority target n-Pentane

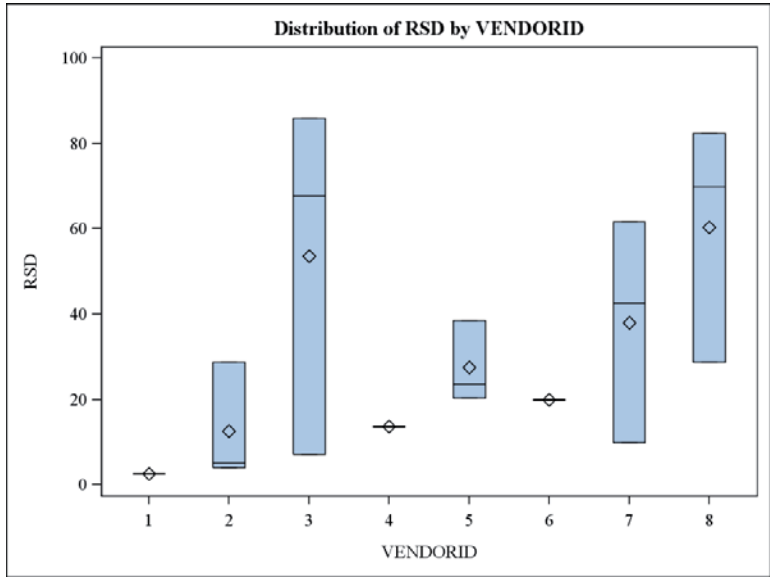


Figure A-51: Distribution of RSD for priority target o-Ethyltoluene

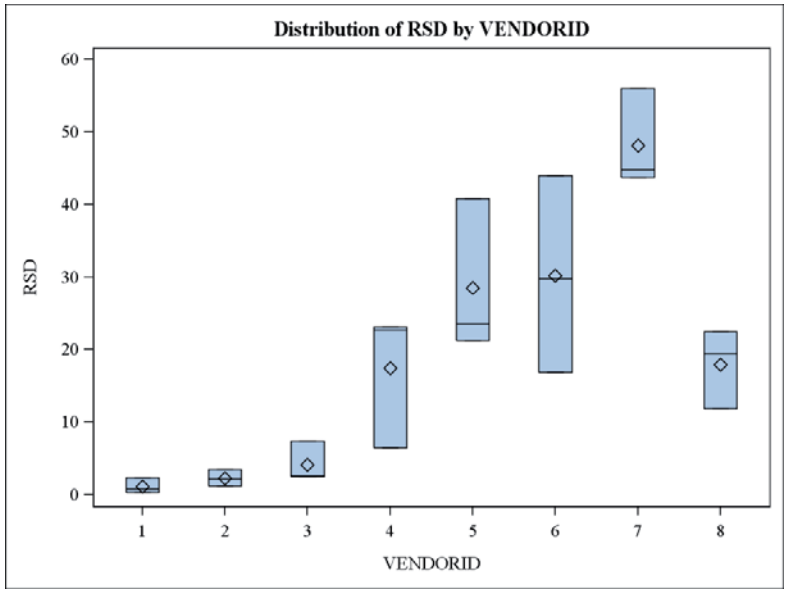


Figure A-52: Distribution of RSD for priority target o-Xylene

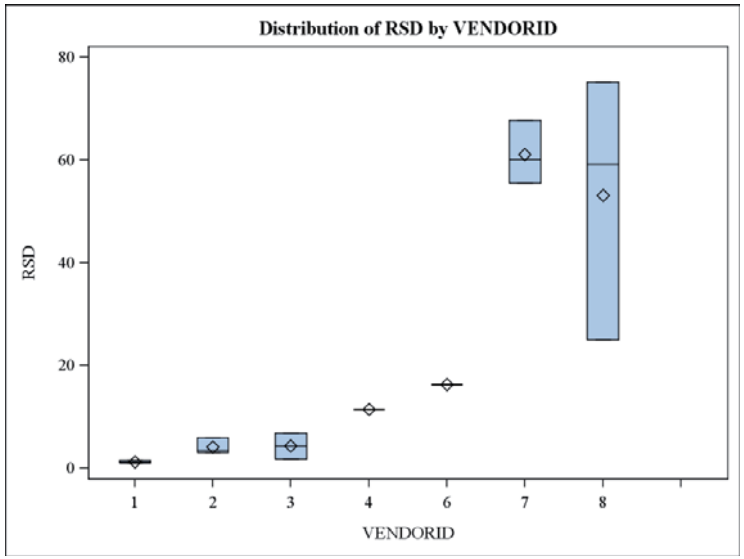


Figure A-53: Distribution of RSD for priority target p-Ethyltoluene

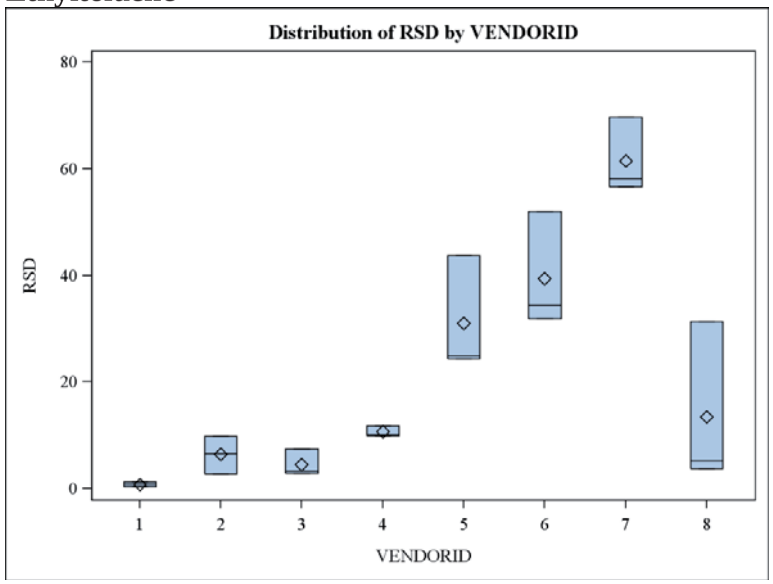


Figure A-54: Distribution of %RSD for priority target 2-butene

Table A1. Descriptive Statistics for Precision – All Vendors

TARGET	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	1,3,5-Trimethylbenzene	1	174	0.6786	31.521	0.2139	0.046
O	1,3,5-Trimethylbenzene	4	175	4.9832	31.265	1.5580	2.427
O	1,3,5-Trimethylbenzene	9	164	10.7734	28.056	3.0226	9.136
O	1-Pentene	1	231	0.9936	44.842	0.4455	0.199
O	1-Pentene	4	234	4.3232	30.424	1.3153	1.730
O	1-Pentene	9	200	9.0494	36.753	3.3259	11.062
O	2,2-Dimethylbutane	1	192	1.4868	47.175	0.7014	0.492
O	2,2-Dimethylbutane	4	40	1.0430	162.523	1.6951	2.873
O	2,2-Dimethylbutane	9	37	0.2422	85.137	0.2062	0.043
O	2,3,4-Trimethylpentane	1	198	0.7689	49.383	0.3797	0.144
O	2,3,4-Trimethylpentane	4	24	1.6566	36.731	0.6085	0.370
O	2,3,4-Trimethylpentane	9	38	5.3706	138.269	7.4258	55.143
O	2,3-Dimethylbutane	1	217	1.6732	68.163	1.1405	1.301
O	2,3-Dimethylbutane	4	39	1.9923	59.495	1.1853	1.405
O	2,3-Dimethylbutane	9	42	1.7151	85.475	1.4660	2.149
O	2,3-Dimethylpentane	1	234	1.3317	61.740	0.8222	0.676
O	2,3-Dimethylpentane	4	55	1.9269	62.617	1.2065	1.456
O	2,3-Dimethylpentane	9	79	5.1446	74.428	3.8290	14.661
O	2,4-Dimethylpentane	1	234	1.2210	32.929	0.4021	0.162
O	2,4-Dimethylpentane	4	73	2.1597	39.871	0.8611	0.741
O	2,4-Dimethylpentane	9	78	3.7577	64.590	2.4271	5.891
O	2-Methylheptane	1	232	0.6994	40.567	0.2837	0.080
O	2-Methylheptane	4	38	0.4157	42.436	0.1764	0.031
O	2-Methylheptane	9	60	0.4367	121.583	0.5310	0.282
O	2-Methylhexane	1	201	0.8955	44.486	0.3984	0.159
O	2-Methylhexane	9	26	0.5464	142.876	0.7807	0.609
O	2-Methylpentane	1	150	0.9784	45.312	0.4433	0.197
O	2-Methylpentane	4	23	2.7896	81.014	2.2599	5.107
O	2-Methylpentane	9	46	4.9515	85.043	4.2109	17.732
O	3-Methylheptane	1	230	0.7464	44.722	0.3338	0.111
O	3-Methylheptane	4	106	1.0365	90.299	0.9359	0.876
O	3-Methylheptane	9	118	2.5656	119.574	3.0678	9.411
O	3-Methylhexane	1	227	0.8541	42.497	0.3630	0.132
O	3-Methylhexane	4	46	5.0292	136.145	6.8470	46.882
O	3-Methylhexane	9	66	16.8132	152.360	25.6165	656.207
O	3-Methylpentane	1	187	1.3711	44.692	0.6128	0.375
O	3-Methylpentane	4	27	0.7648	312.595	2.3908	5.716
O	3-Methylpentane	9	36	0.6742	124.197	0.8373	0.701
O	Acetylene	1	30	0.1802	46.166	0.0832	0.007

TARGET	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	Acetylene	4	167	4.3790	54.334	2.3793	5.661
O	Acetylene	9	159	7.8278	72.969	5.7119	32.625
O	Cyclohexane	1	200	1.3061	24.356	0.3181	0.101
O	Cyclohexane	4	202	3.8393	26.261	1.0082	1.017
O	Cyclohexane	9	174	9.0350	35.448	3.2028	10.258
O	Cyclopentane	1	224	0.8353	39.882	0.3331	0.111
O	Cyclopentane	4	92	0.4329	83.457	0.3613	0.131
O	Cyclopentane	9	76	0.7621	71.675	0.5462	0.298
O	Isopropylbenzene	1	234	0.9178	33.024	0.3031	0.092
O	Isopropylbenzene	4	235	4.3265	32.282	1.3967	1.951
O	Isopropylbenzene	9	213	10.5494	42.768	4.5117	20.356
O	Methylcyclohexane	1	202	0.8310	31.333	0.2604	0.068
O	Methylcyclohexane	4	28	1.1428	21.964	0.2510	0.063
O	Methylcyclohexane	9	41	2.0085	58.749	1.1800	1.392
O	Methylcyclopentane	1	127	0.6386	32.953	0.2104	0.044
O	Methylcyclopentane	4	41	0.2549	315.030	0.8030	0.645
O	Methylcyclopentane	9	37	0.6658	234.126	1.5588	2.430
O	cis-2-Pentene	1	199	1.3639	54.670	0.7457	0.556
O	cis-2-Pentene	4	129	4.5271	31.009	1.4038	1.971
O	cis-2-Pentene	9	105	8.7913	30.625	2.6924	7.249
O	m-Diethylbenzene	1	196	0.7261	25.276	0.1835	0.034
O	m-Diethylbenzene	4	39	0.4352	165.072	0.7184	0.516
O	m-Diethylbenzene	9	43	0.8218	117.705	0.9673	0.936
O	n-Decane	1	232	0.6407	40.050	0.2566	0.066
O	n-Decane	4	235	7.7686	63.300	4.9175	24.182
O	n-Decane	9	206	17.2845	57.660	9.9662	99.325
O	n-Heptane	1	228	0.7417	38.335	0.2843	0.081
O	n-Heptane	4	183	4.1240	35.837	1.4779	2.184
O	n-Heptane	9	193	8.6174	43.903	3.7833	14.313
O	n-Nonane	1	230	0.6957	44.450	0.3093	0.096
O	n-Nonane	4	235	4.4125	37.239	1.6432	2.700
O	n-Nonane	9	213	10.1870	42.349	4.3140	18.611
O	n-Octane	1	227	0.7872	30.901	0.2432	0.059
O	n-Octane	4	235	3.8589	36.661	1.4147	2.001
O	n-Octane	9	210	8.3719	39.817	3.3334	11.112
O	n-Propylbenzene	1	234	0.6693	29.906	0.2002	0.040
O	n-Propylbenzene	4	235	5.0327	58.663	2.9524	8.716
O	n-Propylbenzene	9	213	11.2024	61.130	6.8480	46.895
O	n-Undecane	1	225	0.6966	41.068	0.2861	0.082
O	n-Undecane	4	225	5.2376	54.257	2.8418	8.076

TARGET	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	n-Undecane	9	208	12.5983	64.074	8.0722	65.160
O	p-Diethylbenzene	1	164	0.5446	31.390	0.1709	0.029
O	p-Diethylbenzene	4	60	2.3776	99.443	2.3644	5.590
O	p-Diethylbenzene	9	45	6.9366	111.604	7.7414	59.930
O	trans-2-Pentene	1	234	0.9760	41.224	0.4023	0.162
O	trans-2-Pentene	4	234	4.1554	33.238	1.3812	1.908
O	trans-2-Pentene	9	201	9.4490	34.851	3.2931	10.844
P	1,2,3-Trimethylbenzene	1	231	0.5402	35.526	0.1919	0.037
P	1,2,3-Trimethylbenzene	4	101	4.4658	69.605	3.1084	9.662
P	1,2,3-Trimethylbenzene	9	120	15.0117	116.302	17.4589	304.812
P	1,2,4-Trimethylbenzene	1	224	0.8187	26.887	0.2201	0.048
P	1,2,4-Trimethylbenzene	4	205	8.1518	54.082	4.4087	19.436
P	1,2,4-Trimethylbenzene	9	188	17.7257	56.990	10.1019	102.048
P	1-Butene	1	234	1.2819	36.918	0.4732	0.224
P	1-Butene	4	235	4.3333	30.607	1.3263	1.759
P	1-Butene	9	213	9.4043	36.776	3.4586	11.962
P	2,2,4-Trimethylpentane	1	229	0.7813	30.244	0.2363	0.056
P	2,2,4-Trimethylpentane	4	213	4.1014	38.522	1.5799	2.496
P	2,2,4-Trimethylpentane	9	206	9.4056	42.396	3.9876	15.901
P	Benzene	1	234	1.1153	52.892	0.5899	0.348
P	Benzene	4	235	3.8487	29.862	1.1493	1.321
P	Benzene	9	213	8.9683	36.930	3.3120	10.969
P	Ethane	1	205	2.1714	59.916	1.3010	1.693
P	Ethane	4	205	3.6656	58.707	2.1520	4.631
P	Ethane	9	188	7.6516	67.350	5.1534	26.557
P	Ethylbenzene	1	234	0.7017	39.381	0.2763	0.076
P	Ethylbenzene	4	233	4.0099	33.446	1.3411	1.799
P	Ethylbenzene	9	213	9.2025	37.321	3.4345	11.796
P	Ethylene	1	234	1.7821	72.195	1.2866	1.655
P	Ethylene	4	235	3.7525	53.180	1.9956	3.982
P	Ethylene	9	213	7.8207	63.879	4.9958	24.958
P	Isobutane	1	231	1.0637	30.732	0.3269	0.107
P	Isobutane	4	175	3.5692	26.216	0.9357	0.876
P	Isobutane	9	163	7.7799	32.501	2.5285	6.393
P	Isopentane	1	233	1.4005	34.890	0.4886	0.239
P	Isopentane	4	235	3.8147	30.802	1.1750	1.381
P	Isopentane	9	212	8.5576	35.793	3.0630	9.382
P	Isoprene	1	233	1.4942	61.776	0.9230	0.852
P	Isoprene	4	234	3.9510	45.195	1.7857	3.189
P	Isoprene	9	200	8.0631	42.775	3.4490	11.895

TARGET	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	Propane	1	204	2.4082	46.894	1.1293	1.275
P	Propane	4	205	3.9884	49.283	1.9656	3.863
P	Propane	9	188	8.5970	56.486	4.8562	23.582
P	Propylene	1	234	1.4469	50.430	0.7297	0.532
P	Propylene	4	235	4.3053	47.404	2.0409	4.165
P	Propylene	9	212	9.3187	53.498	4.9853	24.853
P	Styrene	1	232	0.8055	31.617	0.2547	0.065
P	Styrene	4	235	4.0265	36.166	1.4562	2.121
P	Styrene	9	213	10.8620	53.134	5.7714	33.309
P	Toluene	1	234	1.1676	40.355	0.4712	0.222
P	Toluene	4	205	3.9477	37.457	1.4787	2.186
P	Toluene	9	186	9.6508	42.967	4.1467	17.195
P	cis-2-Butene	1	234	1.3661	37.293	0.5095	0.260
P	cis-2-Butene	4	235	3.8405	29.050	1.1156	1.245
P	cis-2-Butene	9	202	8.4721	31.987	2.7100	7.344
P	m,p-Xylene	1	223	1.2021	42.531	0.5113	0.261
P	m,p-Xylene	4	205	9.1478	28.873	2.6413	6.976
P	m,p-Xylene	9	188	21.3568	32.501	6.9412	48.181
P	m-Ethyltoluene	1	147	0.4897	31.475	0.1541	0.024
P	m-Ethyltoluene	4	10	0.2056	2.946	0.0061	0.000
P	m-Ethyltoluene	9	7	2.1086	205.602	4.3353	18.794
P	n-Butane	1	234	1.5732	37.144	0.5843	0.341
P	n-Butane	4	233	3.7485	29.586	1.1090	1.230
P	n-Butane	9	211	8.3577	31.879	2.6644	7.099
P	n-Hexane	1	218	1.4946	156.058	2.3324	5.440
P	n-Hexane	4	231	4.0644	65.128	2.6470	7.007
P	n-Hexane	9	191	8.3588	30.476	2.5474	6.489
P	n-Pentane	1	234	1.1785	40.598	0.4784	0.229
P	n-Pentane	4	235	4.6127	35.982	1.6597	2.755
P	n-Pentane	9	212	10.9889	153.279	16.8436	283.707
P	o-Ethyltoluene	1	234	0.7016	23.359	0.1639	0.027
P	o-Ethyltoluene	4	140	0.2716	88.557	0.2406	0.058
P	o-Ethyltoluene	9	112	0.5640	73.276	0.4133	0.171
P	o-Xylene	1	234	0.6988	32.226	0.2252	0.051
P	o-Xylene	4	235	4.4993	43.436	1.9543	3.819
P	o-Xylene	9	213	10.5447	46.974	4.9533	24.535
P	p-Ethyltoluene	1	197	0.8918	44.669	0.3984	0.159
P	p-Ethyltoluene	4	111	3.7216	59.651	2.2199	4.928
P	p-Ethyltoluene	9	95	7.5586	38.573	2.9155	8.500
P	trans-2-Butene	1	233	1.0787	30.828	0.3325	0.111

TARGET	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	trans-2-Butene	4	235	3.9647	27.909	1.1065	1.224
P	trans-2-Butene	9	208	8.4933	34.649	2.9428	8.660

Table A2. Descriptive Statistics for Precision – By Vendor

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	1	1,3,5-Trimethylbenzene	1	30	0.4597	2.019	0.0093	0.00
O	1	1,3,5-Trimethylbenzene	4	30	3.4413	1.373	0.0473	0.00
O	1	1,3,5-Trimethylbenzene	9	26	7.6342	0.493	0.0376	0.00
O	2	1,3,5-Trimethylbenzene	1	30	0.6842	6.237	0.0427	0.00
O	2	1,3,5-Trimethylbenzene	4	30	4.8805	2.785	0.1359	0.02
O	2	1,3,5-Trimethylbenzene	9	25	12.1298	4.251	0.5157	0.27
O	3	1,3,5-Trimethylbenzene	1	30	0.8532	7.196	0.0614	0.00
O	3	1,3,5-Trimethylbenzene	4	30	3.7360	2.793	0.1043	0.01
O	3	1,3,5-Trimethylbenzene	9	25	8.8724	2.786	0.2472	0.06
O	4	1,3,5-Trimethylbenzene	1	29	0.6007	19.085	0.1146	0.01
O	4	1,3,5-Trimethylbenzene	4	30	5.1650	5.421	0.2800	0.08
O	4	1,3,5-Trimethylbenzene	9	26	11.8762	4.697	0.5578	0.31
O	5	1,3,5-Trimethylbenzene	1	33	0.9208	23.985	0.2209	0.05
O	5	1,3,5-Trimethylbenzene	4	33	6.6240	20.600	1.3645	1.86
O	5	1,3,5-Trimethylbenzene	9	33	12.6078	39.922	5.0333	25.33
O	6	1,3,5-Trimethylbenzene	9	1	9.5000	.	.	.
O	8	1,3,5-Trimethylbenzene	1	22	0.4709	29.562	0.1392	0.02
O	8	1,3,5-Trimethylbenzene	4	22	6.2173	38.116	2.3698	5.62
O	8	1,3,5-Trimethylbenzene	9	28	11.0339	19.429	2.1437	4.60
O	1	1-Pentene	1	30	1.0103	0.609	0.0061	0.00
O	1	1-Pentene	4	30	4.4567	2.401	0.1070	0.01
O	1	1-Pentene	9	26	9.9258	1.864	0.1851	0.03
O	2	1-Pentene	1	30	0.9613	2.537	0.0244	0.00
O	2	1-Pentene	4	30	4.2822	6.374	0.2730	0.07
O	2	1-Pentene	9	25	9.5542	4.844	0.4628	0.21
O	3	1-Pentene	1	30	0.8217	6.688	0.0550	0.00
O	3	1-Pentene	4	30	3.8444	2.482	0.0954	0.01
O	3	1-Pentene	9	25	9.1698	2.444	0.2241	0.05
O	4	1-Pentene	1	29	1.3131	11.735	0.1541	0.02
O	4	1-Pentene	4	30	6.5050	7.178	0.4669	0.22
O	4	1-Pentene	9	26	14.7135	7.547	1.1104	1.23
O	5	1-Pentene	1	33	0.9703	26.243	0.2546	0.06
O	5	1-Pentene	4	33	4.2518	25.619	1.0893	1.19

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	5	1-Pentene	9	33	8.1534	43.729	3.5654	12.71
O	6	1-Pentene	1	30	0.6243	11.174	0.0698	0.00
O	6	1-Pentene	4	30	3.0373	16.919	0.5139	0.26
O	6	1-Pentene	9	25	7.7816	24.180	1.8816	3.54
O	7	1-Pentene	1	30	1.5077	59.314	0.8943	0.80
O	7	1-Pentene	4	29	3.6166	56.254	2.0344	4.14
O	7	1-Pentene	9	15	3.7247	96.147	3.5811	12.82
O	8	1-Pentene	1	19	0.6132	34.477	0.2114	0.04
O	8	1-Pentene	4	22	4.6668	18.329	0.8554	0.73
O	8	1-Pentene	9	25	7.2676	21.721	1.5786	2.49
O	1	2,2-Dimethylbutane	1	30	1.3537	0.494	0.0067	0.00
O	2	2,2-Dimethylbutane	1	30	2.0958	1.289	0.0270	0.00
O	2	2,2-Dimethylbutane	4	22	0.0436	112.167	0.0489	0.00
O	2	2,2-Dimethylbutane	9	15	0.0607	58.184	0.0353	0.00
O	3	2,2-Dimethylbutane	1	30	1.0720	9.851	0.1056	0.01
O	3	2,2-Dimethylbutane	9	7	0.2604	44.653	0.1163	0.01
O	4	2,2-Dimethylbutane	1	29	2.3655	11.094	0.2624	0.07
O	6	2,2-Dimethylbutane	1	30	0.5267	9.609	0.0506	0.00
O	7	2,2-Dimethylbutane	1	30	1.4233	63.531	0.9043	0.82
O	7	2,2-Dimethylbutane	4	9	0.4011	72.433	0.2905	0.08
O	7	2,2-Dimethylbutane	9	7	0.4600	54.996	0.2530	0.06
O	8	2,2-Dimethylbutane	1	13	1.7485	2.661	0.0465	0.00
O	8	2,2-Dimethylbutane	4	9	4.1278	1.026	0.0424	0.00
O	8	2,2-Dimethylbutane	9	8	0.3763	27.728	0.1043	0.01
O	1	2,3,4-Trimethylpentane	1	30	0.6283	0.603	0.0038	0.00
O	2	2,3,4-Trimethylpentane	1	30	0.5715	1.262	0.0072	0.00
O	3	2,3,4-Trimethylpentane	1	30	0.6111	5.710	0.0349	0.00
O	3	2,3,4-Trimethylpentane	4	2	0.0360	3.928	0.0014	0.00
O	3	2,3,4-Trimethylpentane	9	1	0.0510	.	.	.
O	4	2,3,4-Trimethylpentane	1	29	0.6583	16.457	0.1083	0.01
O	5	2,3,4-Trimethylpentane	1	33	0.9228	29.685	0.2739	0.08
O	5	2,3,4-Trimethylpentane	4	22	1.8039	20.190	0.3642	0.13
O	5	2,3,4-Trimethylpentane	9	27	3.3541	33.212	1.1139	1.24
O	6	2,3,4-Trimethylpentane	1	30	1.3750	41.102	0.5652	0.32
O	8	2,3,4-Trimethylpentane	1	16	0.4450	9.812	0.0437	0.00
O	8	2,3,4-Trimethylpentane	9	10	11.3470	114.257	12.9647	168.08
O	1	2,3-Dimethylbutane	1	30	0.7130	39.740	0.2833	0.08
O	2	2,3-Dimethylbutane	1	30	2.3238	1.529	0.0355	0.00
O	2	2,3-Dimethylbutane	4	30	1.3517	1.965	0.0266	0.00
O	2	2,3-Dimethylbutane	9	22	3.0395	18.256	0.5549	0.31
O	3	2,3-Dimethylbutane	1	30	1.6454	7.251	0.1193	0.01

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	4	2,3-Dimethylbutane	1	29	3.0483	11.370	0.3466	0.12
O	5	2,3-Dimethylbutane	1	32	0.9151	26.943	0.2466	0.06
O	5	2,3-Dimethylbutane	9	7	0.0690	88.943	0.0614	0.00
O	6	2,3-Dimethylbutane	1	30	0.5267	9.609	0.0506	0.00
O	7	2,3-Dimethylbutane	1	23	2.8870	68.417	1.9752	3.90
O	7	2,3-Dimethylbutane	9	5	0.3340	49.542	0.1655	0.03
O	8	2,3-Dimethylbutane	1	13	1.7485	2.661	0.0465	0.00
O	8	2,3-Dimethylbutane	4	9	4.1278	1.026	0.0424	0.00
O	8	2,3-Dimethylbutane	9	8	0.3763	27.728	0.1043	0.01
O	1	2,3-Dimethylpentane	1	30	1.4457	0.647	0.0094	0.00
O	2	2,3-Dimethylpentane	1	30	0.7307	3.940	0.0288	0.00
O	2	2,3-Dimethylpentane	4	30	2.8692	13.117	0.3764	0.14
O	2	2,3-Dimethylpentane	9	25	7.3568	12.928	0.9511	0.90
O	3	2,3-Dimethylpentane	1	30	1.1069	18.397	0.2036	0.04
O	3	2,3-Dimethylpentane	4	2	1.0695	0.727	0.0078	0.00
O	4	2,3-Dimethylpentane	1	29	1.5631	9.540	0.1491	0.02
O	5	2,3-Dimethylpentane	1	33	1.0085	26.518	0.2674	0.07
O	5	2,3-Dimethylpentane	4	13	0.0541	4.165	0.0023	0.00
O	5	2,3-Dimethylpentane	9	26	0.0932	28.074	0.0262	0.00
O	6	2,3-Dimethylpentane	1	30	2.5723	60.562	1.5579	2.43
O	7	2,3-Dimethylpentane	1	30	1.2737	54.924	0.6996	0.49
O	8	2,3-Dimethylpentane	1	22	0.8695	6.905	0.0600	0.00
O	8	2,3-Dimethylpentane	4	10	1.7060	10.918	0.1863	0.03
O	8	2,3-Dimethylpentane	9	28	7.8600	27.875	2.1910	4.80
O	1	2,4-Dimethylpentane	1	30	1.1433	0.773	0.0088	0.00
O	2	2,4-Dimethylpentane	1	30	0.9475	3.249	0.0308	0.00
O	2	2,4-Dimethylpentane	4	30	1.4648	38.766	0.5679	0.32
O	2	2,4-Dimethylpentane	9	25	3.1896	31.518	1.0053	1.01
O	3	2,4-Dimethylpentane	1	30	0.8634	9.522	0.0822	0.01
O	4	2,4-Dimethylpentane	1	29	1.1803	12.008	0.1417	0.02
O	5	2,4-Dimethylpentane	1	33	1.0159	25.881	0.2629	0.07
O	5	2,4-Dimethylpentane	4	33	2.8004	25.198	0.7056	0.50
O	5	2,4-Dimethylpentane	9	33	5.5851	43.901	2.4519	6.01
O	6	2,4-Dimethylpentane	1	30	1.4023	32.948	0.4620	0.21
O	7	2,4-Dimethylpentane	1	30	1.7020	31.642	0.5386	0.29
O	7	2,4-Dimethylpentane	4	10	2.1300	3.915	0.0834	0.01
O	7	2,4-Dimethylpentane	9	10	2.1650	3.927	0.0850	0.01
O	8	2,4-Dimethylpentane	1	22	1.6455	9.136	0.1503	0.02
O	8	2,4-Dimethylpentane	9	10	0.7400	66.569	0.4926	0.24
O	1	2-Methylheptane	1	30	1.0030	13.199	0.1324	0.02
O	2	2-Methylheptane	1	30	0.6053	1.470	0.0089	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	2	2-Methylheptane	9	6	0.0175	23.905	0.0042	0.00
O	3	2-Methylheptane	1	30	0.5964	5.649	0.0337	0.00
O	3	2-Methylheptane	4	5	0.0740	4.428	0.0033	0.00
O	3	2-Methylheptane	9	6	0.1500	2.921	0.0044	0.00
O	4	2-Methylheptane	1	29	0.6166	21.339	0.1316	0.02
O	5	2-Methylheptane	1	33	1.0336	25.626	0.2649	0.07
O	5	2-Methylheptane	4	33	0.4674	26.180	0.1224	0.01
O	5	2-Methylheptane	9	29	0.3186	59.689	0.1902	0.04
O	6	2-Methylheptane	1	30	0.3153	11.711	0.0369	0.00
O	7	2-Methylheptane	1	28	0.5589	50.610	0.2829	0.08
O	7	2-Methylheptane	9	9	0.1167	64.571	0.0753	0.01
O	8	2-Methylheptane	1	22	0.8645	14.057	0.1215	0.01
O	8	2-Methylheptane	9	10	1.4910	28.175	0.4201	0.18
O	1	2-Methylhexane	1	30	0.7207	0.624	0.0045	0.00
O	3	2-Methylhexane	1	30	0.5886	9.988	0.0588	0.00
O	3	2-Methylhexane	9	15	0.0155	95.207	0.0147	0.00
O	4	2-Methylhexane	1	29	0.5890	19.424	0.1144	0.01
O	5	2-Methylhexane	1	33	1.2707	26.525	0.3370	0.11
O	5	2-Methylhexane	9	1	0.1247	.	.	.
O	6	2-Methylhexane	1	30	1.1067	33.139	0.3667	0.13
O	7	2-Methylhexane	1	27	0.6167	47.284	0.2916	0.09
O	8	2-Methylhexane	1	22	1.4482	7.685	0.1113	0.01
O	8	2-Methylhexane	9	10	1.3850	46.887	0.6494	0.42
O	1	2-Methylpentane	1	30	1.5940	0.748	0.0119	0.00
O	2	2-Methylpentane	9	5	2.3910	34.307	0.8203	0.67
O	3	2-Methylpentane	1	30	0.6210	5.860	0.0364	0.00
O	3	2-Methylpentane	4	6	0.0100	39.194	0.0039	0.00
O	3	2-Methylpentane	9	8	0.0131	68.443	0.0090	0.00
O	4	2-Methylpentane	1	29	1.2159	12.389	0.1506	0.02
O	6	2-Methylpentane	1	30	0.5267	9.609	0.0506	0.00
O	7	2-Methylpentane	1	9	0.3356	90.565	0.3039	0.09
O	7	2-Methylpentane	9	6	0.1900	68.462	0.1301	0.02
O	8	2-Methylpentane	1	22	1.1923	6.130	0.0731	0.01
O	8	2-Methylpentane	4	17	3.7706	46.716	1.7615	3.10
O	8	2-Methylpentane	9	27	7.9470	33.923	2.6959	7.27
O	1	3-Methylheptane	1	30	0.6370	1.022	0.0065	0.00
O	2	3-Methylheptane	1	30	0.6315	3.341	0.0211	0.00
O	2	3-Methylheptane	4	30	1.9202	58.375	1.1209	1.26
O	2	3-Methylheptane	9	25	4.4510	66.551	2.9622	8.77
O	3	3-Methylheptane	1	30	0.9906	5.311	0.0526	0.00
O	3	3-Methylheptane	4	30	0.0504	17.815	0.0090	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	3	3-Methylheptane	9	25	0.0896	13.951	0.0125	0.00
O	4	3-Methylheptane	1	29	0.6738	16.245	0.1095	0.01
O	5	3-Methylheptane	1	33	1.2526	29.367	0.3678	0.14
O	5	3-Methylheptane	4	32	1.1413	19.738	0.2253	0.05
O	5	3-Methylheptane	9	30	2.0766	23.109	0.4799	0.23
O	6	3-Methylheptane	1	30	0.3157	8.471	0.0267	0.00
O	7	3-Methylheptane	1	28	0.5371	50.172	0.2695	0.07
O	7	3-Methylheptane	9	10	0.0740	6.978	0.0052	0.00
O	8	3-Methylheptane	1	20	0.9255	10.734	0.0993	0.01
O	8	3-Methylheptane	4	14	1.0164	27.438	0.2789	0.08
O	8	3-Methylheptane	9	28	4.5068	92.277	4.1587	17.29
O	1	3-Methylhexane	1	30	0.7213	1.012	0.0073	0.00
O	1	3-Methylhexane	4	30	0.5417	1.290	0.0070	0.00
O	1	3-Methylhexane	9	26	1.2438	2.739	0.0341	0.00
O	2	3-Methylhexane	1	30	0.6563	1.057	0.0069	0.00
O	2	3-Methylhexane	9	3	0.0267	21.651	0.0058	0.00
O	3	3-Methylhexane	1	30	0.6179	8.470	0.0523	0.00
O	3	3-Methylhexane	4	5	6.2869	2.154	0.1354	0.02
O	3	3-Methylhexane	9	6	15.1835	0.759	0.1153	0.01
O	4	3-Methylhexane	1	29	0.6962	18.178	0.1266	0.02
O	5	3-Methylhexane	1	33	1.1902	26.068	0.3103	0.10
O	5	3-Methylhexane	9	9	0.1511	10.662	0.0161	0.00
O	6	3-Methylhexane	1	30	1.1840	41.302	0.4890	0.24
O	7	3-Methylhexane	1	27	0.5819	48.186	0.2804	0.08
O	7	3-Methylhexane	9	5	0.6840	7.207	0.0493	0.00
O	8	3-Methylhexane	1	18	1.2956	14.317	0.1855	0.03
O	8	3-Methylhexane	4	11	16.6964	0.856	0.1428	0.02
O	8	3-Methylhexane	9	17	57.7276	24.621	14.2133	202.02
O	1	3-Methylpentane	1	30	1.3713	0.952	0.0131	0.00
O	2	3-Methylpentane	1	30	1.4158	1.574	0.0223	0.00
O	2	3-Methylpentane	4	19	0.0184	55.074	0.0101	0.00
O	2	3-Methylpentane	9	21	0.0438	38.008	0.0167	0.00
O	3	3-Methylpentane	1	30	1.2182	7.455	0.0908	0.01
O	4	3-Methylpentane	1	29	2.4386	10.775	0.2628	0.07
O	6	3-Methylpentane	1	30	0.5267	9.609	0.0506	0.00
O	7	3-Methylpentane	1	16	1.0525	78.324	0.8244	0.68
O	7	3-Methylpentane	4	3	5.4500	110.189	6.0053	36.06
O	8	3-Methylpentane	1	22	1.4941	6.828	0.1020	0.01
O	8	3-Methylpentane	4	5	0.7900	12.627	0.0997	0.01
O	8	3-Methylpentane	9	15	1.5567	36.441	0.5673	0.32
O	1	Acetylene	4	30	4.3893	0.846	0.0371	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	1	Acetylene	9	26	9.5692	2.433	0.2328	0.05
O	2	Acetylene	1	28	0.1713	14.207	0.0243	0.00
O	2	Acetylene	4	30	4.3268	1.454	0.0629	0.00
O	2	Acetylene	9	25	9.4916	0.995	0.0944	0.01
O	3	Acetylene	4	30	7.3176	4.420	0.3234	0.10
O	3	Acetylene	9	25	18.2882	2.623	0.4797	0.23
O	4	Acetylene	9	1	2.5500	.	.	.
O	5	Acetylene	4	33	3.2144	25.287	0.8128	0.66
O	5	Acetylene	9	33	6.8457	34.690	2.3748	5.64
O	6	Acetylene	1	1	0.5800	.	.	.
O	7	Acetylene	1	1	0.0300	.	.	.
O	7	Acetylene	4	22	1.4300	52.955	0.7573	0.57
O	7	Acetylene	9	21	1.9529	74.488	1.4547	2.12
O	8	Acetylene	4	22	5.1250	84.720	4.3419	18.85
O	8	Acetylene	9	28	1.1375	32.142	0.3656	0.13
O	1	Cyclohexane	1	30	1.3733	0.481	0.0066	0.00
O	1	Cyclohexane	4	30	4.3590	0.547	0.0238	0.00
O	1	Cyclohexane	9	26	9.6938	0.444	0.0430	0.00
O	2	Cyclohexane	1	30	1.1623	2.325	0.0270	0.00
O	2	Cyclohexane	4	30	4.5698	7.419	0.3390	0.11
O	2	Cyclohexane	9	25	10.9116	11.040	1.2046	1.45
O	3	Cyclohexane	1	30	1.1887	6.950	0.0826	0.01
O	3	Cyclohexane	4	30	3.6979	2.743	0.1014	0.01
O	3	Cyclohexane	9	25	8.8519	2.765	0.2448	0.06
O	4	Cyclohexane	1	29	1.0576	14.263	0.1508	0.02
O	4	Cyclohexane	4	30	3.5853	9.322	0.3342	0.11
O	4	Cyclohexane	9	26	8.1519	8.126	0.6624	0.44
O	6	Cyclohexane	1	30	1.1420	30.981	0.3538	0.13
O	6	Cyclohexane	4	30	3.4603	35.620	1.2326	1.52
O	6	Cyclohexane	9	25	8.4192	52.100	4.3864	19.24
O	7	Cyclohexane	1	29	1.4472	18.815	0.2723	0.07
O	7	Cyclohexane	4	30	2.4703	30.862	0.7624	0.58
O	7	Cyclohexane	9	19	3.1963	69.018	2.2060	4.87
O	8	Cyclohexane	1	22	1.9355	8.075	0.1563	0.02
O	8	Cyclohexane	4	22	5.0573	17.639	0.8921	0.80
O	8	Cyclohexane	9	28	12.2429	16.647	2.0381	4.15
O	1	Cyclopentane	1	30	0.8140	0.692	0.0056	0.00
O	2	Cyclopentane	1	30	0.8377	4.542	0.0381	0.00
O	2	Cyclopentane	4	19	0.3347	17.838	0.0597	0.00
O	2	Cyclopentane	9	17	0.8635	7.055	0.0609	0.00
O	3	Cyclopentane	1	30	0.7896	6.732	0.0532	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	4	Cyclopentane	1	29	1.0200	11.529	0.1176	0.01
O	4	Cyclopentane	4	10	0.2580	20.897	0.0539	0.00
O	5	Cyclopentane	1	33	1.4113	19.193	0.2709	0.07
O	5	Cyclopentane	4	33	0.8672	20.551	0.1782	0.03
O	5	Cyclopentane	9	33	1.2172	26.664	0.3246	0.11
O	6	Cyclopentane	1	30	0.5267	9.609	0.0506	0.00
O	7	Cyclopentane	1	27	0.4600	67.283	0.3095	0.10
O	7	Cyclopentane	4	30	0.0757	117.731	0.0891	0.01
O	7	Cyclopentane	9	22	0.1241	188.264	0.2336	0.05
O	8	Cyclopentane	1	15	0.6327	7.230	0.0457	0.00
O	8	Cyclopentane	9	4	0.0850	24.490	0.0208	0.00
O	1	Isopropylbenzene	1	30	0.8937	0.905	0.0081	0.00
O	1	Isopropylbenzene	4	30	4.3737	0.634	0.0277	0.00
O	1	Isopropylbenzene	9	26	9.7573	0.375	0.0366	0.00
O	2	Isopropylbenzene	1	30	0.9197	3.243	0.0298	0.00
O	2	Isopropylbenzene	4	30	4.6175	1.923	0.0888	0.01
O	2	Isopropylbenzene	9	25	10.4536	1.438	0.1503	0.02
O	3	Isopropylbenzene	1	30	0.7920	5.647	0.0447	0.00
O	3	Isopropylbenzene	4	30	3.6743	2.474	0.0909	0.01
O	3	Isopropylbenzene	9	25	8.7666	2.735	0.2398	0.06
O	4	Isopropylbenzene	1	29	0.9917	12.566	0.1246	0.02
O	4	Isopropylbenzene	4	30	5.3587	9.214	0.4937	0.24
O	4	Isopropylbenzene	9	26	12.2631	7.795	0.9559	0.91
O	5	Isopropylbenzene	1	33	0.9687	23.044	0.2232	0.05
O	5	Isopropylbenzene	4	33	5.0134	23.212	1.1637	1.35
O	5	Isopropylbenzene	9	33	12.5115	43.439	5.4349	29.54
O	6	Isopropylbenzene	1	30	0.6573	12.621	0.0830	0.01
O	6	Isopropylbenzene	4	30	3.4540	28.115	0.9711	0.94
O	6	Isopropylbenzene	9	25	8.5156	42.175	3.5915	12.90
O	7	Isopropylbenzene	1	30	0.7443	57.737	0.4298	0.18
O	7	Isopropylbenzene	4	30	2.1750	53.415	1.1618	1.35
O	7	Isopropylbenzene	9	25	3.9028	66.467	2.5941	6.73
O	8	Isopropylbenzene	1	22	1.5377	17.986	0.2766	0.08
O	8	Isopropylbenzene	4	22	6.4409	13.611	0.8767	0.77
O	8	Isopropylbenzene	9	28	16.8086	18.817	3.1629	10.00
O	1	Methylcyclohexane	1	30	0.8157	22.250	0.1815	0.03
O	2	Methylcyclohexane	1	30	0.8325	1.614	0.0134	0.00
O	2	Methylcyclohexane	4	27	1.0957	2.999	0.0329	0.00
O	2	Methylcyclohexane	9	25	2.4442	9.899	0.2420	0.06
O	3	Methylcyclohexane	1	30	0.7291	7.566	0.0552	0.00
O	3	Methylcyclohexane	9	6	3.4222	1.468	0.0502	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	4	Methylcyclohexane	1	20	1.0050	25.872	0.2600	0.07
O	5	Methylcyclohexane	1	33	0.8895	29.108	0.2589	0.07
O	5	Methylcyclohexane	4	1	2.4129	.	.	.
O	6	Methylcyclohexane	1	30	0.8653	39.680	0.3434	0.12
O	7	Methylcyclohexane	1	29	0.7286	54.114	0.3943	0.16
O	7	Methylcyclohexane	9	10	0.0710	7.995	0.0057	0.00
O	1	Methylcyclopentane	1	30	0.8517	0.821	0.0070	0.00
O	3	Methylcyclopentane	1	30	0.7846	6.348	0.0498	0.00
O	3	Methylcyclopentane	4	23	0.0253	27.218	0.0069	0.00
O	3	Methylcyclopentane	9	25	0.0782	11.654	0.0091	0.00
O	4	Methylcyclopentane	1	29	0.6021	18.262	0.1099	0.01
O	6	Methylcyclopentane	1	30	0.3853	14.291	0.0551	0.00
O	7	Methylcyclopentane	1	8	0.3738	75.256	0.2813	0.08
O	7	Methylcyclopentane	4	18	0.5483	212.271	1.1640	1.35
O	7	Methylcyclopentane	9	12	1.8900	124.446	2.3520	5.53
O	1	cis-2-Pentene	1	30	1.4190	0.623	0.0088	0.00
O	1	cis-2-Pentene	4	30	4.5607	5.244	0.2392	0.06
O	1	cis-2-Pentene	9	26	10.0973	3.762	0.3799	0.14
O	2	cis-2-Pentene	1	30	1.3062	2.007	0.0262	0.00
O	2	cis-2-Pentene	4	30	4.5635	14.196	0.6479	0.42
O	2	cis-2-Pentene	9	25	10.1010	13.313	1.3447	1.81
O	3	cis-2-Pentene	1	30	0.9378	6.715	0.0630	0.00
O	3	cis-2-Pentene	4	30	3.8662	3.213	0.1242	0.02
O	3	cis-2-Pentene	9	25	9.3086	2.839	0.2643	0.07
O	4	cis-2-Pentene	1	29	1.7841	11.844	0.2113	0.04
O	4	cis-2-Pentene	4	10	6.7490	0.744	0.0502	0.00
O	4	cis-2-Pentene	9	1	14.3500	.	.	.
O	6	cis-2-Pentene	1	30	0.5267	9.609	0.0506	0.00
O	7	cis-2-Pentene	1	30	2.2363	58.673	1.3121	1.72
O	7	cis-2-Pentene	4	29	4.3721	57.132	2.4978	6.24
O	7	cis-2-Pentene	9	16	4.5675	86.189	3.9367	15.50
O	8	cis-2-Pentene	1	20	1.3450	34.408	0.4628	0.21
O	8	cis-2-Pentene	9	12	7.3242	24.918	1.8250	3.33
O	1	m-Diethylbenzene	1	30	0.7853	2.310	0.0181	0.00
O	2	m-Diethylbenzene	1	30	0.7580	12.319	0.0934	0.01
O	3	m-Diethylbenzene	1	30	0.7696	6.612	0.0509	0.00
O	3	m-Diethylbenzene	4	27	0.0294	10.021	0.0029	0.00
O	3	m-Diethylbenzene	9	19	0.0321	17.385	0.0056	0.00
O	4	m-Diethylbenzene	1	29	0.7986	14.980	0.1196	0.01
O	6	m-Diethylbenzene	1	30	0.5567	8.391	0.0467	0.00
O	7	m-Diethylbenzene	1	27	0.6407	52.722	0.3378	0.11

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	8	m-Diethylbenzene	1	20	0.7880	33.438	0.2635	0.07
O	8	m-Diethylbenzene	4	12	1.3483	50.808	0.6851	0.47
O	8	m-Diethylbenzene	9	24	1.4471	61.248	0.8863	0.79
O	1	n-Decane	1	30	0.5613	7.198	0.0404	0.00
O	1	n-Decane	4	30	6.3920	1.019	0.0651	0.00
O	1	n-Decane	9	26	14.4204	0.899	0.1297	0.02
O	2	n-Decane	1	30	0.6853	11.564	0.0793	0.01
O	2	n-Decane	4	30	7.8583	4.626	0.3635	0.13
O	2	n-Decane	9	25	17.7894	7.017	1.2483	1.56
O	3	n-Decane	1	30	0.5299	8.872	0.0470	0.00
O	3	n-Decane	4	30	3.9387	3.515	0.1384	0.02
O	3	n-Decane	9	25	9.3015	2.412	0.2244	0.05
O	4	n-Decane	1	29	0.6359	14.893	0.0947	0.01
O	4	n-Decane	4	30	5.1567	9.610	0.4955	0.25
O	4	n-Decane	9	26	11.8912	7.060	0.8395	0.70
O	5	n-Decane	1	33	1.0212	19.657	0.2007	0.04
O	5	n-Decane	4	33	12.8896	22.044	2.8414	8.07
O	5	n-Decane	9	33	30.2698	40.837	12.3612	152.80
O	6	n-Decane	1	30	0.3243	4.260	0.0138	0.00
O	6	n-Decane	4	30	3.2603	23.772	0.7751	0.60
O	6	n-Decane	9	25	9.5972	21.483	2.0618	4.25
O	7	n-Decane	1	28	0.6571	60.638	0.3985	0.16
O	7	n-Decane	4	30	7.2733	59.794	4.3490	18.91
O	7	n-Decane	9	25	14.0232	72.862	10.2175	104.40
O	8	n-Decane	1	22	0.6855	25.372	0.1739	0.03
O	8	n-Decane	4	22	17.4491	30.034	5.2406	27.46
O	8	n-Decane	9	21	29.0390	4.171	1.2113	1.47
O	1	n-Heptane	1	30	0.7057	0.887	0.0063	0.00
O	1	n-Heptane	4	30	4.0923	0.555	0.0227	0.00
O	1	n-Heptane	9	26	9.1585	0.352	0.0322	0.00
O	2	n-Heptane	1	30	0.7145	10.313	0.0737	0.01
O	2	n-Heptane	4	30	5.0722	9.083	0.4607	0.21
O	2	n-Heptane	9	25	10.9840	2.011	0.2209	0.05
O	3	n-Heptane	1	30	0.3738	11.839	0.0443	0.00
O	3	n-Heptane	4	30	3.5606	2.582	0.0919	0.01
O	3	n-Heptane	9	25	8.9604	2.404	0.2154	0.05
O	4	n-Heptane	1	29	0.6645	16.867	0.1121	0.01
O	4	n-Heptane	4	30	4.5147	6.625	0.2991	0.09
O	4	n-Heptane	9	26	10.2800	5.361	0.5512	0.30
O	5	n-Heptane	1	33	1.0662	25.428	0.2711	0.07
O	5	n-Heptane	4	33	5.6761	24.699	1.4020	1.97

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	5	n-Heptane	9	33	11.2813	43.111	4.8635	23.65
O	6	n-Heptane	1	30	0.8470	38.465	0.3258	0.11
O	6	n-Heptane	9	5	10.7660	19.397	2.0883	4.36
O	7	n-Heptane	1	26	0.5692	45.222	0.2574	0.07
O	7	n-Heptane	4	30	1.6730	55.269	0.9247	0.85
O	7	n-Heptane	9	25	2.9596	66.298	1.9622	3.85
O	8	n-Heptane	1	20	1.0315	8.436	0.0870	0.01
O	8	n-Heptane	9	28	5.6804	63.380	3.6002	12.96
O	1	n-Nonane	1	30	0.5707	5.365	0.0306	0.00
O	1	n-Nonane	4	30	4.3207	0.838	0.0362	0.00
O	1	n-Nonane	9	26	9.6135	0.397	0.0382	0.00
O	2	n-Nonane	1	30	0.5815	2.359	0.0137	0.00
O	2	n-Nonane	4	30	4.5467	1.174	0.0534	0.00
O	2	n-Nonane	9	25	10.3920	2.045	0.2125	0.05
O	3	n-Nonane	1	30	0.4773	8.788	0.0419	0.00
O	3	n-Nonane	4	30	3.8074	2.272	0.0865	0.01
O	3	n-Nonane	9	25	9.0989	2.486	0.2262	0.05
O	4	n-Nonane	1	29	0.5597	16.894	0.0945	0.01
O	4	n-Nonane	4	30	5.0140	20.143	1.0100	1.02
O	4	n-Nonane	9	26	12.0473	4.622	0.5568	0.31
O	5	n-Nonane	1	33	1.0075	24.542	0.2473	0.06
O	5	n-Nonane	4	33	6.0792	21.961	1.3350	1.78
O	5	n-Nonane	9	33	10.1533	39.114	3.9713	15.77
O	6	n-Nonane	1	30	0.6453	5.921	0.0382	0.00
O	6	n-Nonane	4	30	3.2070	27.023	0.8666	0.75
O	6	n-Nonane	9	25	8.5628	41.666	3.5677	12.73
O	7	n-Nonane	1	26	0.5088	48.424	0.2464	0.06
O	7	n-Nonane	4	30	1.9697	52.721	1.0384	1.08
O	7	n-Nonane	9	25	3.5716	65.942	2.3552	5.55
O	8	n-Nonane	1	22	1.3214	25.683	0.3394	0.12
O	8	n-Nonane	4	22	6.8350	16.210	1.1079	1.23
O	8	n-Nonane	9	28	17.1768	20.503	3.5217	12.40
O	1	n-Octane	1	30	0.7480	0.816	0.0061	0.00
O	1	n-Octane	4	30	4.2313	0.685	0.0290	0.00
O	1	n-Octane	9	26	9.4612	0.339	0.0320	0.00
O	2	n-Octane	1	30	0.7230	1.840	0.0133	0.00
O	2	n-Octane	4	30	5.4195	1.610	0.0873	0.01
O	2	n-Octane	9	25	12.3548	0.909	0.1123	0.01
O	3	n-Octane	1	30	0.6594	6.427	0.0424	0.00
O	3	n-Octane	4	30	3.7908	2.078	0.0788	0.01
O	3	n-Octane	9	25	9.0592	2.492	0.2258	0.05

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	4	n-Octane	1	29	0.7721	12.631	0.0975	0.01
O	4	n-Octane	4	30	4.5980	10.802	0.4967	0.25
O	4	n-Octane	9	26	10.4054	10.561	1.0989	1.21
O	5	n-Octane	1	33	0.9566	26.579	0.2543	0.06
O	5	n-Octane	4	33	4.8225	24.596	1.1861	1.41
O	5	n-Octane	9	33	8.6191	42.732	3.6831	13.57
O	6	n-Octane	1	30	0.6717	23.622	0.1587	0.03
O	6	n-Octane	4	30	3.8850	27.725	1.0771	1.16
O	6	n-Octane	9	25	8.1904	37.371	3.0608	9.37
O	7	n-Octane	1	23	0.6117	60.189	0.3682	0.14
O	7	n-Octane	4	30	1.4537	45.650	0.6636	0.44
O	7	n-Octane	9	25	2.2484	56.145	1.2624	1.59
O	8	n-Octane	1	22	1.2091	14.311	0.1730	0.03
O	8	n-Octane	4	22	2.1068	20.189	0.4254	0.18
O	8	n-Octane	9	25	6.4324	11.164	0.7181	0.52
O	1	n-Propylbenzene	1	30	0.6667	1.326	0.0088	0.00
O	1	n-Propylbenzene	4	30	4.4420	0.641	0.0285	0.00
O	1	n-Propylbenzene	9	26	10.1319	0.364	0.0369	0.00
O	2	n-Propylbenzene	1	30	0.6372	5.975	0.0381	0.00
O	2	n-Propylbenzene	4	30	5.0618	1.700	0.0860	0.01
O	2	n-Propylbenzene	9	25	11.6684	2.281	0.2661	0.07
O	3	n-Propylbenzene	1	30	0.6268	7.433	0.0466	0.00
O	3	n-Propylbenzene	4	30	3.7907	2.793	0.1059	0.01
O	3	n-Propylbenzene	9	25	9.0380	2.591	0.2341	0.05
O	4	n-Propylbenzene	1	29	0.6907	14.911	0.1030	0.01
O	4	n-Propylbenzene	4	30	5.3547	7.104	0.3804	0.14
O	4	n-Propylbenzene	9	26	12.1585	5.802	0.7054	0.50
O	5	n-Propylbenzene	1	33	0.9445	23.330	0.2203	0.05
O	5	n-Propylbenzene	4	33	11.2017	22.285	2.4963	6.23
O	5	n-Propylbenzene	9	33	22.9222	41.505	9.5138	90.51
O	6	n-Propylbenzene	1	30	0.6190	9.366	0.0580	0.00
O	6	n-Propylbenzene	4	30	2.9893	20.718	0.6193	0.38
O	6	n-Propylbenzene	9	25	8.4664	31.505	2.6674	7.11
O	7	n-Propylbenzene	1	30	0.5810	59.897	0.3480	0.12
O	7	n-Propylbenzene	4	30	2.0453	55.477	1.1347	1.29
O	7	n-Propylbenzene	9	25	3.6128	67.978	2.4559	6.03
O	8	n-Propylbenzene	1	22	0.5232	26.137	0.1367	0.02
O	8	n-Propylbenzene	4	22	4.6595	40.614	1.8924	3.58
O	8	n-Propylbenzene	9	28	8.2314	26.783	2.2046	4.86
O	1	n-Undecane	1	30	0.7340	11.575	0.0850	0.01
O	1	n-Undecane	4	30	5.2143	0.977	0.0510	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	1	n-Undecane	9	26	11.7038	0.616	0.0721	0.01
O	2	n-Undecane	1	30	0.7058	8.047	0.0568	0.00
O	2	n-Undecane	4	30	4.9278	1.900	0.0936	0.01
O	2	n-Undecane	9	25	11.0614	1.611	0.1782	0.03
O	3	n-Undecane	1	30	0.4923	11.241	0.0553	0.00
O	3	n-Undecane	4	30	3.9500	2.805	0.1108	0.01
O	3	n-Undecane	9	25	9.4051	2.149	0.2021	0.04
O	4	n-Undecane	1	29	0.5600	18.771	0.1051	0.01
O	4	n-Undecane	4	20	4.7980	10.139	0.4865	0.24
O	4	n-Undecane	9	26	11.6292	8.454	0.9831	0.97
O	5	n-Undecane	1	33	1.1028	19.668	0.2169	0.05
O	5	n-Undecane	4	33	9.9750	19.652	1.9603	3.84
O	5	n-Undecane	9	33	24.6002	40.804	10.0379	100.76
O	6	n-Undecane	1	30	0.4317	5.774	0.0249	0.00
O	6	n-Undecane	4	30	2.8740	75.053	2.1570	4.65
O	6	n-Undecane	9	25	5.9324	23.468	1.3922	1.94
O	7	n-Undecane	1	21	0.7605	28.476	0.2166	0.05
O	7	n-Undecane	4	30	2.8920	63.728	1.8430	3.40
O	7	n-Undecane	9	20	5.7285	55.675	3.1894	10.17
O	8	n-Undecane	1	22	0.7827	65.581	0.5133	0.26
O	8	n-Undecane	4	22	7.1623	46.812	3.3528	11.24
O	8	n-Undecane	9	28	15.2654	64.670	9.8721	97.46
O	1	p-Diethylbenzene	1	30	0.4810	4.241	0.0204	0.00
O	2	p-Diethylbenzene	1	30	0.6475	19.355	0.1253	0.02
O	2	p-Diethylbenzene	4	30	4.7197	3.308	0.1561	0.02
O	2	p-Diethylbenzene	9	25	12.4280	50.369	6.2599	39.19
O	3	p-Diethylbenzene	1	30	0.7651	6.382	0.0488	0.00
O	3	p-Diethylbenzene	4	30	0.0356	79.427	0.0283	0.00
O	3	p-Diethylbenzene	9	20	0.0723	133.404	0.0964	0.01
O	4	p-Diethylbenzene	1	29	0.4697	22.006	0.1034	0.01
O	6	p-Diethylbenzene	1	30	0.4540	14.856	0.0674	0.00
O	7	p-Diethylbenzene	1	15	0.3507	73.273	0.2569	0.07
O	1	trans-2-Pentene	1	30	1.0020	0.550	0.0055	0.00
O	1	trans-2-Pentene	4	30	4.1267	3.423	0.1413	0.02
O	1	trans-2-Pentene	9	26	9.1685	2.409	0.2209	0.05
O	2	trans-2-Pentene	1	30	0.9798	2.440	0.0239	0.00
O	2	trans-2-Pentene	4	30	4.2025	11.027	0.4634	0.21
O	2	trans-2-Pentene	9	25	10.5450	15.811	1.6673	2.78
O	3	trans-2-Pentene	1	30	0.6917	7.343	0.0508	0.00
O	3	trans-2-Pentene	4	30	3.2642	30.217	0.9863	0.97
O	3	trans-2-Pentene	9	25	9.3190	2.662	0.2481	0.06

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
O	4	trans-2-Pentene	1	29	1.3514	11.887	0.1606	0.03
O	4	trans-2-Pentene	4	30	6.2490	6.491	0.4057	0.16
O	4	trans-2-Pentene	9	26	14.1935	6.612	0.9385	0.88
O	5	trans-2-Pentene	1	33	0.9886	26.169	0.2587	0.07
O	5	trans-2-Pentene	4	33	4.6353	23.995	1.1122	1.24
O	5	trans-2-Pentene	9	30	9.7254	28.465	2.7683	7.66
O	6	trans-2-Pentene	1	30	0.5267	9.609	0.0506	0.00
O	6	trans-2-Pentene	4	30	3.0547	18.726	0.5720	0.33
O	6	trans-2-Pentene	9	25	7.7680	26.528	2.0607	4.25
O	7	trans-2-Pentene	1	30	1.3183	60.581	0.7987	0.64
O	7	trans-2-Pentene	4	29	2.7066	59.138	1.6006	2.56
O	7	trans-2-Pentene	9	16	2.5750	95.190	2.4511	6.01
O	8	trans-2-Pentene	1	22	0.9550	5.965	0.0570	0.00
O	8	trans-2-Pentene	4	22	5.1823	2.805	0.1454	0.02
O	8	trans-2-Pentene	9	28	9.5739	29.545	2.8286	8.00
P	1	1,2,3-Trimethylbenzene	1	30	0.5640	4.624	0.0261	0.00
P	2	1,2,3-Trimethylbenzene	1	30	0.5785	8.460	0.0489	0.00
P	2	1,2,3-Trimethylbenzene	4	30	4.9755	4.712	0.2345	0.05
P	2	1,2,3-Trimethylbenzene	9	25	12.2546	27.667	3.3905	11.50
P	3	1,2,3-Trimethylbenzene	1	30	0.5591	7.768	0.0434	0.00
P	3	1,2,3-Trimethylbenzene	4	20	0.0319	40.272	0.0128	0.00
P	3	1,2,3-Trimethylbenzene	9	25	0.0348	46.014	0.0160	0.00
P	4	1,2,3-Trimethylbenzene	1	29	0.5172	18.297	0.0946	0.01
P	5	1,2,3-Trimethylbenzene	1	33	0.7990	17.161	0.1371	0.02
P	5	1,2,3-Trimethylbenzene	4	33	5.5258	21.190	1.1709	1.37
P	5	1,2,3-Trimethylbenzene	9	33	36.3073	44.968	16.3267	266.56
P	6	1,2,3-Trimethylbenzene	1	30	0.2660	10.383	0.0276	0.00
P	7	1,2,3-Trimethylbenzene	1	27	0.5341	53.437	0.2854	0.08
P	7	1,2,3-Trimethylbenzene	9	9	0.0178	24.804	0.0044	0.00
P	8	1,2,3-Trimethylbenzene	1	22	0.4536	37.789	0.1714	0.03
P	8	1,2,3-Trimethylbenzene	4	18	6.5994	73.571	4.8553	23.57
P	8	1,2,3-Trimethylbenzene	9	28	10.5668	117.000	12.3631	152.85
P	1	1,2,4-Trimethylbenzene	1	30	0.8630	3.165	0.0273	0.00
P	1	1,2,4-Trimethylbenzene	4	30	9.1697	0.653	0.0599	0.00
P	1	1,2,4-Trimethylbenzene	9	26	20.5488	0.454	0.0933	0.01
P	2	1,2,4-Trimethylbenzene	1	30	0.9297	8.805	0.0819	0.01
P	2	1,2,4-Trimethylbenzene	4	30	9.8847	1.967	0.1944	0.04
P	2	1,2,4-Trimethylbenzene	9	25	23.0494	11.474	2.6446	6.99
P	3	1,2,4-Trimethylbenzene	1	30	0.6797	6.974	0.0474	0.00
P	3	1,2,4-Trimethylbenzene	4	30	3.7659	2.673	0.1007	0.01
P	3	1,2,4-Trimethylbenzene	9	25	8.9489	2.629	0.2352	0.06

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	4	1,2,4-Trimethylbenzene	1	29	0.7263	35.660	0.2590	0.07
P	4	1,2,4-Trimethylbenzene	4	30	6.6717	34.412	2.2959	5.27
P	4	1,2,4-Trimethylbenzene	9	26	11.5852	7.342	0.8505	0.72
P	5	1,2,4-Trimethylbenzene	1	33	0.9575	15.043	0.1440	0.02
P	5	1,2,4-Trimethylbenzene	4	33	15.0219	22.748	3.4172	11.68
P	5	1,2,4-Trimethylbenzene	9	33	32.4257	41.627	13.4978	182.19
P	6	1,2,4-Trimethylbenzene	1	30	0.6220	9.378	0.0583	0.00
P	6	1,2,4-Trimethylbenzene	4	30	2.9700	17.495	0.5196	0.27
P	6	1,2,4-Trimethylbenzene	9	25	9.9896	20.429	2.0408	4.16
P	7	1,2,4-Trimethylbenzene	1	20	1.1900	13.765	0.1638	0.03
P	8	1,2,4-Trimethylbenzene	1	22	0.6405	31.687	0.2029	0.04
P	8	1,2,4-Trimethylbenzene	4	22	9.1609	39.839	3.6496	13.32
P	8	1,2,4-Trimethylbenzene	9	28	13.4711	4.388	0.5911	0.35
P	1	1-Butene	1	30	1.5843	1.888	0.0299	0.00
P	1	1-Butene	4	30	4.2313	3.326	0.1407	0.02
P	1	1-Butene	9	26	9.1977	0.282	0.0260	0.00
P	2	1-Butene	1	30	1.4748	1.657	0.0244	0.00
P	2	1-Butene	4	30	4.2673	4.002	0.1708	0.03
P	2	1-Butene	9	25	9.6634	4.485	0.4334	0.19
P	3	1-Butene	1	30	1.1688	11.380	0.1330	0.02
P	3	1-Butene	4	30	3.9446	4.529	0.1787	0.03
P	3	1-Butene	9	25	9.6790	2.697	0.2610	0.07
P	4	1-Butene	1	29	1.8952	11.787	0.2234	0.05
P	4	1-Butene	4	30	5.4857	22.230	1.2194	1.49
P	4	1-Butene	9	26	12.0800	13.558	1.6378	2.68
P	5	1-Butene	1	33	0.9820	26.438	0.2596	0.07
P	5	1-Butene	4	33	5.3491	27.108	1.4500	2.10
P	5	1-Butene	9	33	11.5956	45.178	5.2386	27.44
P	6	1-Butene	1	30	0.6077	51.987	0.3159	0.10
P	6	1-Butene	4	30	4.1697	31.928	1.3313	1.77
P	6	1-Butene	9	25	8.4616	34.395	2.9104	8.47
P	7	1-Butene	1	30	1.0560	52.774	0.5573	0.31
P	7	1-Butene	4	30	2.4053	54.696	1.3156	1.73
P	7	1-Butene	9	25	4.7804	71.121	3.3999	11.56
P	8	1-Butene	1	22	1.6291	6.407	0.1044	0.01
P	8	1-Butene	4	22	4.8491	2.102	0.1019	0.01
P	8	1-Butene	9	28	9.0229	29.685	2.6784	7.17
P	1	2,2,4-Trimethylpentane	1	30	0.7307	4.574	0.0334	0.00
P	1	2,2,4-Trimethylpentane	4	30	4.0777	0.747	0.0305	0.00
P	1	2,2,4-Trimethylpentane	9	26	9.0650	0.363	0.0329	0.00
P	2	2,2,4-Trimethylpentane	1	30	0.7165	1.117	0.0080	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	2	2,2,4-Trimethylpentane	4	30	5.4675	2.883	0.1577	0.02
P	2	2,2,4-Trimethylpentane	9	25	12.4276	0.557	0.0692	0.00
P	3	2,2,4-Trimethylpentane	1	30	0.6698	7.190	0.0482	0.00
P	3	2,2,4-Trimethylpentane	4	30	3.8022	2.655	0.1010	0.01
P	3	2,2,4-Trimethylpentane	9	25	9.0386	2.174	0.1965	0.04
P	4	2,2,4-Trimethylpentane	1	29	0.8307	14.406	0.1197	0.01
P	4	2,2,4-Trimethylpentane	4	10	4.9460	3.335	0.1649	0.03
P	4	2,2,4-Trimethylpentane	9	20	11.5115	3.611	0.4157	0.17
P	5	2,2,4-Trimethylpentane	1	33	1.0543	26.381	0.2781	0.08
P	5	2,2,4-Trimethylpentane	4	33	5.4607	25.086	1.3699	1.88
P	5	2,2,4-Trimethylpentane	9	33	10.8371	43.414	4.7048	22.14
P	6	2,2,4-Trimethylpentane	1	30	0.6437	23.207	0.1494	0.02
P	6	2,2,4-Trimethylpentane	4	30	3.3777	20.923	0.7067	0.50
P	6	2,2,4-Trimethylpentane	9	25	7.9064	32.313	2.5548	6.53
P	7	2,2,4-Trimethylpentane	1	29	0.6507	56.453	0.3673	0.13
P	7	2,2,4-Trimethylpentane	4	30	1.2183	50.702	0.6177	0.38
P	7	2,2,4-Trimethylpentane	9	25	1.8784	60.349	1.1336	1.29
P	8	2,2,4-Trimethylpentane	1	18	1.0194	8.860	0.0903	0.01
P	8	2,2,4-Trimethylpentane	4	20	5.2820	20.630	1.0897	1.19
P	8	2,2,4-Trimethylpentane	9	27	12.3237	25.954	3.1985	10.23
P	1	Benzene	1	30	1.0203	1.374	0.0140	0.00
P	1	Benzene	4	30	4.3153	0.508	0.0219	0.00
P	1	Benzene	9	26	9.6450	0.368	0.0355	0.00
P	2	Benzene	1	30	0.9707	0.686	0.0067	0.00
P	2	Benzene	4	30	4.1400	3.397	0.1406	0.02
P	2	Benzene	9	25	9.3182	1.799	0.1676	0.03
P	3	Benzene	1	30	0.8828	6.588	0.0582	0.00
P	3	Benzene	4	30	3.7658	2.749	0.1035	0.01
P	3	Benzene	9	25	8.9935	2.170	0.1952	0.04
P	4	Benzene	1	29	0.7941	17.020	0.1352	0.02
P	4	Benzene	4	30	3.6127	9.735	0.3517	0.12
P	4	Benzene	9	26	8.1177	8.466	0.6872	0.47
P	5	Benzene	1	33	0.9486	23.293	0.2210	0.05
P	5	Benzene	4	33	4.0648	24.197	0.9835	0.97
P	5	Benzene	9	33	10.1806	43.387	4.4171	19.51
P	6	Benzene	1	30	1.1503	31.048	0.3572	0.13
P	6	Benzene	4	30	3.3740	36.578	1.2341	1.52
P	6	Benzene	9	25	8.3888	52.869	4.4351	19.67
P	7	Benzene	1	30	0.8627	51.780	0.4467	0.20
P	7	Benzene	4	30	2.2587	50.851	1.1485	1.32
P	7	Benzene	9	25	4.1252	63.937	2.6375	6.96

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	8	Benzene	1	22	2.7295	15.411	0.4207	0.18
P	8	Benzene	4	22	5.7414	15.818	0.9082	0.82
P	8	Benzene	9	28	12.2079	13.905	1.6975	2.88
P	1	Ethane	1	30	2.8443	1.262	0.0359	0.00
P	1	Ethane	4	30	4.6033	1.457	0.0671	0.00
P	1	Ethane	9	26	9.9723	0.718	0.0716	0.01
P	2	Ethane	1	30	2.5253	10.201	0.2576	0.07
P	2	Ethane	4	30	4.3070	7.065	0.3043	0.09
P	2	Ethane	9	25	9.3574	4.615	0.4318	0.19
P	3	Ethane	1	30	4.7238	9.501	0.4488	0.20
P	3	Ethane	4	30	7.9648	4.470	0.3561	0.13
P	3	Ethane	9	25	18.5778	3.098	0.5755	0.33
P	4	Ethane	1	29	1.5731	8.916	0.1403	0.02
P	4	Ethane	4	30	2.7433	9.801	0.2689	0.07
P	4	Ethane	9	26	6.2365	5.377	0.3353	0.11
P	5	Ethane	1	33	0.9568	27.157	0.2598	0.07
P	5	Ethane	4	33	1.6574	29.372	0.4868	0.24
P	5	Ethane	9	33	3.3528	21.559	0.7228	0.52
P	6	Ethane	1	1	0.5800	.	.	.
P	7	Ethane	1	30	1.3213	54.209	0.7163	0.51
P	7	Ethane	4	30	2.1627	57.918	1.2526	1.57
P	7	Ethane	9	25	4.6380	73.741	3.4201	11.70
P	8	Ethane	1	22	1.1323	5.403	0.0612	0.00
P	8	Ethane	4	22	1.9695	5.226	0.1029	0.01
P	8	Ethane	9	28	3.2889	34.216	1.1253	1.27
P	1	Ethylbenzene	1	30	0.6227	1.395	0.0087	0.00
P	1	Ethylbenzene	4	30	4.2303	0.625	0.0265	0.00
P	1	Ethylbenzene	9	26	9.4704	0.314	0.0297	0.00
P	2	Ethylbenzene	1	30	0.6543	3.081	0.0202	0.00
P	2	Ethylbenzene	4	30	4.4990	2.109	0.0949	0.01
P	2	Ethylbenzene	9	25	10.1678	0.896	0.0911	0.01
P	3	Ethylbenzene	1	30	0.5138	7.726	0.0397	0.00
P	3	Ethylbenzene	4	30	3.7286	2.665	0.0994	0.01
P	3	Ethylbenzene	9	25	8.9995	2.458	0.2213	0.05
P	4	Ethylbenzene	1	29	0.6024	17.363	0.1046	0.01
P	4	Ethylbenzene	4	30	4.6457	9.827	0.4565	0.21
P	4	Ethylbenzene	9	26	10.5623	8.847	0.9344	0.87
P	5	Ethylbenzene	1	33	1.0561	22.344	0.2360	0.06
P	5	Ethylbenzene	4	33	5.5431	22.278	1.2349	1.52
P	5	Ethylbenzene	9	33	10.1306	40.818	4.1351	17.10
P	6	Ethylbenzene	1	30	0.5113	18.615	0.0952	0.01

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	6	Ethylbenzene	4	30	2.7937	32.766	0.9154	0.84
P	6	Ethylbenzene	9	25	7.7528	48.779	3.7817	14.30
P	7	Ethylbenzene	1	30	0.5730	51.802	0.2968	0.09
P	7	Ethylbenzene	4	30	1.8477	51.499	0.9515	0.91
P	7	Ethylbenzene	9	25	3.1948	64.588	2.0635	4.26
P	8	Ethylbenzene	1	22	1.1645	16.598	0.1933	0.04
P	8	Ethylbenzene	4	20	4.9520	13.294	0.6583	0.43
P	8	Ethylbenzene	9	28	12.5750	15.970	2.0082	4.03
P	1	Ethylene	1	30	2.0977	0.716	0.0150	0.00
P	1	Ethylene	4	30	3.5653	1.265	0.0451	0.00
P	1	Ethylene	9	26	8.0531	0.862	0.0694	0.00
P	2	Ethylene	1	30	3.2402	13.681	0.4433	0.20
P	2	Ethylene	4	30	5.0450	8.364	0.4220	0.18
P	2	Ethylene	9	25	10.3972	7.671	0.7976	0.64
P	3	Ethylene	1	30	4.1978	9.042	0.3796	0.14
P	3	Ethylene	4	30	7.4654	6.203	0.4631	0.21
P	3	Ethylene	9	25	19.0043	3.800	0.7222	0.52
P	4	Ethylene	1	29	1.2579	5.452	0.0686	0.00
P	4	Ethylene	4	30	2.2753	9.124	0.2076	0.04
P	4	Ethylene	9	26	5.1908	5.540	0.2876	0.08
P	5	Ethylene	1	33	0.9534	26.055	0.2484	0.06
P	5	Ethylene	4	33	1.6538	34.168	0.5651	0.32
P	5	Ethylene	9	33	3.1111	36.891	1.1477	1.32
P	6	Ethylene	1	30	0.6077	51.987	0.3159	0.10
P	6	Ethylene	4	30	4.1697	31.928	1.3313	1.77
P	6	Ethylene	9	25	8.4616	34.395	2.9104	8.47
P	7	Ethylene	1	30	1.0803	52.595	0.5682	0.32
P	7	Ethylene	4	30	1.6687	57.088	0.9526	0.91
P	7	Ethylene	9	25	3.3796	73.068	2.4694	6.10
P	8	Ethylene	1	22	0.5618	9.053	0.0509	0.00
P	8	Ethylene	4	22	4.6177	9.152	0.4226	0.18
P	8	Ethylene	9	28	6.7050	32.116	2.1534	4.64
P	1	Isobutane	1	30	1.2900	0.644	0.0083	0.00
P	1	Isobutane	4	30	4.1913	1.282	0.0537	0.00
P	1	Isobutane	9	26	9.4238	0.949	0.0894	0.01
P	2	Isobutane	1	30	1.2525	3.145	0.0394	0.00
P	2	Isobutane	4	30	4.0167	1.545	0.0621	0.00
P	2	Isobutane	9	25	8.9546	1.176	0.1053	0.01
P	3	Isobutane	1	30	1.0409	7.637	0.0795	0.01
P	3	Isobutane	4	30	3.8275	3.016	0.1154	0.01
P	3	Isobutane	9	25	9.2699	2.412	0.2236	0.05

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	4	Isobutane	1	29	1.3355	10.514	0.1404	0.02
P	4	Isobutane	9	1	11.4700	.	.	.
P	5	Isobutane	1	33	1.0120	25.947	0.2626	0.07
P	5	Isobutane	4	33	3.1648	25.160	0.7963	0.63
P	5	Isobutane	9	33	6.5378	34.348	2.2456	5.04
P	6	Isobutane	1	30	0.6077	51.987	0.3159	0.10
P	7	Isobutane	1	27	0.7978	56.136	0.4478	0.20
P	7	Isobutane	4	30	2.3637	59.965	1.4174	2.01
P	7	Isobutane	9	25	5.2380	74.558	3.9054	15.25
P	8	Isobutane	1	22	1.1964	5.578	0.0667	0.00
P	8	Isobutane	4	22	4.0086	3.220	0.1291	0.02
P	8	Isobutane	9	28	7.4757	27.931	2.0880	4.36
P	1	Isopentane	1	30	1.6230	0.946	0.0153	0.00
P	1	Isopentane	4	30	4.1530	0.573	0.0238	0.00
P	1	Isopentane	9	26	9.2638	0.242	0.0225	0.00
P	2	Isopentane	1	30	1.6025	2.311	0.0370	0.00
P	2	Isopentane	4	30	3.9608	1.566	0.0620	0.00
P	2	Isopentane	9	25	8.9574	1.461	0.1309	0.02
P	3	Isopentane	1	30	1.4770	6.572	0.0971	0.01
P	3	Isopentane	4	30	3.8952	3.019	0.1176	0.01
P	3	Isopentane	9	25	9.3521	2.427	0.2270	0.05
P	4	Isopentane	1	29	2.2338	11.268	0.2517	0.06
P	4	Isopentane	4	30	6.0883	9.706	0.5909	0.35
P	4	Isopentane	9	26	13.8573	9.107	1.2621	1.59
P	5	Isopentane	1	33	1.0397	27.454	0.2854	0.08
P	5	Isopentane	4	33	2.9323	25.700	0.7536	0.57
P	5	Isopentane	9	33	7.2140	43.080	3.1078	9.66
P	6	Isopentane	1	30	0.6243	11.174	0.0698	0.00
P	6	Isopentane	4	30	3.0373	16.919	0.5139	0.26
P	6	Isopentane	9	25	7.7816	24.180	1.8816	3.54
P	7	Isopentane	1	29	1.2128	30.738	0.3728	0.14
P	7	Isopentane	4	30	2.6920	46.368	1.2482	1.56
P	7	Isopentane	9	24	5.3792	65.177	3.5060	12.29
P	8	Isopentane	1	22	1.4659	5.821	0.0853	0.01
P	8	Isopentane	4	22	3.8591	3.464	0.1337	0.02
P	8	Isopentane	9	28	6.9150	28.621	1.9791	3.92
P	1	Isoprene	1	30	1.6180	0.657	0.0106	0.00
P	1	Isoprene	4	30	4.5847	0.708	0.0325	0.00
P	1	Isoprene	9	26	10.2700	0.702	0.0721	0.01
P	2	Isoprene	1	30	1.3053	13.097	0.1710	0.03
P	2	Isoprene	4	30	3.5917	6.586	0.2365	0.06

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	2	Isoprene	9	25	8.0368	3.917	0.3148	0.10
P	3	Isoprene	1	30	1.4266	6.452	0.0920	0.01
P	3	Isoprene	4	30	3.9149	2.815	0.1102	0.01
P	3	Isoprene	9	25	9.2547	2.605	0.2411	0.06
P	4	Isoprene	1	29	1.9310	27.046	0.5223	0.27
P	4	Isoprene	4	30	5.3307	31.927	1.7019	2.90
P	4	Isoprene	9	26	11.6904	9.739	1.1385	1.30
P	5	Isoprene	1	33	0.9879	26.992	0.2666	0.07
P	5	Isoprene	4	33	3.0878	26.005	0.8030	0.64
P	5	Isoprene	9	33	6.8648	44.162	3.0316	9.19
P	6	Isoprene	1	30	0.5267	9.609	0.0506	0.00
P	6	Isoprene	4	30	3.0547	18.726	0.5720	0.33
P	6	Isoprene	9	25	7.7680	26.528	2.0607	4.25
P	7	Isoprene	1	29	3.3683	29.321	0.9876	0.98
P	7	Isoprene	4	29	6.5838	26.368	1.7360	3.01
P	7	Isoprene	9	20	8.1665	59.674	4.8733	23.75
P	8	Isoprene	1	22	0.7073	6.663	0.0471	0.00
P	8	Isoprene	4	22	0.7914	4.096	0.0324	0.00
P	8	Isoprene	9	20	1.2645	41.420	0.5238	0.27
P	1	Propane	1	30	2.7980	1.431	0.0400	0.00
P	1	Propane	4	30	4.4263	1.695	0.0750	0.01
P	1	Propane	9	26	9.9992	1.708	0.1707	0.03
P	2	Propane	1	30	2.4598	2.686	0.0661	0.00
P	2	Propane	4	30	4.0218	2.068	0.0832	0.01
P	2	Propane	9	25	9.1336	1.139	0.1040	0.01
P	3	Propane	1	30	4.5265	6.497	0.2941	0.09
P	3	Propane	4	30	7.8285	3.239	0.2536	0.06
P	3	Propane	9	25	18.3600	2.765	0.5076	0.26
P	4	Propane	1	29	2.4076	4.090	0.0985	0.01
P	4	Propane	4	30	4.0033	4.850	0.1941	0.04
P	4	Propane	9	26	9.1504	2.946	0.2695	0.07
P	5	Propane	1	33	1.0185	25.187	0.2565	0.07
P	5	Propane	4	33	1.6310	27.722	0.4521	0.20
P	5	Propane	9	33	3.1859	33.578	1.0698	1.14
P	6	Propane	1	1	0.5800	.	.	.
P	7	Propane	1	29	1.3917	56.144	0.7814	0.61
P	7	Propane	4	30	2.1980	59.815	1.3147	1.73
P	7	Propane	9	25	4.3292	88.153	3.8163	14.56
P	8	Propane	1	22	2.4259	5.953	0.1444	0.02
P	8	Propane	4	22	4.0659	2.837	0.1153	0.01
P	8	Propane	9	28	7.7732	27.678	2.1515	4.63

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	1	Propylene	1	30	1.6997	0.780	0.0133	0.00
P	1	Propylene	4	30	4.6267	1.065	0.0493	0.00
P	1	Propylene	9	26	10.3600	0.890	0.0922	0.01
P	2	Propylene	1	30	2.7157	11.065	0.3005	0.09
P	2	Propylene	4	30	5.0773	9.262	0.4703	0.22
P	2	Propylene	9	25	10.0386	5.558	0.5579	0.31
P	3	Propylene	1	30	1.9952	11.955	0.2385	0.06
P	3	Propylene	4	30	7.3866	4.318	0.3189	0.10
P	3	Propylene	9	25	18.9977	3.210	0.6099	0.37
P	4	Propylene	1	29	1.1559	11.969	0.1383	0.02
P	4	Propylene	4	30	3.2287	10.092	0.3258	0.11
P	4	Propylene	9	26	7.2142	6.466	0.4665	0.22
P	5	Propylene	1	33	0.7850	23.727	0.1862	0.03
P	5	Propylene	4	33	1.9678	24.310	0.4784	0.23
P	5	Propylene	9	33	3.8853	40.399	1.5696	2.46
P	6	Propylene	1	30	0.6077	51.987	0.3159	0.10
P	6	Propylene	4	30	4.1697	31.928	1.3313	1.77
P	6	Propylene	9	25	8.4616	34.395	2.9104	8.47
P	7	Propylene	1	30	1.2263	61.231	0.7509	0.56
P	7	Propylene	4	30	1.9157	63.562	1.2176	1.48
P	7	Propylene	9	24	4.4567	76.982	3.4308	11.77
P	8	Propylene	1	22	1.4459	5.906	0.0854	0.01
P	8	Propylene	4	22	7.0309	6.390	0.4493	0.20
P	8	Propylene	9	28	12.3579	29.226	3.6117	13.04
P	1	Styrene	1	30	0.9867	2.050	0.0202	0.00
P	1	Styrene	4	30	4.6997	0.994	0.0467	0.00
P	1	Styrene	9	26	10.4342	0.715	0.0746	0.01
P	2	Styrene	1	30	0.8032	13.509	0.1085	0.01
P	2	Styrene	4	30	3.9090	5.967	0.2333	0.05
P	2	Styrene	9	25	8.9324	3.156	0.2819	0.08
P	3	Styrene	1	30	0.8217	6.582	0.0541	0.00
P	3	Styrene	4	30	3.7718	2.404	0.0907	0.01
P	3	Styrene	9	25	8.9536	2.956	0.2647	0.07
P	4	Styrene	1	29	0.7438	16.448	0.1223	0.01
P	4	Styrene	4	30	3.8657	14.762	0.5707	0.33
P	4	Styrene	9	26	8.6673	13.350	1.1571	1.34
P	5	Styrene	1	33	0.9659	25.082	0.2423	0.06
P	5	Styrene	4	33	5.1449	22.999	1.1833	1.40
P	5	Styrene	9	33	17.9086	39.059	6.9950	48.93
P	6	Styrene	1	30	0.5297	14.745	0.0781	0.01
P	6	Styrene	4	30	2.6743	38.132	1.0198	1.04

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	6	Styrene	9	25	7.7772	49.453	3.8460	14.79
P	7	Styrene	1	28	0.8779	55.035	0.4831	0.23
P	7	Styrene	4	30	2.1870	57.205	1.2511	1.57
P	7	Styrene	9	25	3.6492	69.418	2.5332	6.42
P	8	Styrene	1	22	0.6645	32.012	0.2127	0.05
P	8	Styrene	4	22	6.5105	12.732	0.8289	0.69
P	8	Styrene	9	28	17.6132	14.742	2.5965	6.74
P	1	Toluene	1	30	1.1480	1.524	0.0175	0.00
P	1	Toluene	4	30	4.1180	0.620	0.0255	0.00
P	1	Toluene	9	26	9.2142	0.375	0.0345	0.00
P	2	Toluene	1	30	1.2137	3.560	0.0432	0.00
P	2	Toluene	4	30	4.3432	1.320	0.0573	0.00
P	2	Toluene	9	25	9.7564	0.908	0.0886	0.01
P	3	Toluene	1	30	0.9474	6.984	0.0662	0.00
P	3	Toluene	4	30	3.6596	2.871	0.1051	0.01
P	3	Toluene	9	25	8.9000	2.596	0.2310	0.05
P	4	Toluene	1	29	1.1159	12.289	0.1371	0.02
P	4	Toluene	4	30	4.1710	10.443	0.4356	0.19
P	4	Toluene	9	26	9.3869	9.373	0.8799	0.77
P	5	Toluene	1	33	0.8048	25.032	0.2015	0.04
P	5	Toluene	4	33	2.8469	24.008	0.6835	0.47
P	5	Toluene	9	33	8.9705	43.815	3.9305	15.45
P	6	Toluene	1	30	1.3663	41.586	0.5682	0.32
P	6	Toluene	9	5	14.7760	13.997	2.0681	4.28
P	7	Toluene	1	30	1.0023	54.207	0.5433	0.30
P	7	Toluene	4	30	2.2583	53.190	1.2012	1.44
P	7	Toluene	9	25	4.0400	66.011	2.6668	7.11
P	8	Toluene	1	22	1.9986	32.097	0.6415	0.41
P	8	Toluene	4	22	7.2195	10.750	0.7761	0.60
P	8	Toluene	9	21	17.8148	13.955	2.4861	6.18
P	1	cis-2-Butene	1	30	1.7757	0.604	0.0107	0.00
P	1	cis-2-Butene	4	30	4.4007	0.473	0.0208	0.00
P	1	cis-2-Butene	9	26	9.8281	0.268	0.0264	0.00
P	2	cis-2-Butene	1	30	1.7380	2.480	0.0431	0.00
P	2	cis-2-Butene	4	30	4.2505	1.555	0.0661	0.00
P	2	cis-2-Butene	9	25	9.4482	0.641	0.0606	0.00
P	3	cis-2-Butene	1	30	1.4239	7.406	0.1054	0.01
P	3	cis-2-Butene	4	30	3.8282	3.175	0.1215	0.01
P	3	cis-2-Butene	9	25	9.2738	2.642	0.2450	0.06
P	4	cis-2-Butene	1	29	1.8428	11.062	0.2039	0.04
P	4	cis-2-Butene	4	30	4.9297	9.952	0.4906	0.24

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	4	cis-2-Butene	9	26	11.2762	10.361	1.1683	1.36
P	5	cis-2-Butene	1	33	0.9496	26.812	0.2546	0.06
P	5	cis-2-Butene	4	33	2.6154	26.100	0.6826	0.47
P	5	cis-2-Butene	9	30	7.4832	31.072	2.3252	5.41
P	6	cis-2-Butene	1	30	0.6077	51.987	0.3159	0.10
P	6	cis-2-Butene	4	30	4.1697	31.928	1.3313	1.77
P	6	cis-2-Butene	9	25	8.4616	34.395	2.9104	8.47
P	7	cis-2-Butene	1	30	1.2793	55.926	0.7155	0.51
P	7	cis-2-Butene	4	30	2.6443	56.858	1.5035	2.26
P	7	cis-2-Butene	9	24	5.1000	71.582	3.6507	13.33
P	8	cis-2-Butene	1	22	1.3705	3.164	0.0434	0.00
P	8	cis-2-Butene	4	22	4.0686	11.917	0.4849	0.24
P	8	cis-2-Butene	9	21	6.4838	33.877	2.1965	4.82
P	1	m,p-Xylene	1	30	0.9947	2.041	0.0203	0.00
P	1	m,p-Xylene	4	30	8.9377	0.670	0.0599	0.00
P	1	m,p-Xylene	9	26	20.4150	0.378	0.0771	0.01
P	2	m,p-Xylene	1	30	1.0617	3.768	0.0400	0.00
P	2	m,p-Xylene	4	30	9.7085	3.485	0.3383	0.11
P	2	m,p-Xylene	9	25	22.1834	1.112	0.2466	0.06
P	3	m,p-Xylene	1	30	0.6028	9.665	0.0583	0.00
P	3	m,p-Xylene	4	30	7.3737	3.061	0.2257	0.05
P	3	m,p-Xylene	9	25	17.8532	2.579	0.4604	0.21
P	4	m,p-Xylene	1	28	0.9636	11.715	0.1129	0.01
P	4	m,p-Xylene	4	30	9.9283	7.899	0.7843	0.62
P	4	m,p-Xylene	9	26	22.8438	5.921	1.3526	1.83
P	5	m,p-Xylene	1	33	2.1223	17.728	0.3762	0.14
P	5	m,p-Xylene	4	33	11.2113	19.214	2.1542	4.64
P	5	m,p-Xylene	9	33	20.2497	38.973	7.8919	62.28
P	6	m,p-Xylene	1	30	0.8733	8.988	0.0785	0.01
P	6	m,p-Xylene	4	30	5.1503	54.444	2.8041	7.86
P	6	m,p-Xylene	9	25	14.2356	58.690	8.3549	69.80
P	7	m,p-Xylene	1	20	1.5365	11.467	0.1762	0.03
P	8	m,p-Xylene	1	22	1.5614	18.311	0.2859	0.08
P	8	m,p-Xylene	4	22	12.3809	12.536	1.5520	2.41
P	8	m,p-Xylene	9	28	30.9039	19.929	6.1590	37.93
P	1	m-Ethyltoluene	1	30	0.4987	1.018	0.0051	0.00
P	3	m-Ethyltoluene	1	30	0.5320	6.013	0.0320	0.00
P	3	m-Ethyltoluene	4	10	0.2056	2.946	0.0061	0.00
P	3	m-Ethyltoluene	9	6	0.4700	1.718	0.0081	0.00
P	4	m-Ethyltoluene	1	29	0.5121	20.821	0.1066	0.01
P	6	m-Ethyltoluene	1	30	0.3673	16.427	0.0603	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	7	m-Ethyltoluene	1	28	0.5429	55.101	0.2991	0.09
P	8	m-Ethyltoluene	9	1	11.9400	.	.	.
P	1	n-Butane	1	30	2.0557	0.567	0.0117	0.00
P	1	n-Butane	4	30	4.2970	0.807	0.0347	0.00
P	1	n-Butane	9	26	9.6196	0.655	0.0630	0.00
P	2	n-Butane	1	30	1.9405	1.586	0.0308	0.00
P	2	n-Butane	4	30	4.0592	1.688	0.0685	0.00
P	2	n-Butane	9	25	9.0540	1.099	0.0995	0.01
P	3	n-Butane	1	30	1.7359	7.009	0.1217	0.01
P	3	n-Butane	4	30	3.8429	2.783	0.1069	0.01
P	3	n-Butane	9	25	9.2885	2.354	0.2187	0.05
P	4	n-Butane	1	29	2.1200	10.641	0.2256	0.05
P	4	n-Butane	4	30	4.8467	9.493	0.4601	0.21
P	4	n-Butane	9	26	11.1758	9.626	1.0758	1.16
P	5	n-Butane	1	33	0.9798	26.267	0.2574	0.07
P	5	n-Butane	4	33	2.1489	25.654	0.5513	0.30
P	5	n-Butane	9	33	6.7312	42.396	2.8538	8.14
P	6	n-Butane	1	30	0.6077	51.987	0.3159	0.10
P	6	n-Butane	4	30	4.1697	31.928	1.3313	1.77
P	6	n-Butane	9	25	8.4616	34.395	2.9104	8.47
P	7	n-Butane	1	30	1.4270	40.315	0.5753	0.33
P	7	n-Butane	4	28	2.6718	47.037	1.2567	1.58
P	7	n-Butane	9	23	5.1204	64.497	3.3025	10.91
P	8	n-Butane	1	22	1.8777	6.342	0.1191	0.01
P	8	n-Butane	4	22	4.1464	4.917	0.2039	0.04
P	8	n-Butane	9	28	7.5996	28.888	2.1954	4.82
P	1	n-Hexane	1	30	0.9983	0.748	0.0075	0.00
P	1	n-Hexane	4	30	4.6853	0.665	0.0312	0.00
P	1	n-Hexane	9	26	10.4900	0.552	0.0579	0.00
P	2	n-Hexane	1	30	1.0035	2.110	0.0212	0.00
P	2	n-Hexane	4	30	4.2402	3.446	0.1461	0.02
P	2	n-Hexane	9	25	9.7574	12.921	1.2607	1.59
P	3	n-Hexane	1	30	0.6827	10.351	0.0707	0.00
P	3	n-Hexane	4	30	3.6439	2.888	0.1052	0.01
P	3	n-Hexane	9	25	8.9592	2.243	0.2010	0.04
P	4	n-Hexane	1	29	0.8707	10.382	0.0904	0.01
P	4	n-Hexane	4	30	4.1563	10.164	0.4224	0.18
P	4	n-Hexane	9	26	9.2219	11.299	1.0420	1.09
P	5	n-Hexane	1	33	1.0506	25.507	0.2680	0.07
P	5	n-Hexane	4	33	3.9324	24.596	0.9672	0.94
P	5	n-Hexane	9	33	7.3961	42.354	3.1326	9.81

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	6	n-Hexane	1	30	0.3817	14.369	0.0548	0.00
P	6	n-Hexane	4	30	2.5123	8.270	0.2078	0.04
P	6	n-Hexane	9	25	8.3832	28.053	2.3517	5.53
P	7	n-Hexane	1	28	6.1354	68.232	4.1863	17.53
P	7	n-Hexane	4	30	6.4683	100.557	6.5044	42.31
P	7	n-Hexane	9	11	5.8745	67.021	3.9372	15.50
P	8	n-Hexane	1	8	0.2650	35.571	0.0943	0.01
P	8	n-Hexane	4	18	2.1061	43.187	0.9096	0.83
P	8	n-Hexane	9	20	4.8915	25.929	1.2683	1.61
P	1	n-Pentane	1	30	1.0093	0.634	0.0064	0.00
P	1	n-Pentane	4	30	4.2527	0.586	0.0249	0.00
P	1	n-Pentane	9	26	9.5035	0.292	0.0277	0.00
P	2	n-Pentane	1	30	1.0128	2.872	0.0291	0.00
P	2	n-Pentane	4	30	4.2007	1.407	0.0591	0.00
P	2	n-Pentane	9	25	9.2906	0.655	0.0609	0.00
P	3	n-Pentane	1	30	1.8315	5.886	0.1078	0.01
P	3	n-Pentane	4	30	7.5946	2.544	0.1932	0.04
P	3	n-Pentane	9	25	18.1203	2.431	0.4405	0.19
P	4	n-Pentane	1	29	1.4103	11.279	0.1591	0.03
P	4	n-Pentane	4	30	6.5200	9.235	0.6021	0.36
P	4	n-Pentane	9	26	14.7073	9.208	1.3542	1.83
P	5	n-Pentane	1	33	0.9637	25.768	0.2483	0.06
P	5	n-Pentane	4	33	3.7414	24.762	0.9264	0.86
P	5	n-Pentane	9	33	7.3078	41.576	3.0383	9.23
P	6	n-Pentane	1	30	0.5267	9.609	0.0506	0.00
P	6	n-Pentane	4	30	3.0547	18.726	0.5720	0.33
P	6	n-Pentane	9	25	7.7680	26.528	2.0607	4.25
P	7	n-Pentane	1	30	1.7170	33.567	0.5764	0.33
P	7	n-Pentane	4	30	3.5797	42.624	1.5258	2.33
P	7	n-Pentane	9	24	15.8979	309.885	49.2652	2427.06
P	8	n-Pentane	1	22	0.9159	6.052	0.0554	0.00
P	8	n-Pentane	4	22	3.8391	4.066	0.1561	0.02
P	8	n-Pentane	9	28	7.0707	29.413	2.0797	4.33
P	1	o-Ethyltoluene	1	30	0.8000	2.521	0.0202	0.00
P	2	o-Ethyltoluene	1	30	0.6758	4.001	0.0270	0.00
P	2	o-Ethyltoluene	4	30	0.2203	5.089	0.0112	0.00
P	2	o-Ethyltoluene	9	23	0.4796	28.703	0.1377	0.02
P	3	o-Ethyltoluene	1	30	0.6554	7.167	0.0470	0.00
P	3	o-Ethyltoluene	4	26	0.0072	67.753	0.0049	0.00
P	3	o-Ethyltoluene	9	10	0.0112	85.826	0.0096	0.00
P	4	o-Ethyltoluene	1	29	0.7245	13.582	0.0984	0.01

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	5	o-Ethyltoluene	1	33	0.9171	23.603	0.2165	0.05
P	5	o-Ethyltoluene	4	33	0.3222	20.367	0.0656	0.00
P	5	o-Ethyltoluene	9	31	0.5919	38.512	0.2280	0.05
P	6	o-Ethyltoluene	1	30	0.5270	19.871	0.1047	0.01
P	7	o-Ethyltoluene	1	30	0.7113	9.787	0.0696	0.00
P	7	o-Ethyltoluene	4	29	0.3338	61.608	0.2056	0.04
P	7	o-Ethyltoluene	9	20	0.4595	42.532	0.1954	0.04
P	8	o-Ethyltoluene	1	22	0.5373	28.663	0.1540	0.02
P	8	o-Ethyltoluene	4	22	0.4964	82.406	0.4090	0.17
P	8	o-Ethyltoluene	9	28	0.8746	69.905	0.6114	0.37
P	1	o-Xylene	1	30	0.6150	2.329	0.0143	0.00
P	1	o-Xylene	4	30	5.2613	0.795	0.0418	0.00
P	1	o-Xylene	9	26	11.8035	0.372	0.0439	0.00
P	2	o-Xylene	1	30	0.7250	3.455	0.0251	0.00
P	2	o-Xylene	4	30	5.9092	2.186	0.1292	0.02
P	2	o-Xylene	9	25	13.3572	1.229	0.1642	0.03
P	3	o-Xylene	1	30	0.5535	7.355	0.0407	0.00
P	3	o-Xylene	4	30	3.7008	2.614	0.0967	0.01
P	3	o-Xylene	9	25	8.9294	2.476	0.2211	0.05
P	4	o-Xylene	1	29	0.5565	22.703	0.1263	0.02
P	4	o-Xylene	4	30	3.8520	23.077	0.8889	0.79
P	4	o-Xylene	9	26	8.6986	6.459	0.5618	0.32
P	5	o-Xylene	1	33	0.9342	23.479	0.2193	0.05
P	5	o-Xylene	4	33	7.1222	21.228	1.5119	2.29
P	5	o-Xylene	9	33	14.5446	40.821	5.9373	35.25
P	6	o-Xylene	1	30	0.5787	16.912	0.0979	0.01
P	6	o-Xylene	4	30	3.1087	29.839	0.9276	0.86
P	6	o-Xylene	9	25	8.3940	43.945	3.6887	13.61
P	7	o-Xylene	1	30	0.6703	43.724	0.2931	0.09
P	7	o-Xylene	4	30	1.2550	44.817	0.5625	0.32
P	7	o-Xylene	9	25	1.8468	55.931	1.0329	1.07
P	8	o-Xylene	1	22	1.0127	22.420	0.2271	0.05
P	8	o-Xylene	4	22	5.8950	11.896	0.7013	0.49
P	8	o-Xylene	9	28	14.9932	19.450	2.9161	8.50
P	1	p-Ethyltoluene	1	30	0.8730	1.478	0.0129	0.00
P	1	p-Ethyltoluene	4	30	3.9053	0.969	0.0379	0.00
P	1	p-Ethyltoluene	9	26	9.1150	1.223	0.1115	0.01
P	2	p-Ethyltoluene	1	30	1.3215	5.949	0.0786	0.01
P	2	p-Ethyltoluene	4	30	3.9632	3.064	0.1214	0.01
P	2	p-Ethyltoluene	9	25	9.4226	3.422	0.3225	0.10
P	3	p-Ethyltoluene	1	30	0.8436	6.828	0.0576	0.00

TARGET	VENDORID	CMPDNAME	BENZLVL	N	MEAN	RSD	STDEV	VAR
P	3	p-Ethyltoluene	9	6	10.7488	1.786	0.1920	0.04
P	4	p-Ethyltoluene	1	29	0.9403	11.480	0.1080	0.01
P	6	p-Ethyltoluene	1	30	0.3670	16.241	0.0596	0.00
P	7	p-Ethyltoluene	1	30	0.8640	60.095	0.5192	0.27
P	7	p-Ethyltoluene	4	30	2.0230	55.487	1.1225	1.26
P	7	p-Ethyltoluene	9	25	3.5152	67.699	2.3798	5.66
P	8	p-Ethyltoluene	1	18	1.1306	59.061	0.6677	0.45
P	8	p-Ethyltoluene	4	21	5.5405	75.103	4.1611	17.31
P	8	p-Ethyltoluene	9	13	7.1646	24.992	1.7906	3.21
P	1	trans-2-Butene	1	30	1.2920	0.798	0.0103	0.00
P	1	trans-2-Butene	4	30	4.3013	1.337	0.0575	0.00
P	1	trans-2-Butene	9	26	9.6358	0.289	0.0279	0.00
P	2	trans-2-Butene	1	30	1.2202	2.852	0.0348	0.00
P	2	trans-2-Butene	4	30	4.9810	9.849	0.4906	0.24
P	2	trans-2-Butene	9	25	11.3068	6.594	0.7456	0.56
P	3	trans-2-Butene	1	30	1.2202	7.468	0.0911	0.01
P	3	trans-2-Butene	4	30	3.8271	3.320	0.1271	0.02
P	3	trans-2-Butene	9	25	9.2791	2.874	0.2667	0.07
P	4	trans-2-Butene	1	29	1.2528	11.776	0.1475	0.02
P	4	trans-2-Butene	4	30	4.7203	9.970	0.4706	0.22
P	4	trans-2-Butene	9	26	10.8350	10.162	1.1011	1.21
P	5	trans-2-Butene	1	32	0.9485	24.335	0.2308	0.05
P	5	trans-2-Butene	4	33	3.1959	24.870	0.7948	0.63
P	5	trans-2-Butene	9	33	6.8746	43.763	3.0085	9.05
P	6	trans-2-Butene	1	30	0.6077	51.987	0.3159	0.10
P	6	trans-2-Butene	4	30	4.1697	31.928	1.3313	1.77
P	6	trans-2-Butene	9	25	8.4616	34.395	2.9104	8.47
P	7	trans-2-Butene	1	30	0.9207	58.122	0.5351	0.29
P	7	trans-2-Butene	4	30	2.4277	56.681	1.3760	1.89
P	7	trans-2-Butene	9	25	4.5552	69.679	3.1740	10.07
P	8	trans-2-Butene	1	22	1.2200	5.270	0.0643	0.00
P	8	trans-2-Butene	4	22	4.2464	3.775	0.1603	0.03
P	8	trans-2-Butene	9	23	7.2796	31.362	2.2830	5.21

Appendix B Box and Whisker Comparison of Bias Estimates Across Vendors for Individual Target Analytes.

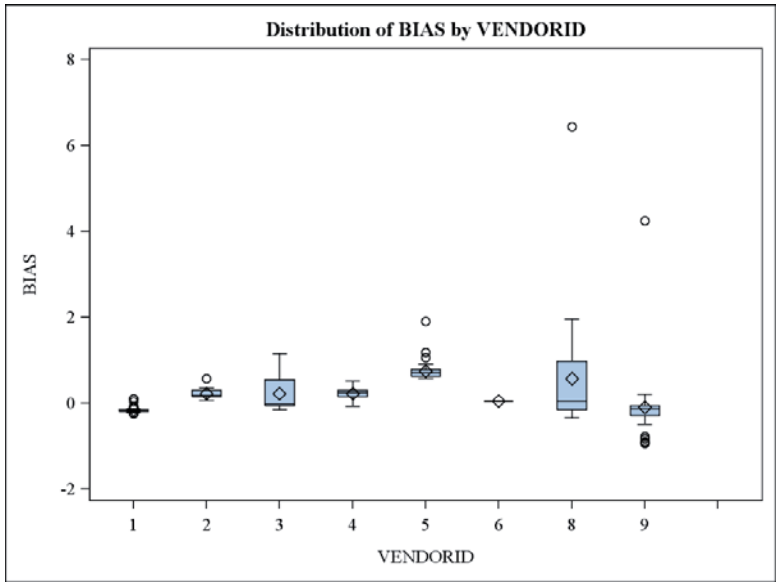


Figure B-1: Distribution of bias for optional target 1,3,5-Trimethylbenzene

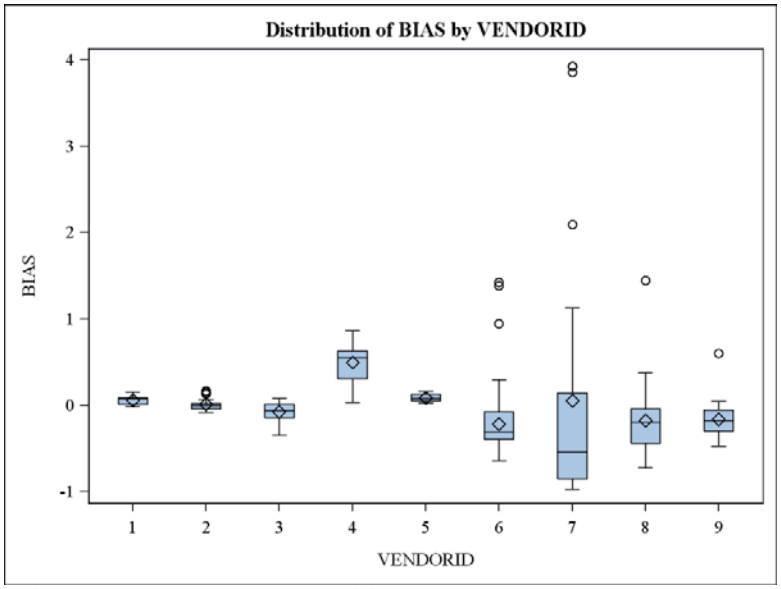


Figure B-2: Distribution of bias for optional target 1-Pentene

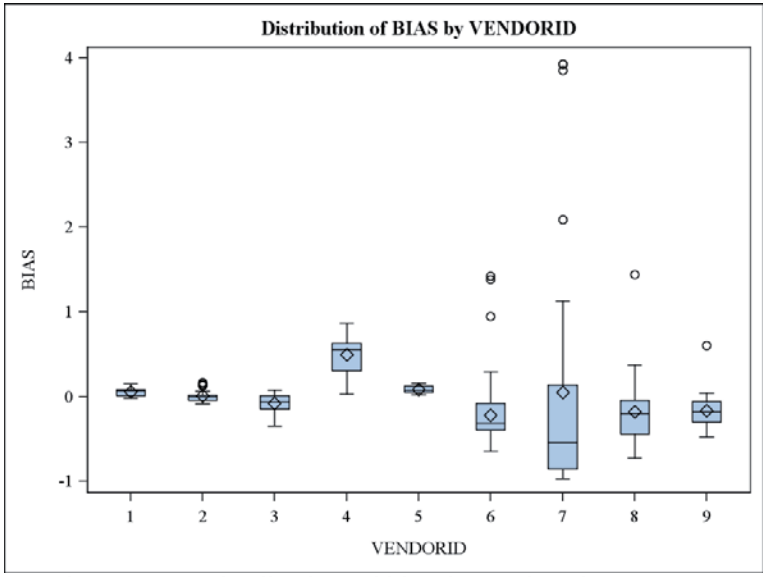


Figure B-3: Distribution of bias for optional target 2,2-Dimethylbutane

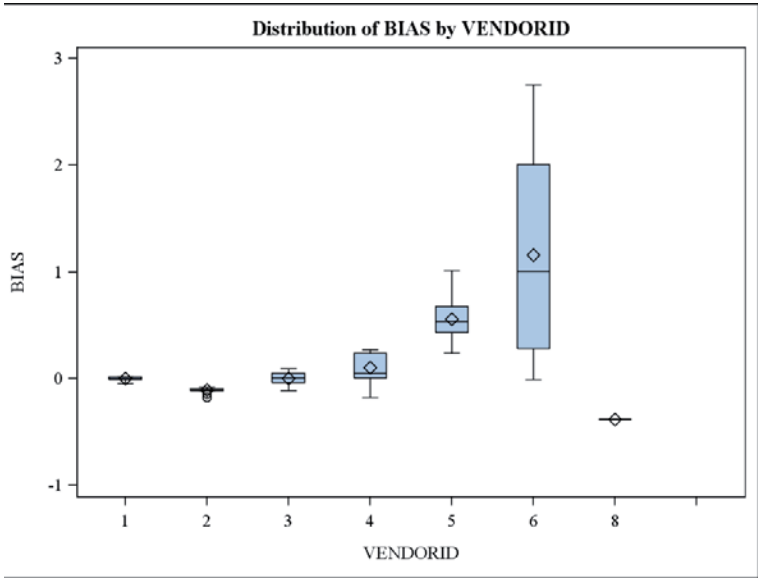


Figure B-4: Distribution of bias for optional target 2,3,4-Trimethylpentane

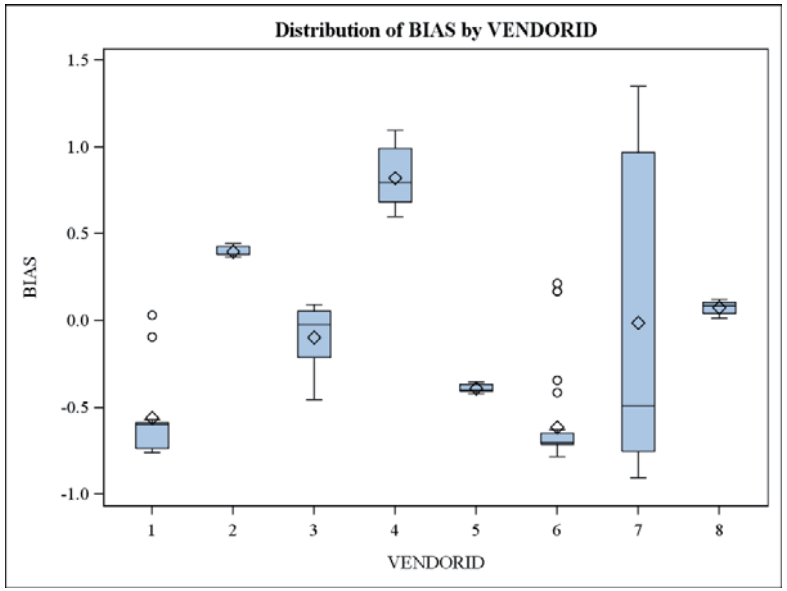


Figure B-5: Distribution of bias for optional target 2,3-Dimethylbutane

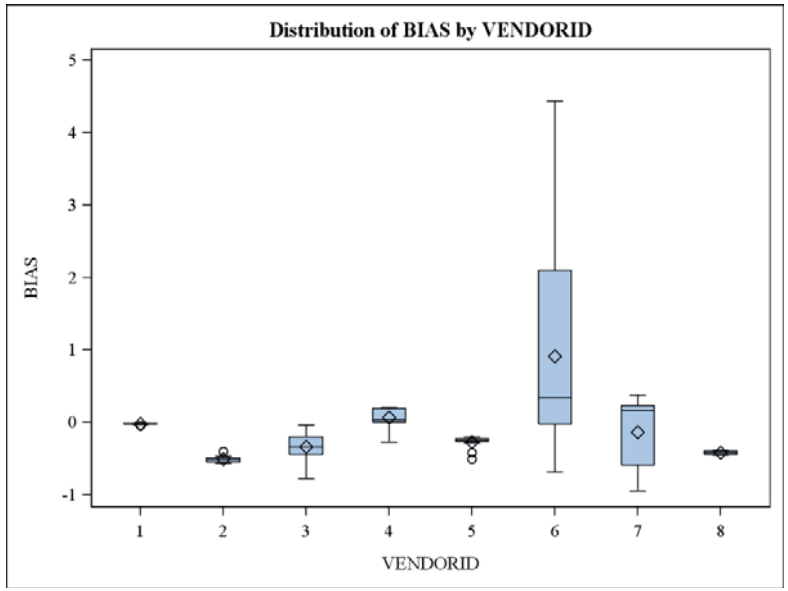


Figure B-6: Distribution of bias for optional target 2,3-Dimethylpentane

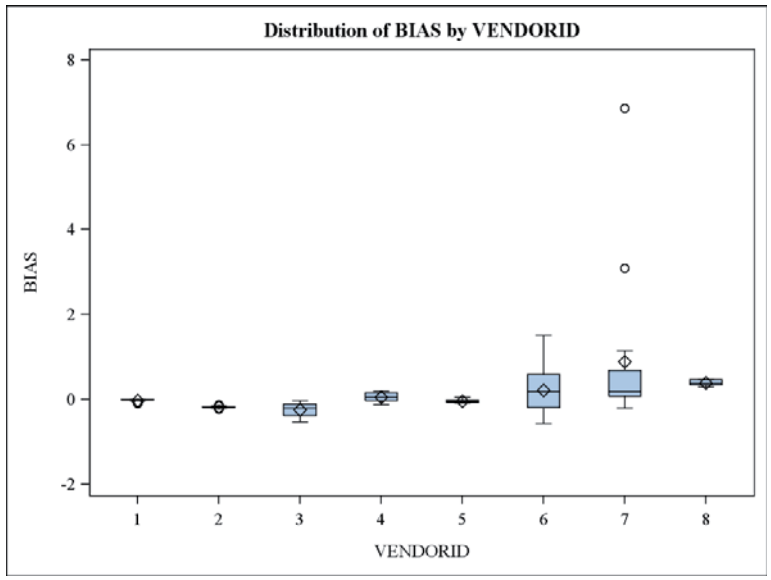


Figure B-7: Distribution of bias for optional target 2,4-Dimethylpentane

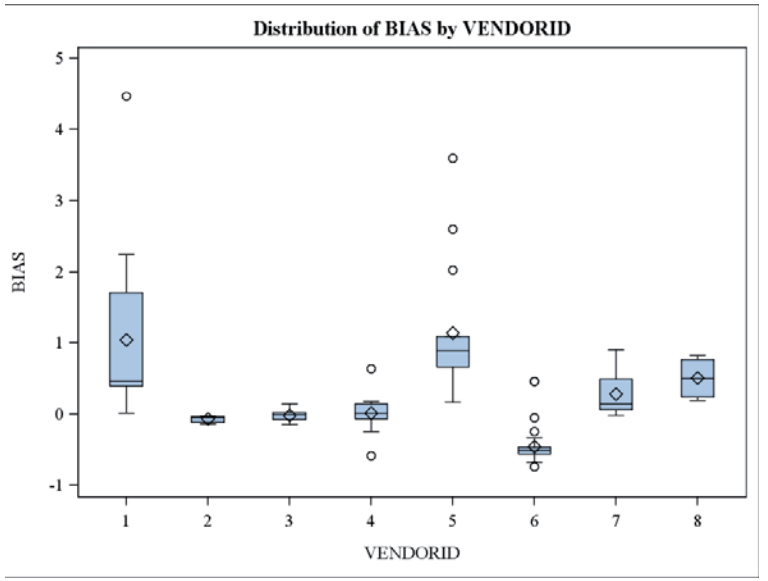


Figure B-8: Distribution of bias for optional target 2-Methylheptane

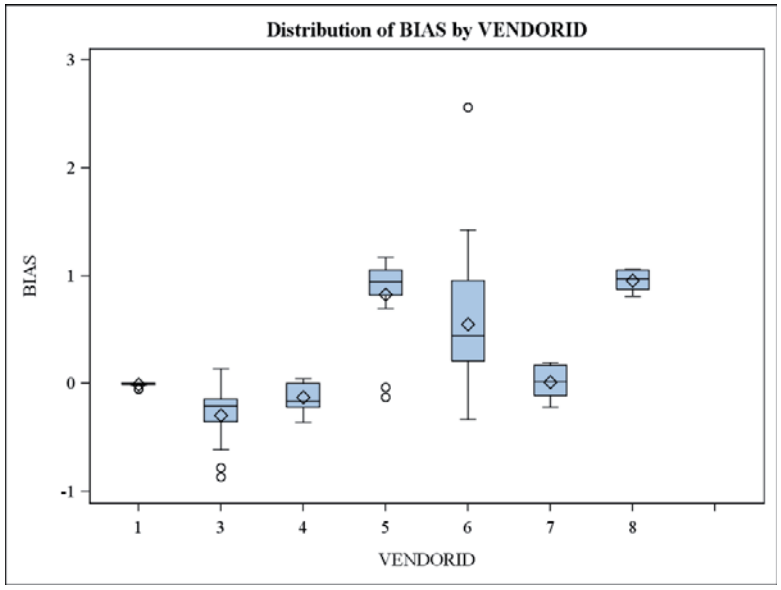


Figure B-9: Distribution of bias for optional target 2-Methylhexane

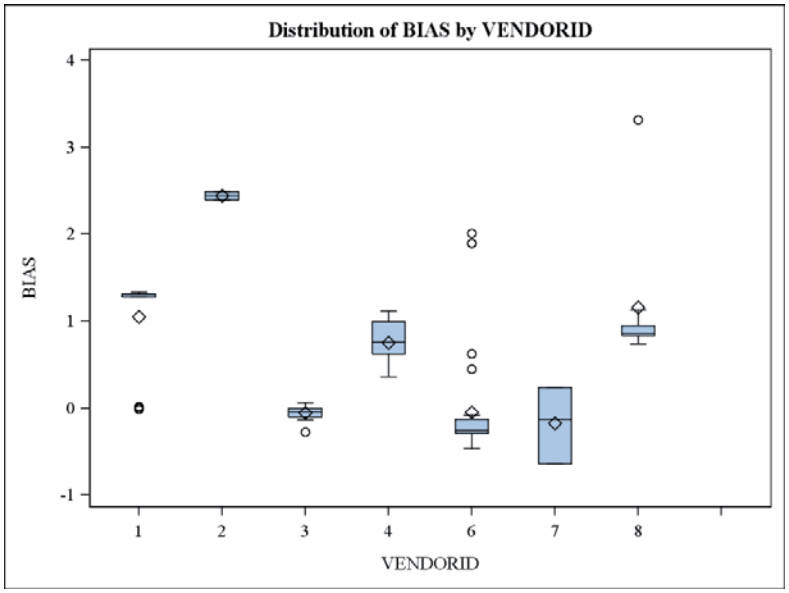


Figure B-10: Distribution of bias for optional target 2-Methylpentane

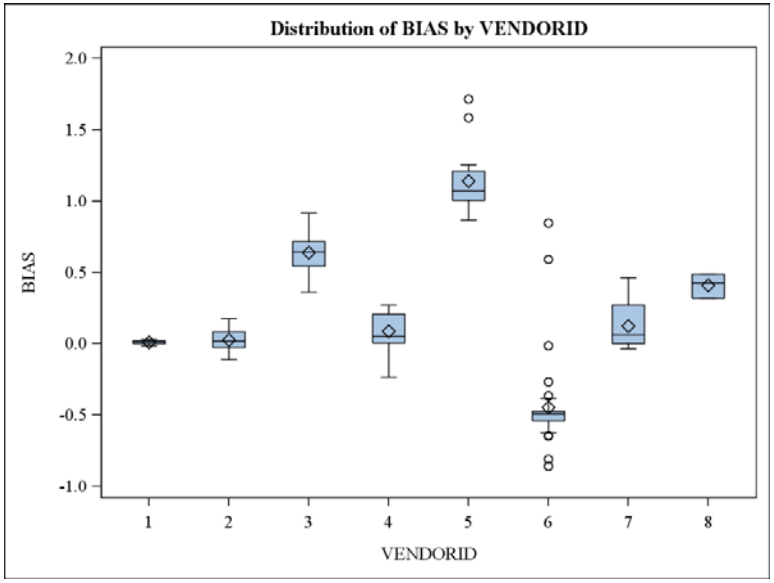


Figure B-11: Distribution of bias for optional target 3-Methylheptane

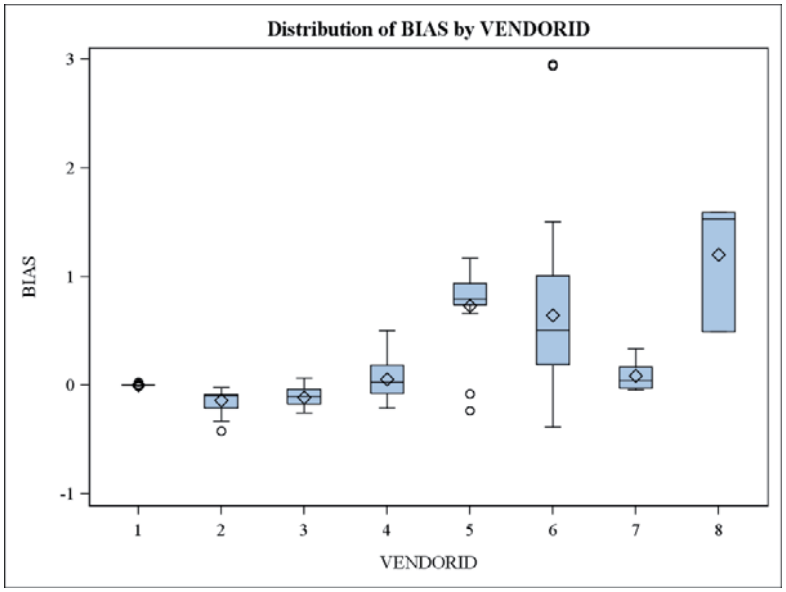


Figure B-12: Distribution of bias for target 3-Methylhexane

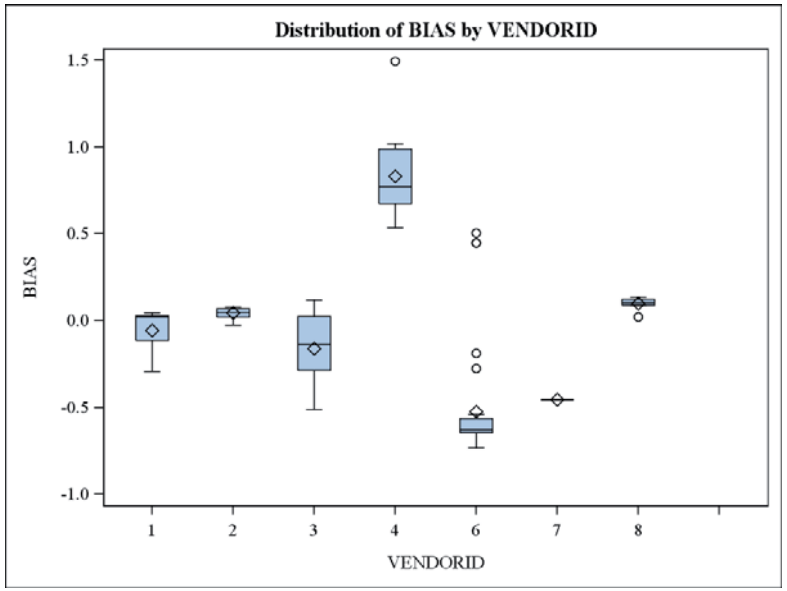


Figure B-13: Distribution of bias for optional target 3-Methylpentane

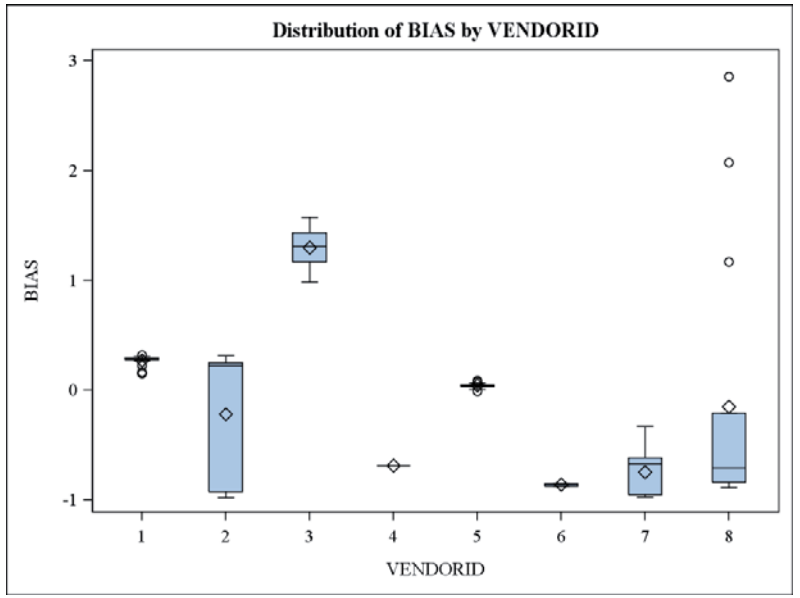


Figure B-14: Distribution of bias for optional target Acetylene

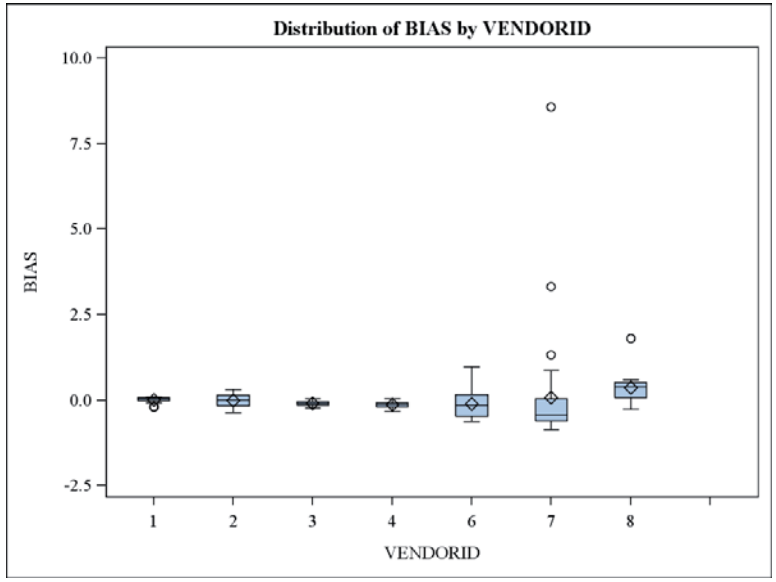


Figure B-15: Distribution of bias for optional target Cyclohexane

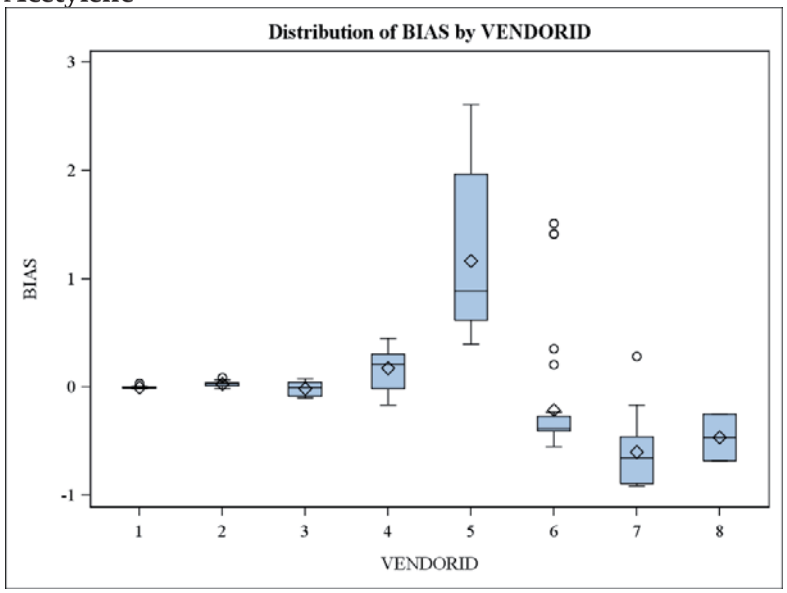


Figure B-16: Distribution of bias for target Cyclopentane

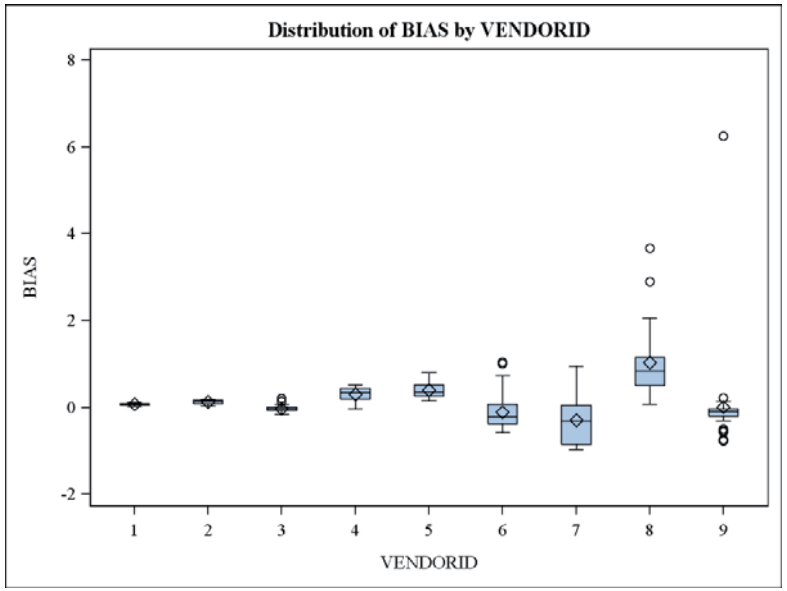


Figure B-17: Distribution for optional target Isopropylbenzene

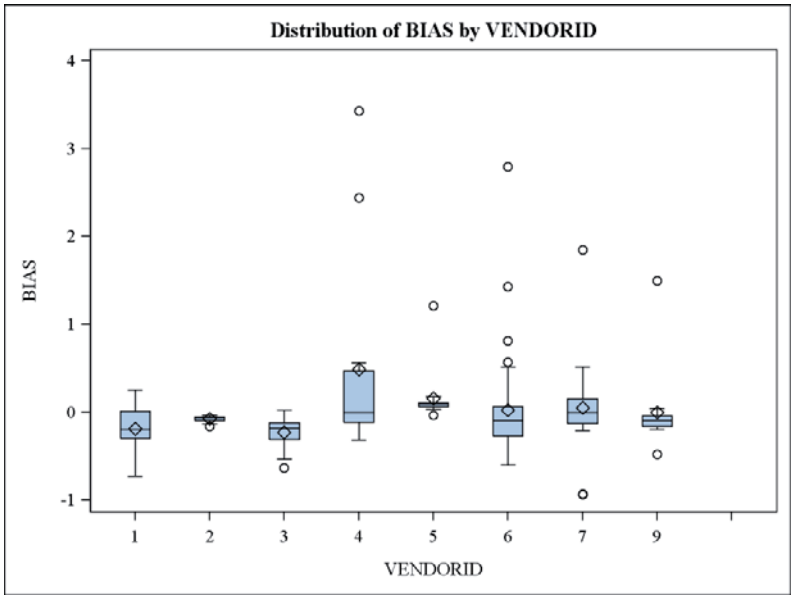


Figure B-18: Distribution of bias for optional target Methylcyclohexane

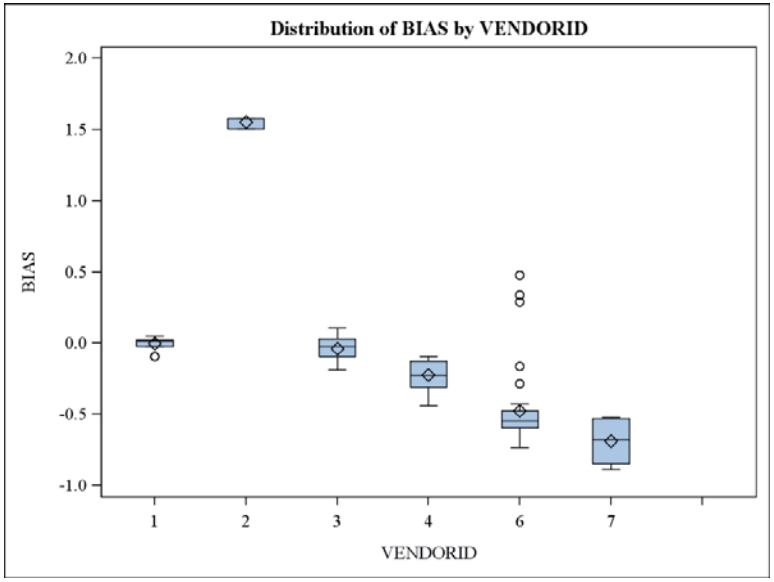


Figure B-19: Distribution of bias for optional target Methylcyclopentane

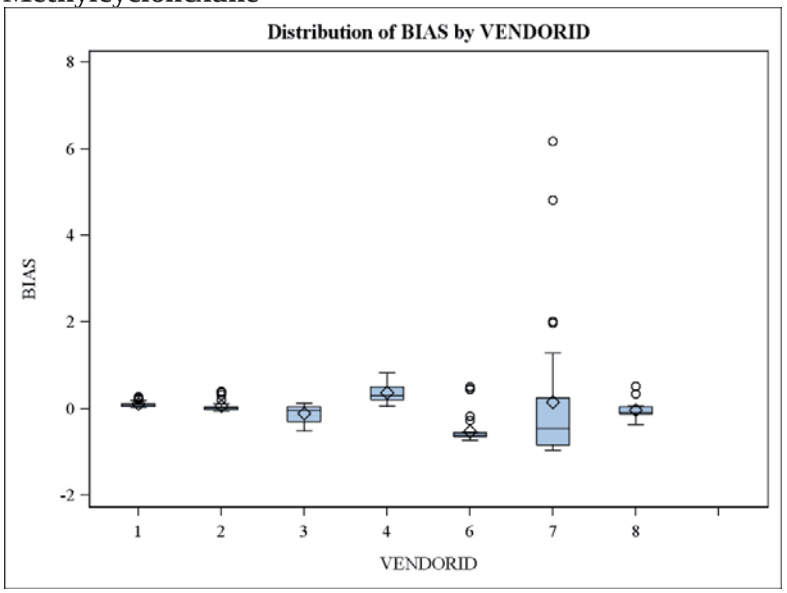


Figure B-20: Distribution of bias for optional target cis-2-Pentene

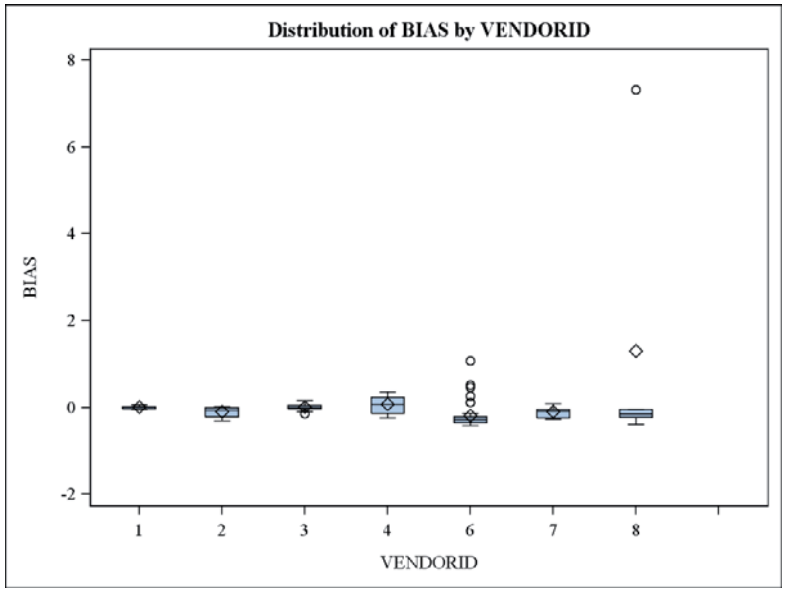


Figure B-21: Distribution of bias for optional target m-Diethylbenzene

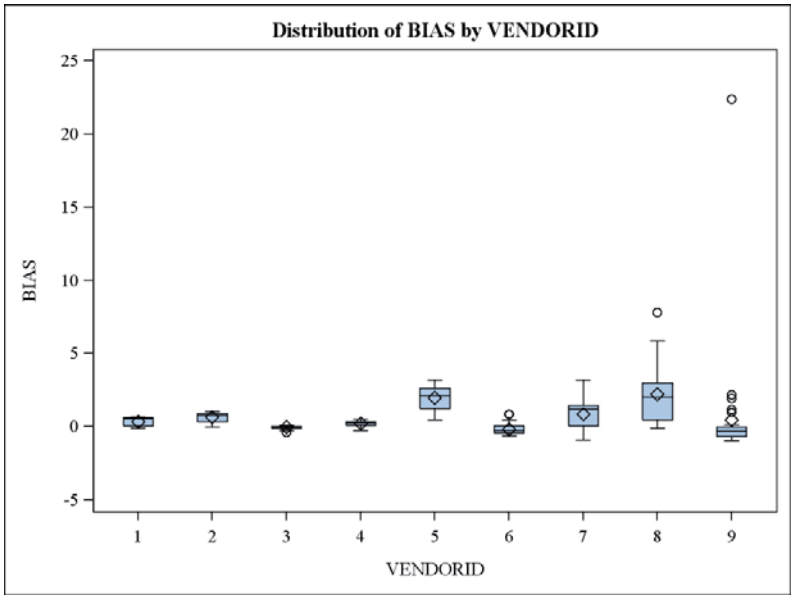


Figure B-22: Distribution of bias for optional target n-Decane

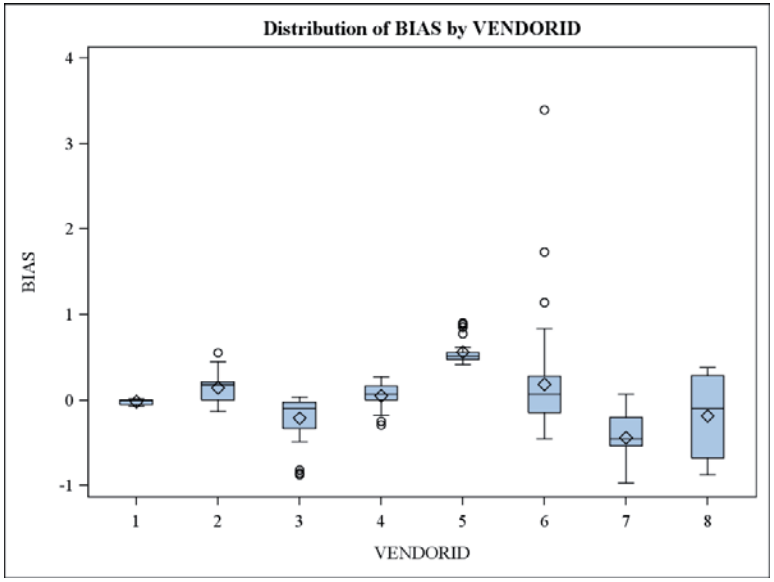


Figure B-23: Distribution of bias for optional target n-Heptane

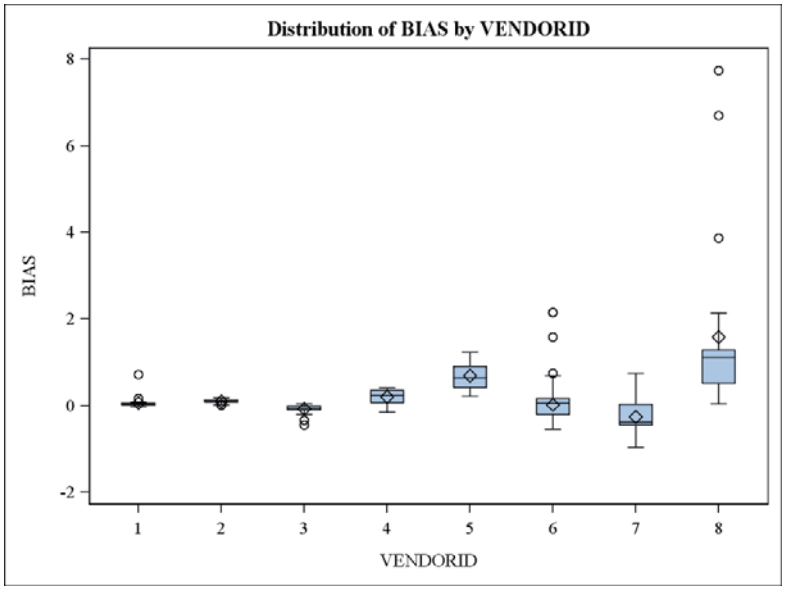


Figure B-24: Distribution of bias for optional target n-Nonane

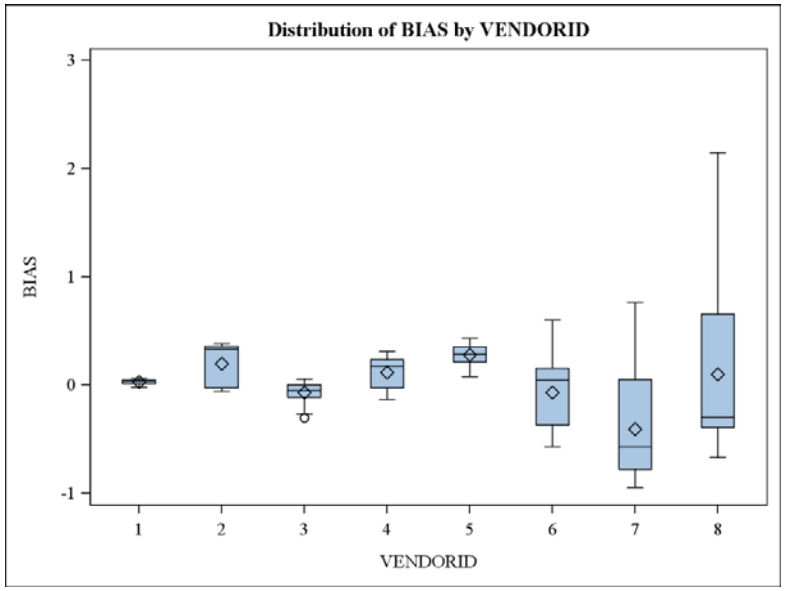


Figure B-25: Distribution of bias for optional target n-Octane

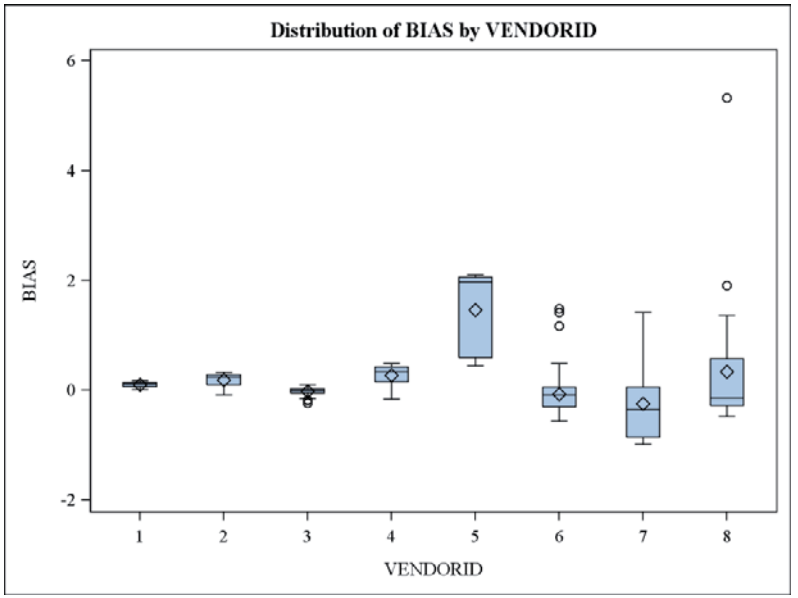


Figure B-26: Distribution of bias for optional target n-Propylbenzene

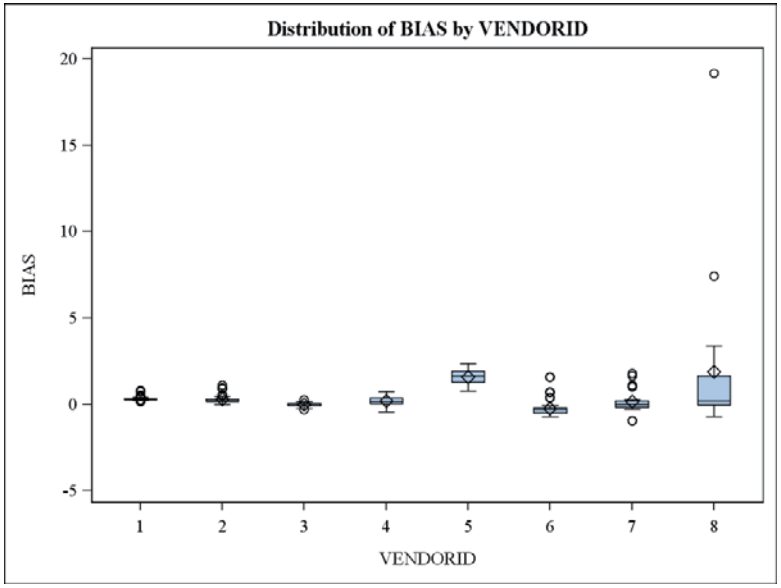


Figure B-27: Distribution of bias for optional target n-Undecane

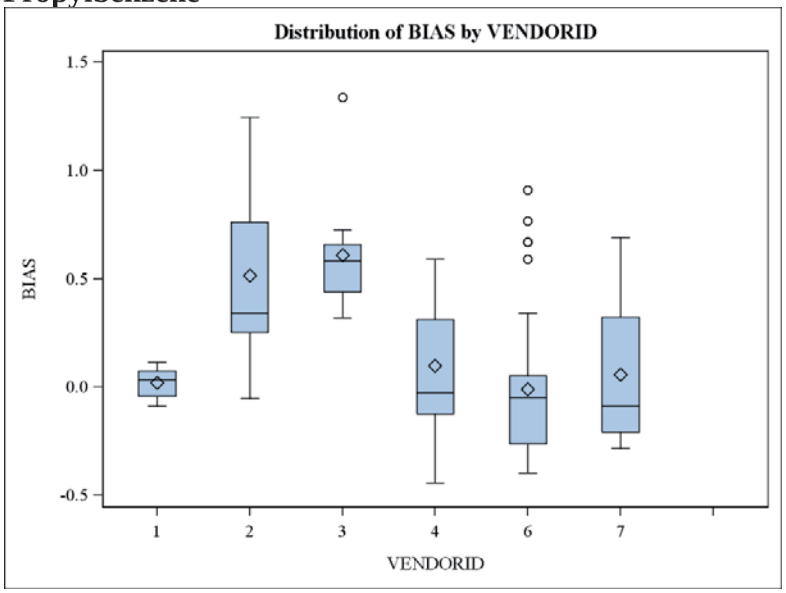


Figure B-28: Distribution of bias for target p-Diethylbenzene

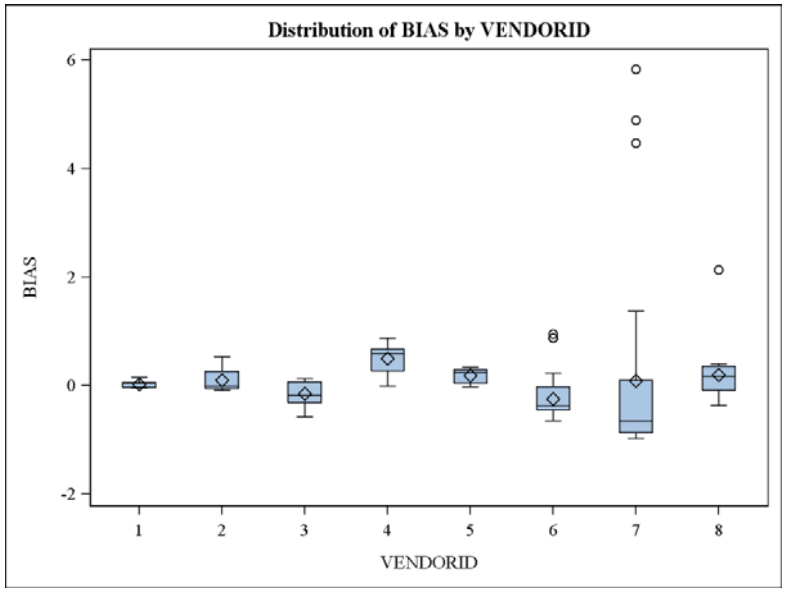


Figure B-29: Distribution of bias for optional target trans-2-Pentene

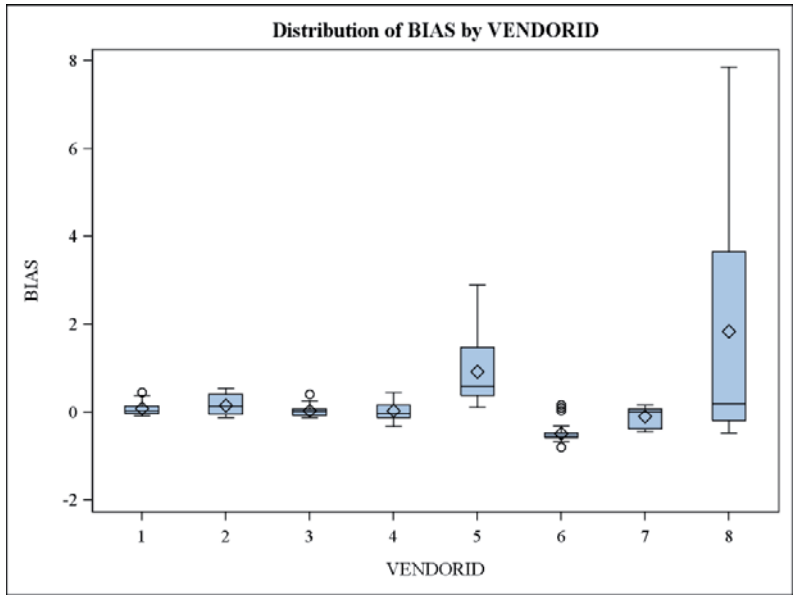


Figure B-30: Distribution of bias for priority target 1,2,3-Trimethylbenzene

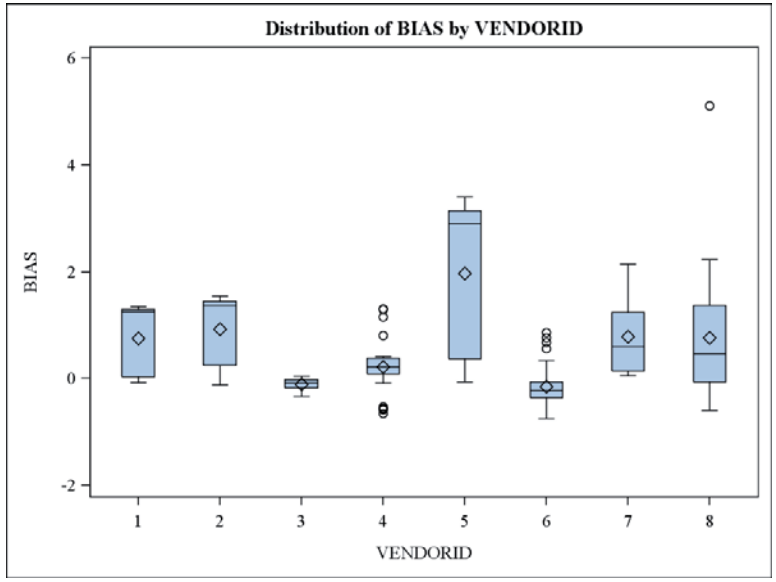


Figure B-31: Distribution of bias for priority target 1,2,4-Trimethylbenzene

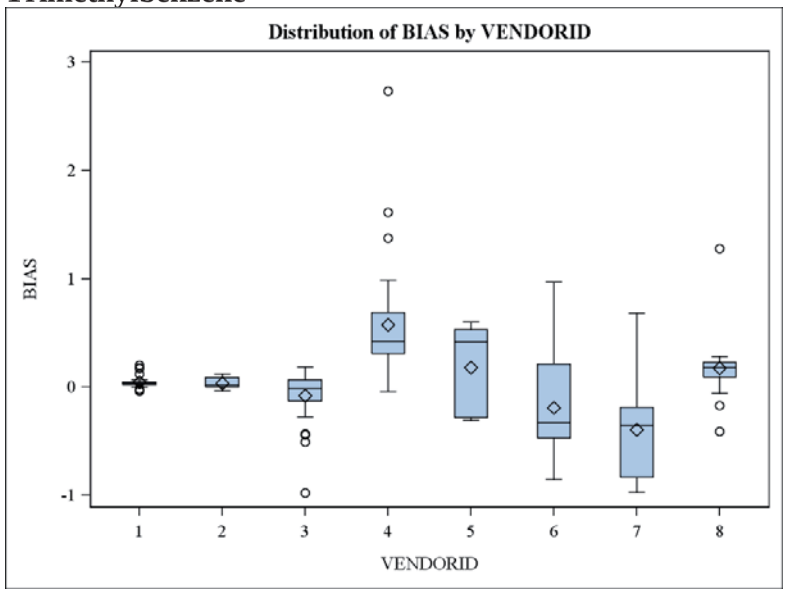


Figure B-32: Distribution of bias for priority target 1-Butene

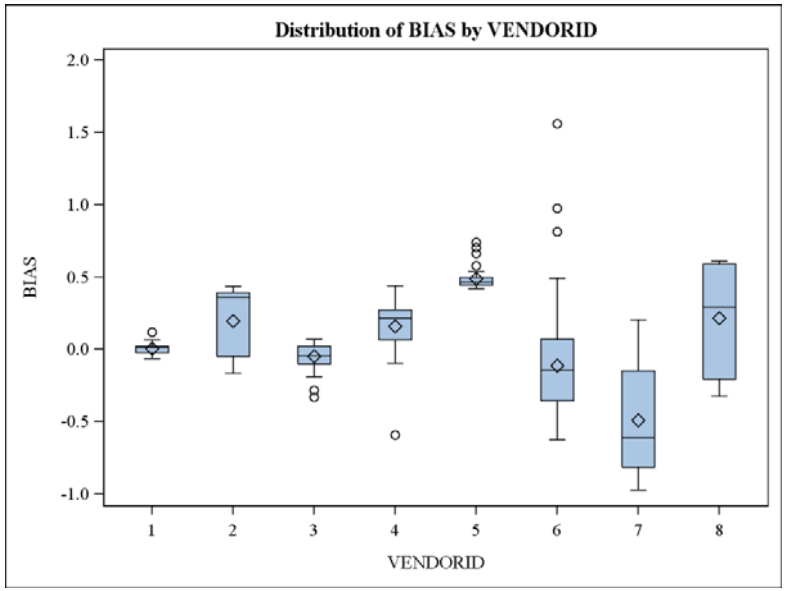


Figure B-33: Distribution of bias for priority target 2,2,4-Trimethlpentane

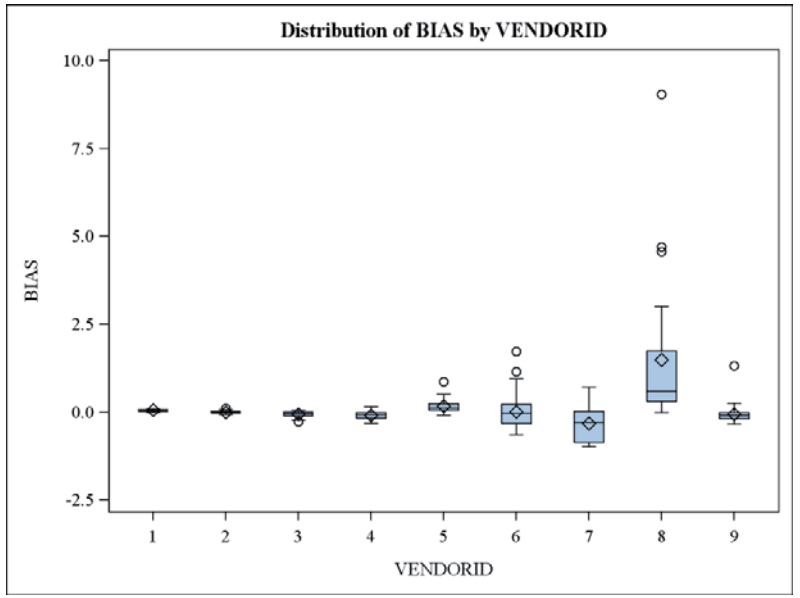


Figure B-34: Distribution of bias for priority target Benzene

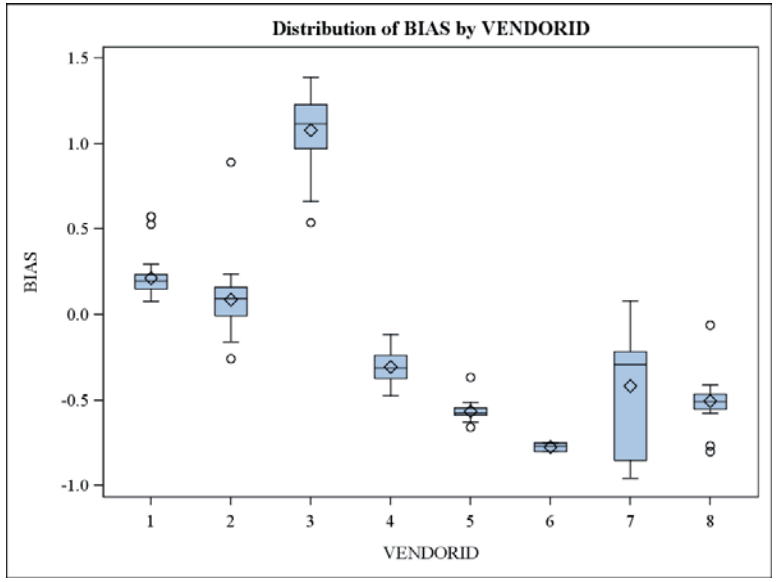


Figure B-35: Distribution of bias for priority target Ethane

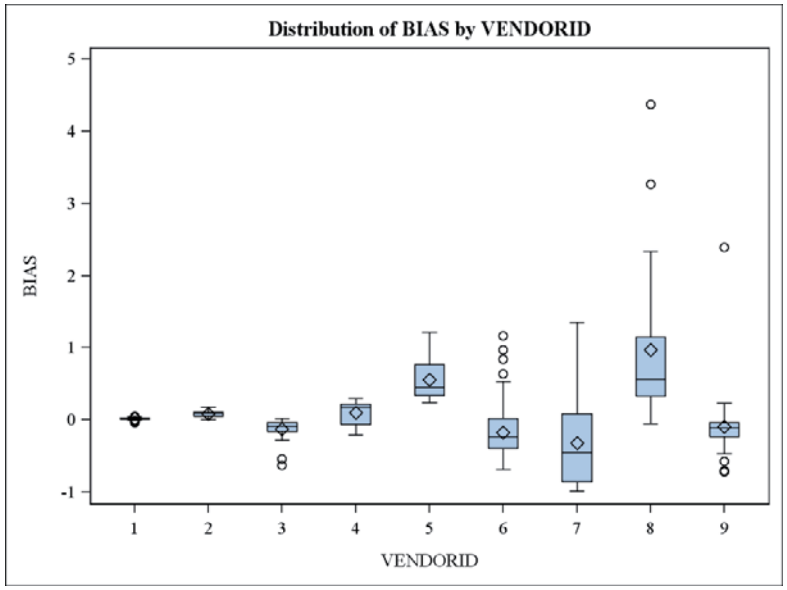


Figure: B-36: Distribution of bias for priority target Ethylbenzene

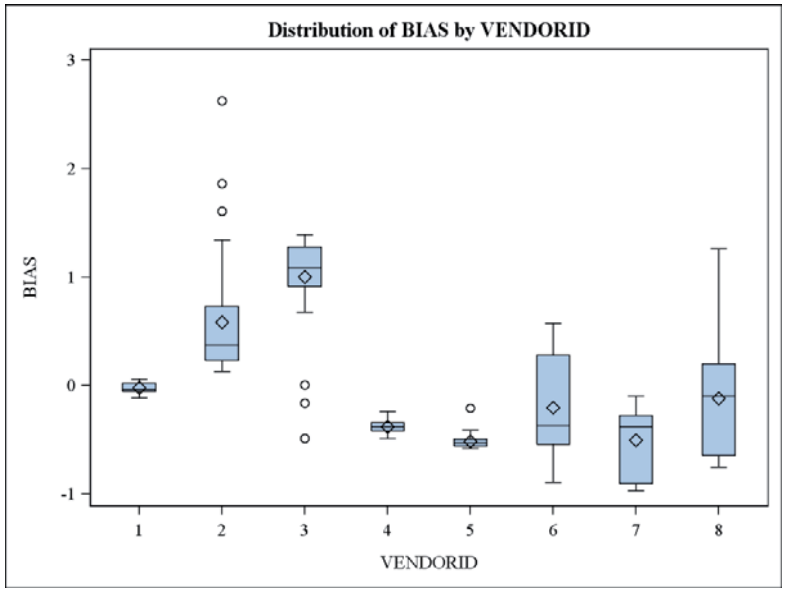


Figure B-37: Distribution of bias for priority target Ethylene

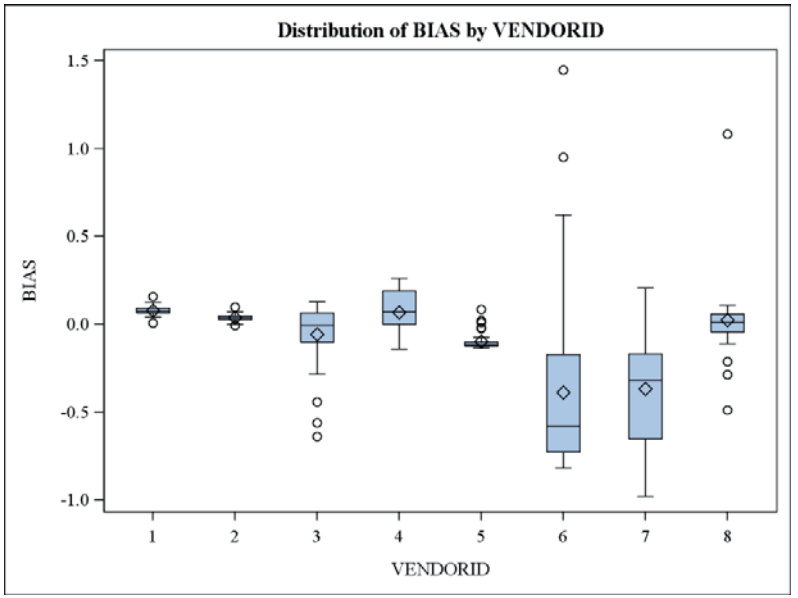


Figure B-38: Distribution of bias for priority target Isobutane

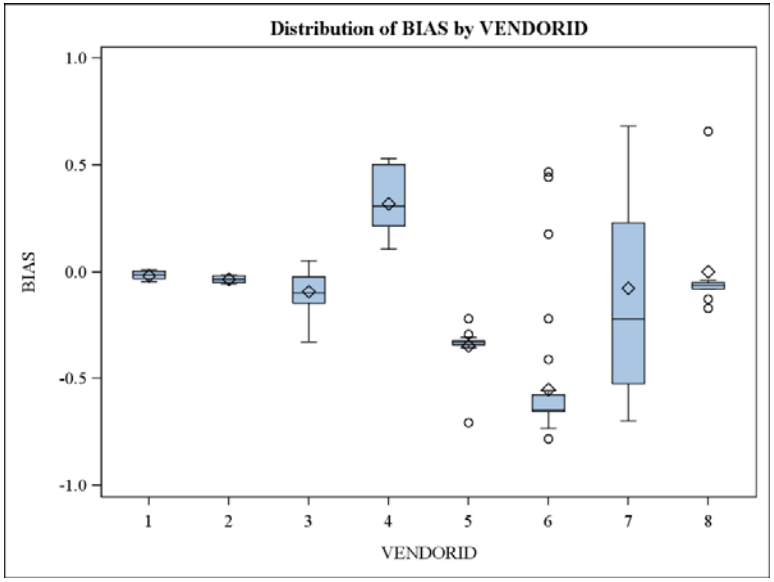


Figure B-39: Distribution of bias for priority target Isopentane

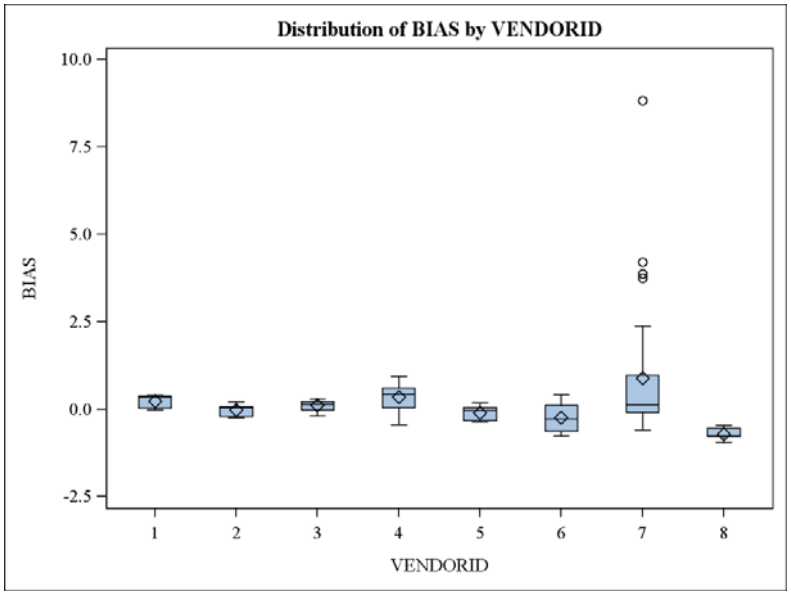


Figure B-40: Distribution of bias for priority target Isoprene

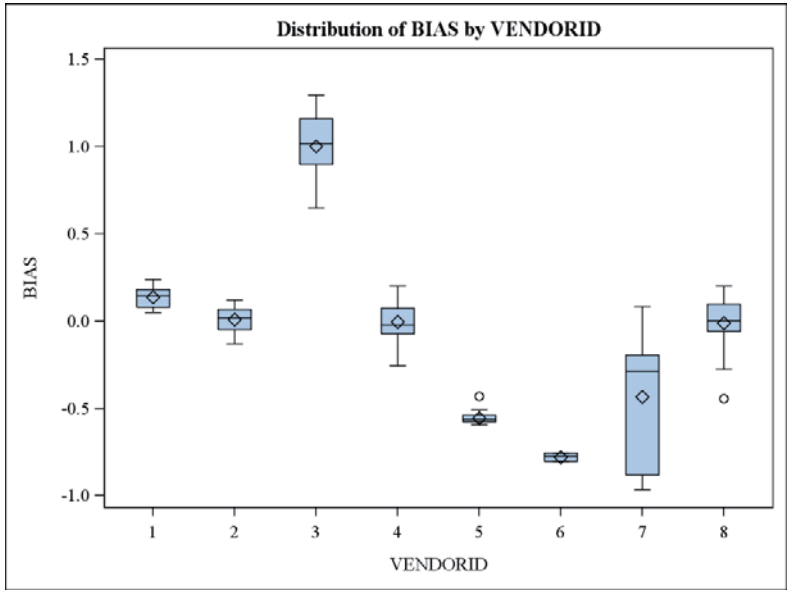


Figure B-41: Distribution of bias for priority target Propane

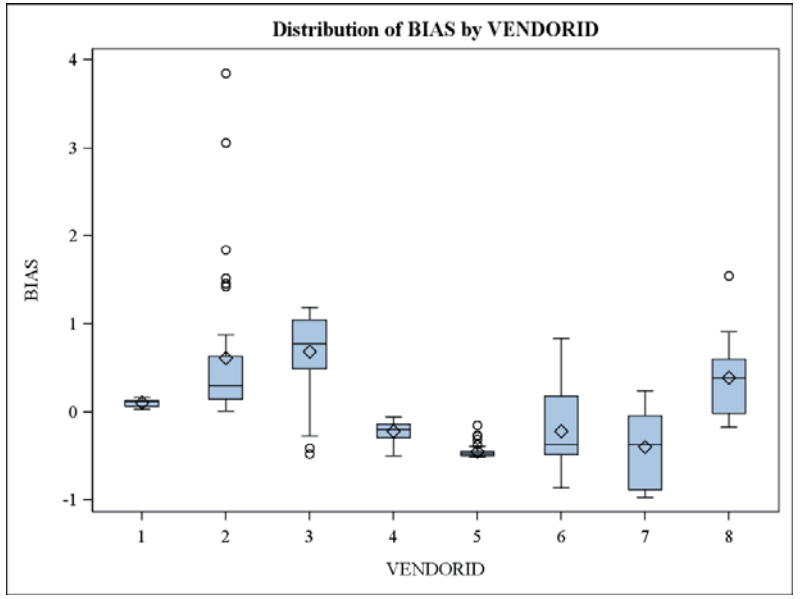


Figure B-42: Distribution of bias for priority target Propylene

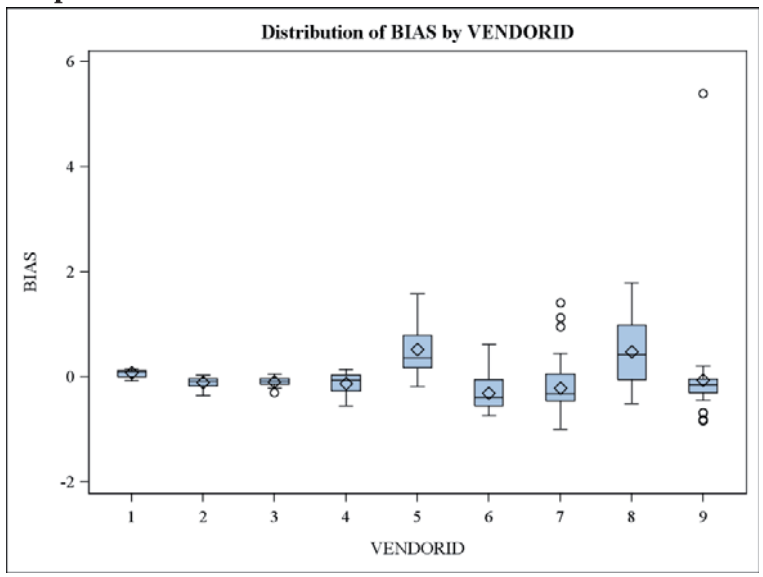


Figure B-43: Distribution of bias for priority target Styrene

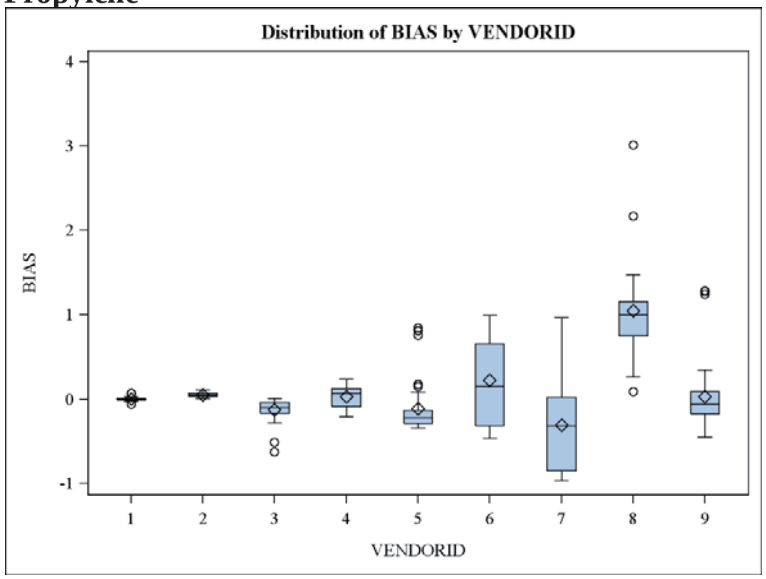


Figure B-44: Distribution of bias for priority target Toluene

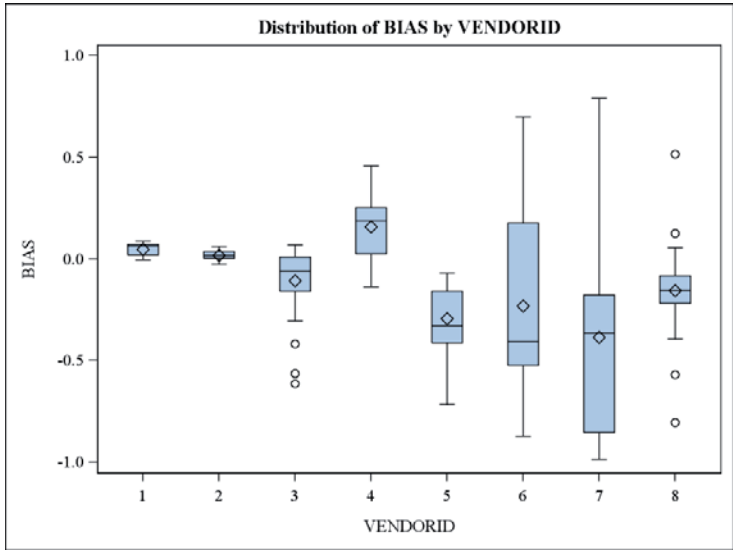


Figure B-45: Distribution of bias for priority target cis-2-Butene

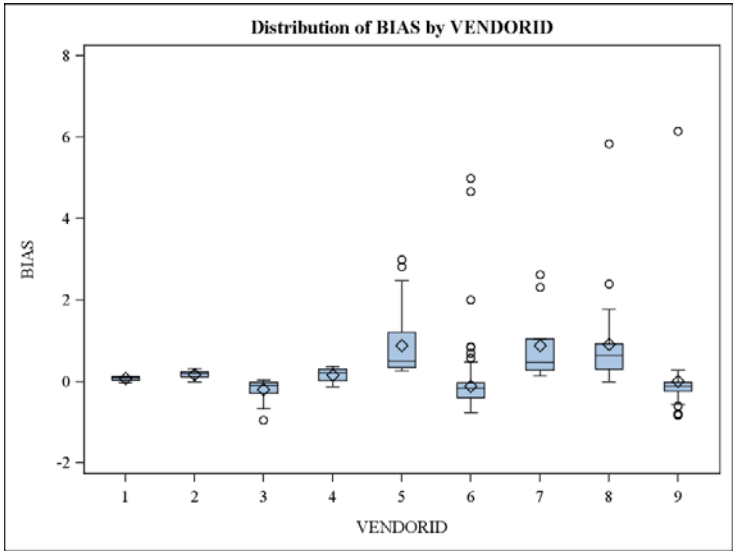


Figure B-46: Distribution of bias for priority target m,p-Xylene

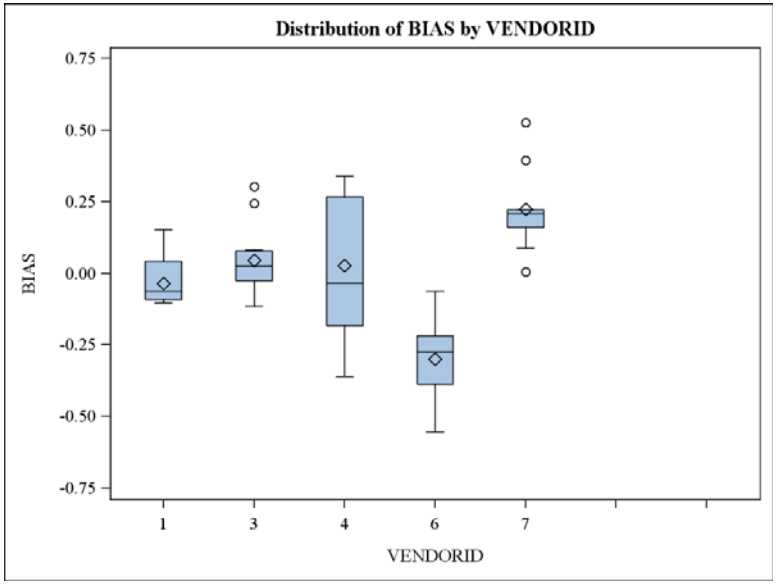


Figure B-47: Distribution of bias for priority target m-Ethyltoluene

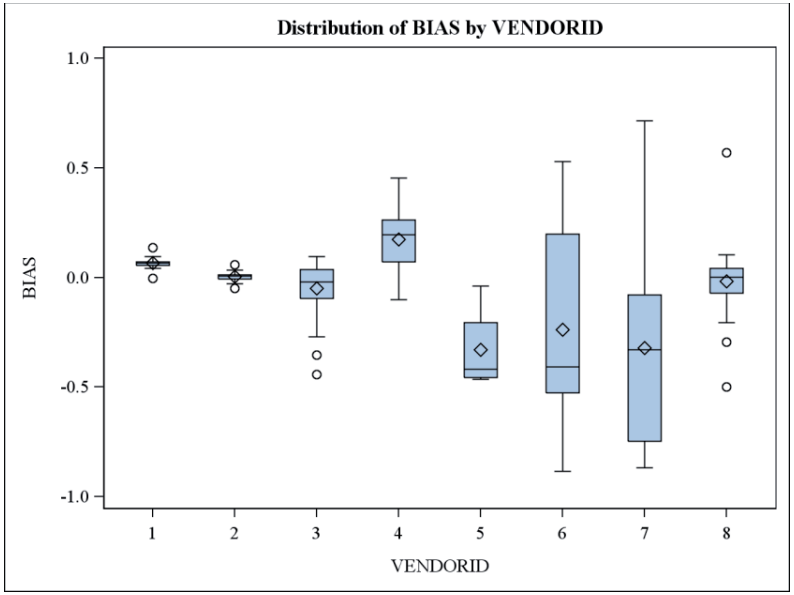


Figure B-48: Distribution of bias for priority target n-Butane

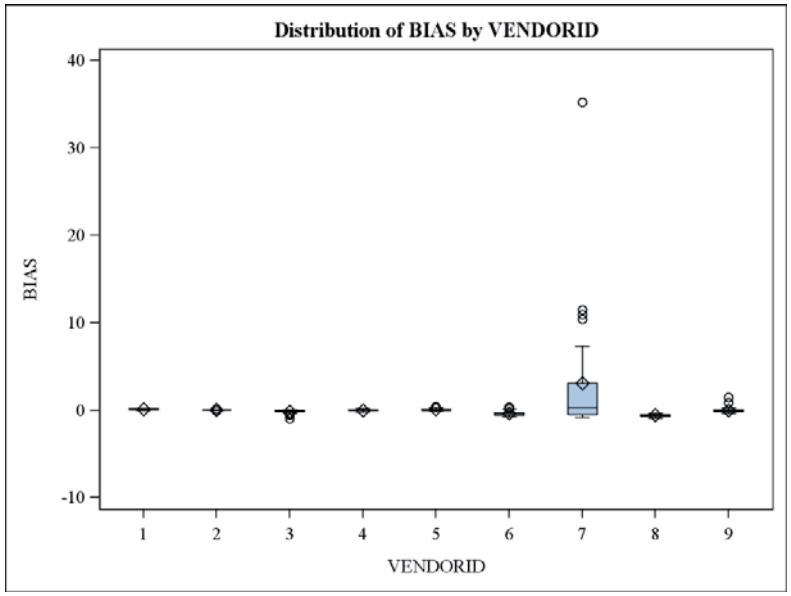


Figure B-49: Distribution of bias for priority target n-Hexane

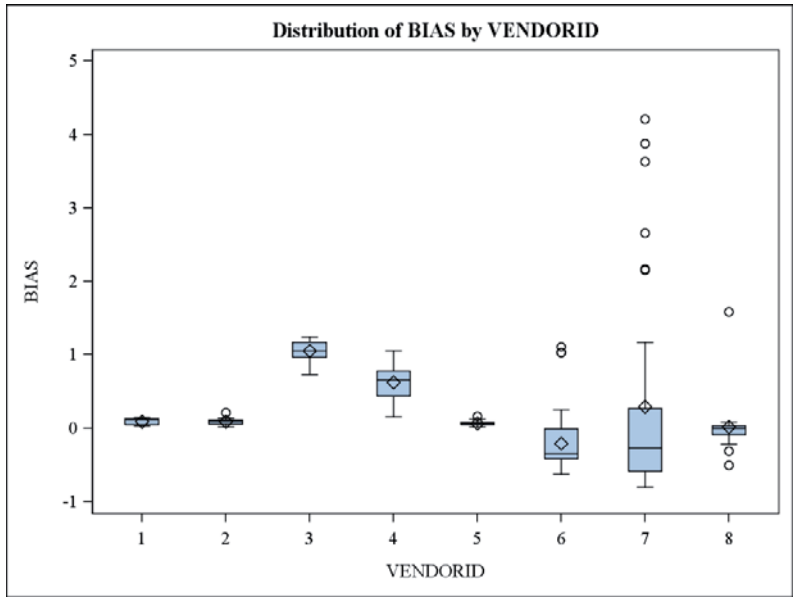


Figure B-50: Distribution of bias for priority target n-Pentane

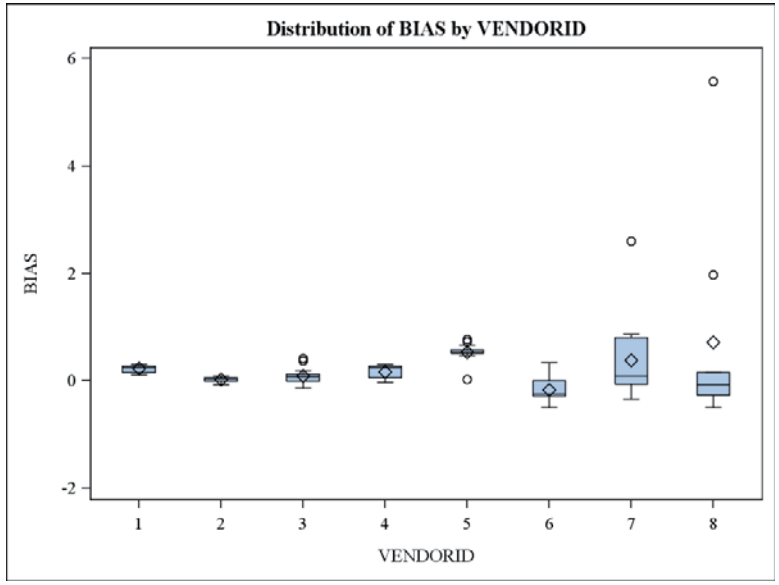


Figure B-51: Distribution of bias for priority target o-Ethyltoluene

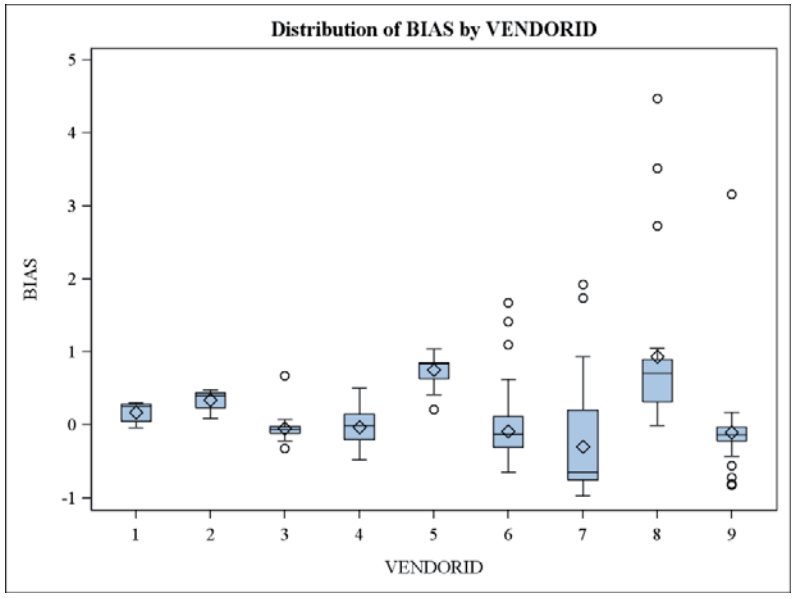


Figure B-52: Distribution of bias for priority target o-Xylene

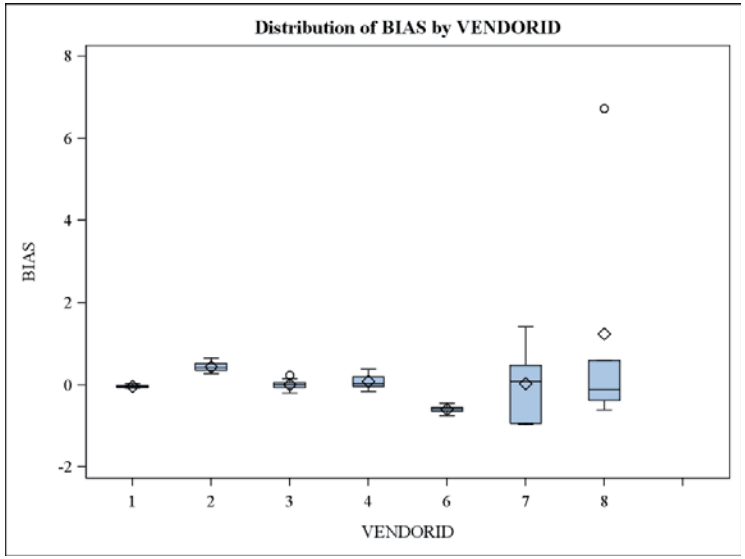


Figure B-53: Distribution of bias for priority target Ethyltoluene

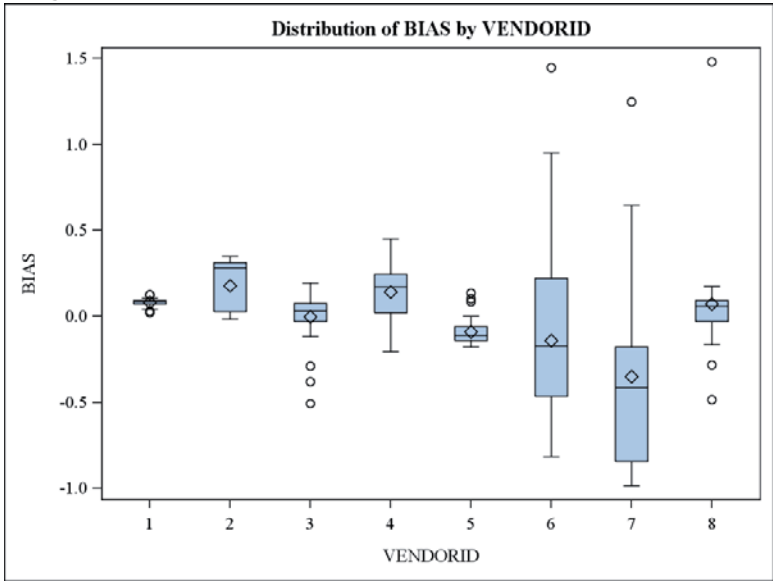


Figure B-54: Distribution of %bias for priority target 2-butene

Table B1 Descriptive Statistics for Bias – All Vendors

TARGET	CMPDNAME	n	mean	stddev	min	p25	median	p75	p90	max
O	1,3,5-Trimethylbenzene	239	0.23125	0.64050	-0.93407	-0.10444	0.12215	0.44667	0.72139	6.4400
O	1-Pentene	373	-0.02991	0.51428	-0.97028	-0.30449	-0.04550	0.07604	0.31154	3.9282
O	2,2-Dimethylbutane	114	-0.02823	0.52694	-0.83762	-0.57190	-0.00767	0.46143	0.66810	1.0667
O	2,3,4-Trimethylpentane	116	0.46852	0.75119	-0.38000	-0.00800	0.16251	0.68729	1.97282	2.7518
O	2,3-Dimethylbutane	130	-0.17787	0.56350	-0.90462	-0.65423	-0.39753	0.16846	0.71454	1.3488
O	2,3-Dimethylpentane	131	0.13306	0.90335	-0.94541	-0.39950	-0.03101	0.18053	1.94792	4.4318
O	2,4-Dimethylpentane	134	0.13279	0.72754	-0.57289	-0.15611	-0.02006	0.18833	0.60741	6.8533
O	2-Methylheptane	130	0.14204	0.77871	-0.72915	-0.45949	-0.02643	0.39897	0.90039	4.4687
O	2-Methylhexane	114	0.28861	0.56496	-0.86646	-0.10974	0.01962	0.81801	1.05047	2.5610
O	2-Methylpentane	100	0.38692	0.77248	-0.64571	-0.25157	-0.00461	0.90429	1.31614	3.3105
O	3-Methylheptane	129	0.09855	0.54793	-0.85869	-0.45949	0.01744	0.46256	0.95131	1.7146
O	3-Methylhexane	128	0.29800	0.58073	-0.42504	-0.07450	0.03266	0.65727	1.03090	2.9505
O	3-Methylpentane	109	-0.10567	0.49513	-0.73210	-0.57190	-0.05524	0.07270	0.72714	1.4948
O	Acetylene	131	0.07806	0.79090	-0.97995	-0.67560	0.14725	0.29066	1.28875	2.8571
O	Cyclohexane	312	-0.03084	0.62637	-0.87037	-0.24503	-0.07721	0.07604	0.32972	8.5740
O	Cyclopentane	133	0.01369	0.60038	-0.91389	-0.38492	-0.01587	0.07959	0.67712	2.6073
O	Isopropylbenzene	383	0.08496	0.55390	-0.97549	-0.18124	0.06950	0.22590	0.49832	6.2469
O	Methylcyclohexane	139	0.01946	0.56952	-0.93671	-0.18792	-0.06419	0.07460	0.35625	3.4304
O	Methylcyclopentane	93	-0.23201	0.43293	-0.88554	-0.54692	-0.24646	-0.00323	0.03588	1.5754
O	cis-2-Pentene	211	-0.03769	0.70327	-0.96264	-0.47019	0.00868	0.10972	0.38362	6.1743
O	m-Diethylbenzene	115	-0.02278	0.72554	-0.42537	-0.25650	-0.06748	0.01746	0.18455	7.3171
O	n-Decane	378	0.48283	1.54107	-0.93950	-0.22500	0.07145	0.74375	2.00380	22.3860
O	n-Heptane	261	0.05444	0.42862	-0.97028	-0.11593	0.00734	0.20606	0.50092	3.3936
O	n-Nonane	343	0.19324	0.73027	-0.96037	-0.04138	0.08000	0.29468	0.75269	7.7277
O	n-Octane	341	0.00866	0.34959	-0.94714	-0.12420	0.03917	0.21750	0.35700	2.1467
O	n-Propylbenzene	347	0.18601	0.66470	-0.98544	-0.10594	0.05400	0.28717	0.73972	5.3240
O	n-Undecane	335	0.30248	1.31699	-0.97477	-0.23967	0.08844	0.36056	1.53046	19.1500
O	p-Diethylbenzene	105	0.17573	0.38085	-0.44359	-0.07265	0.05321	0.47051	0.68910	1.3369
O	trans-2-Pentene	344	0.01289	0.62648	-0.97704	-0.36388	-0.00896	0.19883	0.48264	5.8315
P	1,2,3-Trimethylbenzene	133	0.09034	0.97955	-0.80711	-0.46611	-0.03039	0.17111	0.46389	7.8522
P	1,2,4-Trimethylbenzene	324	0.44939	0.96962	-0.75271	-0.19843	0.05461	0.83538	1.46673	5.1114
P	1-Butene	350	-0.01315	0.44177	-0.97867	-0.31093	0.02751	0.21374	0.47144	2.7333
P	2,2,4-Trimethylpentane	321	0.00856	0.35443	-0.97116	-0.16444	0.01271	0.22667	0.45294	1.5600
P	Benzene	382	0.06558	0.70290	-0.99000	-0.13750	0.00000	0.08500	0.50400	9.0400
P	Ethane	239	-0.03969	0.57580	-0.95417	-0.50277	-0.19356	0.19228	1.04686	1.3899
P	Ethylbenzene	381	0.02033	0.51488	-0.98036	-0.22783	-0.00182	0.15404	0.46782	4.3733
P	Ethylene	348	-0.05140	0.60137	-0.96487	-0.47901	-0.22418	0.27878	0.88952	2.6216
P	Isobutane	255	-0.10868	0.31122	-0.97775	-0.17517	-0.00394	0.06200	0.09558	1.4469
P	Isopentane	138	-0.18906	0.36560	-0.78194	-0.57345	-0.10173	-0.01473	0.30729	0.6822

TARGET	CMPDNAME	n	mean	stddev	min	p25	median	p75	p90	max
P	Isoprene	345	0.02050	0.74044	-0.96800	-0.29500	0.01746	0.19920	0.38900	8.8293
P	Propane	239	0.01861	0.50990	-0.96672	-0.26235	0.00588	0.13912	0.92859	1.2962
P	Propylene	346	-0.01636	0.57213	-0.97520	-0.43927	-0.02489	0.21255	0.65230	3.8443
P	Styrene	379	-0.05530	0.51830	-0.99299	-0.33040	-0.06983	0.08982	0.39648	5.3897
P	Toluene	318	0.05973	0.46192	-0.96213	-0.16018	0.00325	0.10222	0.79252	3.0128
P	cis-2-Butene	349	-0.14247	0.33814	-0.98691	-0.40845	-0.04382	0.07127	0.22482	0.7911
P	m,p-Xylene	357	0.15986	0.78975	-0.94489	-0.16750	0.03333	0.26900	0.69270	6.1413
P	m-Ethyltoluene	94	-0.10088	0.22931	-0.55360	-0.27460	-0.10444	0.05202	0.22016	0.5252
P	n-Butane	348	-0.12253	0.33369	-0.88519	-0.42149	-0.00455	0.07467	0.23600	0.7153
P	n-Hexane	369	0.13470	2.22436	-0.94400	-0.35527	-0.04350	0.04257	0.15636	35.2400
P	n-Pentane	350	0.16257	0.63121	-0.80485	-0.18099	0.06213	0.21244	1.01901	4.2080
P	o-Ethyltoluene	140	0.14744	0.60595	-0.50400	-0.07620	0.05400	0.24775	0.53435	5.5720
P	o-Xylene	384	0.10672	0.57685	-0.96634	-0.16156	0.03333	0.31614	0.79975	4.4687
P	p-Ethyltoluene	120	-0.07872	0.78135	-0.96796	-0.56744	-0.04541	0.15205	0.43786	6.7212
P	trans-2-Butene	350	-0.04549	0.35853	-0.98642	-0.19813	0.02744	0.15811	0.31867	1.4800

Table B2. Descriptive Statistics for Bias – By Vendor

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	1,3,5-Trimethylbenzene	1	36	-0.15279	0.07955	-0.24733	-0.18883	-0.16952	-0.15868	-0.0700	0.1022
O	1,3,5-Trimethylbenzene	2	36	0.21942	0.10153	0.06310	0.14904	0.18811	0.29749	0.3261	0.5672
O	1,3,5-Trimethylbenzene	3	36	0.22439	0.38182	-0.15621	-0.06417	-0.02164	0.54242	0.6912	1.1493
O	1,3,5-Trimethylbenzene	4	36	0.22440	0.13739	-0.07689	0.15018	0.24844	0.30899	0.3634	0.5156
O	1,3,5-Trimethylbenzene	5	36	0.75275	0.23713	0.56940	0.63235	0.70503	0.79084	0.9124	1.9071
O	1,3,5-Trimethylbenzene	6	1	0.04587	.	0.04587	0.04587	0.04587	0.04587	0.0459	0.0459
O	1,3,5-Trimethylbenzene	8	23	0.57431	1.43268	-0.34039	-0.16110	0.05056	0.97009	1.8244	6.4400
O	1,3,5-Trimethylbenzene	9	35	-0.10402	0.81138	-0.93407	-0.29013	-0.13054	-0.05580	0.0670	4.2394
O	1-Pentene	1	36	0.05698	0.04778	-0.01436	0.01243	0.06803	0.08481	0.1246	0.1533
O	1-Pentene	2	36	0.00740	0.06936	-0.08590	-0.04435	-0.00127	0.01922	0.1394	0.1642
O	1-Pentene	3	36	-0.07604	0.10001	-0.34821	-0.14502	-0.06571	0.00969	0.0355	0.0749
O	1-Pentene	4	36	0.49495	0.21550	0.03333	0.30583	0.55670	0.63109	0.7604	0.8628
O	1-Pentene	5	36	0.08503	0.04183	0.02221	0.05152	0.07731	0.12735	0.1442	0.1616
O	1-Pentene	6	111	-0.22080	0.31156	-0.63936	-0.39312	-0.31138	-0.07743	0.0453	1.4244
O	1-Pentene	7	31	0.04916	1.45965	-0.97028	-0.85280	-0.54295	0.14079	2.0901	3.9282
O	1-Pentene	8	21	-0.17764	0.46592	-0.72179	-0.44359	-0.19633	-0.04088	-0.0158	1.4442
O	1-Pentene	9	30	-0.16338	0.19847	-0.47725	-0.29673	-0.17545	-0.06023	0.0010	0.6016
O	2,2-Dimethylbutane	1	15	-0.00359	0.00648	-0.01390	-0.01041	-0.00357	0.00381	0.0038	0.0038
O	2,2-Dimethylbutane	2	12	0.56767	0.05172	0.50899	0.54459	0.54952	0.58690	0.5943	0.7124
O	2,2-Dimethylbutane	3	15	-0.18695	0.18861	-0.50400	-0.32981	-0.16623	-0.02824	0.0717	0.1207

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	2,2-Dimethylbutane	4	15	0.72400	0.17626	0.43190	0.60905	0.72419	0.93381	0.9628	0.9929
O	2,2-Dimethylbutane	6	41	-0.52641	0.29887	-0.73210	-0.64571	-0.63095	-0.56452	-0.2767	0.5057
O	2,2-Dimethylbutane	7	8	0.11476	0.57661	-0.83762	-0.19400	0.10660	0.43190	1.0667	1.0667
O	2,2-Dimethylbutane	8	8	0.32904	0.04810	0.25476	0.28798	0.34224	0.36474	0.3876	0.3876
O	2,3,4-Trimethylpentane	1	15	-0.00042	0.01653	-0.04615	-0.00800	0.00154	0.01744	0.0174	0.0174
O	2,3,4-Trimethylpentane	2	15	-0.10653	0.02387	-0.17333	-0.10974	-0.10503	-0.09385	-0.0779	-0.0779
O	2,3,4-Trimethylpentane	3	15	0.00350	0.05862	-0.11092	-0.03556	0.00472	0.05082	0.0747	0.0925
O	2,3,4-Trimethylpentane	4	15	0.10248	0.13418	-0.17333	0.00472	0.04923	0.23647	0.2559	0.2718
O	2,3,4-Trimethylpentane	5	15	0.55850	0.20591	0.23873	0.43458	0.53378	0.67355	0.8697	1.0113
O	2,3,4-Trimethylpentane	6	40	1.15913	0.88514	-0.00800	0.27974	1.01103	2.00462	2.4100	2.7518
O	2,3,4-Trimethylpentane	8	1	-0.38000	.	-0.38000	-0.38000	-0.38000	-0.38000	-0.3800	-0.3800
O	2,3-Dimethylbutane	1	15	-0.56364	0.22720	-0.76154	-0.73769	-0.59938	-0.58932	-0.0938	0.0302
O	2,3-Dimethylbutane	2	13	0.39796	0.02919	0.36519	0.37910	0.38308	0.42779	0.4427	0.4427
O	2,3-Dimethylbutane	3	15	-0.09671	0.17220	-0.45392	-0.21308	-0.02231	0.05305	0.0678	0.0916
O	2,3-Dimethylbutane	4	15	0.81950	0.15947	0.59769	0.68115	0.79323	0.99115	1.0388	1.0976
O	2,3-Dimethylbutane	5	15	-0.38985	0.02378	-0.41935	-0.40666	-0.39955	-0.36653	-0.3531	-0.3527
O	2,3-Dimethylbutane	6	41	-0.61749	0.24139	-0.78362	-0.71385	-0.70192	-0.64827	-0.4158	0.2162
O	2,3-Dimethylbutane	7	8	-0.01329	0.94309	-0.90462	-0.75260	-0.49208	0.96941	1.3488	1.3488
O	2,3-Dimethylbutane	8	8	0.07345	0.03885	0.01346	0.04029	0.08412	0.10229	0.1208	0.1208
O	2,3-Dimethylpentane	1	15	-0.02174	0.00781	-0.04465	-0.02418	-0.01938	-0.01736	-0.0174	-0.0119
O	2,3-Dimethylpentane	2	15	-0.51022	0.04081	-0.56327	-0.54507	-0.51550	-0.49116	-0.4677	-0.3995
O	2,3-Dimethylpentane	3	14	-0.33734	0.21194	-0.77072	-0.44044	-0.33275	-0.19630	-0.0588	-0.0403
O	2,3-Dimethylpentane	4	15	0.06395	0.12590	-0.26848	0.00084	0.03723	0.19292	0.2147	0.2147
O	2,3-Dimethylpentane	5	15	-0.26981	0.08236	-0.50650	-0.26327	-0.25074	-0.22535	-0.2025	-0.2000
O	2,3-Dimethylpentane	6	40	0.91616	1.27260	-0.68337	-0.02077	0.34772	2.09805	2.4290	4.4318
O	2,3-Dimethylpentane	7	13	-0.13541	0.51239	-0.94541	-0.58511	0.16765	0.23513	0.2556	0.3784
O	2,3-Dimethylpentane	8	4	-0.41637	0.03120	-0.44726	-0.44309	-0.41618	-0.38964	-0.3858	-0.3858
O	2,4-Dimethylpentane	1	15	-0.02746	0.03232	-0.10444	-0.02407	-0.01833	-0.00972	-0.0049	-0.0011
O	2,4-Dimethylpentane	2	15	-0.18577	0.02551	-0.23763	-0.19630	-0.19056	-0.17503	-0.1561	-0.1217
O	2,4-Dimethylpentane	3	12	-0.24699	0.16675	-0.53492	-0.37828	-0.21208	-0.11006	-0.0976	-0.0314
O	2,4-Dimethylpentane	4	15	0.05173	0.09708	-0.12167	-0.03683	0.05400	0.15389	0.1711	0.1969
O	2,4-Dimethylpentane	5	15	-0.04391	0.03647	-0.08626	-0.07152	-0.05347	-0.01351	-0.0025	0.0488
O	2,4-Dimethylpentane	6	42	0.20672	0.48010	-0.57289	-0.19056	0.18833	0.58444	0.8256	1.5144
O	2,4-Dimethylpentane	7	15	0.88111	1.83777	-0.20778	0.06778	0.17800	0.68089	3.0817	6.8533
O	2,4-Dimethylpentane	8	5	0.38798	0.07705	0.29167	0.33951	0.37778	0.46389	0.4671	0.4671
O	2-Methylheptane	1	15	1.04434	1.14319	0.01744	0.39897	0.46256	1.70256	2.2431	4.4687
O	2-Methylheptane	2	15	-0.06255	0.03652	-0.13094	-0.10974	-0.04223	-0.03344	-0.0226	-0.0223
O	2-Methylheptane	3	15	-0.01563	0.07500	-0.14389	-0.07159	-0.00418	0.03015	0.0670	0.1510
O	2-Methylheptane	4	15	0.02176	0.25674	-0.58031	-0.06205	0.01744	0.14462	0.1828	0.6368
O	2-Methylheptane	5	15	1.14168	0.91997	0.17291	0.66542	0.89309	1.09019	2.6049	3.5963

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	2-Methylheptane	6	41	-0.44819	0.23806	-0.72915	-0.55487	-0.50718	-0.45949	-0.3323	0.4626
O	2-Methylheptane	7	10	0.28670	0.34277	-0.01436	0.06831	0.14756	0.49436	0.8759	0.9077
O	2-Methylheptane	8	4	0.50746	0.31048	0.19231	0.24383	0.50613	0.77109	0.8253	0.8253
O	2-Methylhexane	1	15	-0.00865	0.01911	-0.05410	-0.01083	0.00154	0.00154	0.0015	0.0015
O	2-Methylhexane	3	15	-0.29175	0.26864	-0.86646	-0.35178	-0.20763	-0.14535	-0.0623	0.1362
O	2-Methylhexane	4	15	-0.12836	0.12993	-0.36013	-0.22103	-0.16538	0.00154	0.0294	0.0433
O	2-Methylhexane	5	15	0.82278	0.38640	-0.12727	0.81801	0.94521	1.05017	1.1299	1.1689
O	2-Methylhexane	6	40	0.55273	0.58935	-0.33231	0.21019	0.44280	0.95439	1.2256	2.5610
O	2-Methylhexane	7	9	0.01323	0.15387	-0.22103	-0.10974	0.01545	0.16846	0.1963	0.1963
O	2-Methylhexane	8	5	0.95251	0.10945	0.80833	0.87531	0.96969	1.05047	1.0587	1.0587
O	2-Methylpentane	1	15	1.04744	0.54216	-0.01981	1.27443	1.30286	1.31762	1.3324	1.3324
O	2-Methylpentane	2	2	2.43657	0.06680	2.38933	2.38933	2.43657	2.48381	2.4838	2.4838
O	2-Methylpentane	3	15	-0.05741	0.08263	-0.27962	-0.10543	-0.04048	-0.00210	0.0215	0.0629
O	2-Methylpentane	4	15	0.75224	0.23102	0.35810	0.62381	0.75667	0.99286	1.0339	1.1104
O	2-Methylpentane	6	41	-0.05283	0.59773	-0.46420	-0.29143	-0.26190	-0.12905	0.4467	2.0114
O	2-Methylpentane	7	3	-0.17825	0.44490	-0.64571	-0.64571	-0.12905	0.24000	0.2400	0.2400
O	2-Methylpentane	8	9	1.15396	0.81662	0.73862	0.83048	0.86000	0.94857	3.3105	3.3105
O	3-Methylheptane	1	15	0.01011	0.01298	-0.01436	0.00095	0.01744	0.01744	0.0174	0.0302
O	3-Methylheptane	2	15	0.02724	0.07293	-0.10974	-0.02653	0.01861	0.08103	0.1128	0.1764
O	3-Methylheptane	3	15	0.63988	0.13304	0.36247	0.54364	0.64189	0.71692	0.7742	0.9141
O	3-Methylheptane	4	15	0.08536	0.14541	-0.23692	0.00472	0.04923	0.20821	0.2600	0.2718
O	3-Methylheptane	5	15	1.13922	0.23459	0.86699	1.00626	1.07048	1.20911	1.5846	1.7146
O	3-Methylheptane	6	41	-0.44560	0.29647	-0.85869	-0.53897	-0.49128	-0.47538	-0.3641	0.8441
O	3-Methylheptane	7	10	0.12229	0.16063	-0.03344	0.00154	0.06248	0.27179	0.3672	0.4626
O	3-Methylheptane	8	3	0.41079	0.08514	0.31949	0.31949	0.42488	0.48800	0.4880	0.4880
O	3-Methylhexane	1	15	0.00224	0.00893	-0.01083	0.00154	0.00154	0.00154	0.0098	0.0294
O	3-Methylhexane	2	15	-0.14024	0.11057	-0.42504	-0.20712	-0.09583	-0.08639	-0.0611	-0.0170
O	3-Methylhexane	3	15	-0.10905	0.09335	-0.25441	-0.17054	-0.10273	-0.03602	0.0154	0.0661
O	3-Methylhexane	4	15	0.05335	0.18367	-0.20712	-0.07265	0.02936	0.18495	0.2519	0.5023
O	3-Methylhexane	5	15	0.73093	0.38282	-0.23243	0.73989	0.79053	0.93888	1.0409	1.1706
O	3-Methylhexane	6	40	0.63990	0.73603	-0.38795	0.18933	0.50926	1.01003	1.3230	2.9505
O	3-Methylhexane	7	10	0.08765	0.13178	-0.04297	-0.02628	0.04605	0.16846	0.3076	0.3354
O	3-Methylhexane	8	3	1.20435	0.61575	0.49406	0.49406	1.53167	1.58731	1.5873	1.5873
O	3-Methylpentane	1	15	-0.05733	0.12436	-0.29143	-0.11429	0.01857	0.02743	0.0333	0.0443
O	3-Methylpentane	2	15	0.04249	0.02946	-0.02571	0.01956	0.04810	0.06581	0.0727	0.0776
O	3-Methylpentane	3	15	-0.16097	0.21245	-0.51286	-0.28552	-0.13780	0.02300	0.0977	0.1166
O	3-Methylpentane	4	15	0.83208	0.23430	0.53524	0.67105	0.77143	0.98990	1.0175	1.4948
O	3-Methylpentane	6	41	-0.52641	0.29887	-0.73210	-0.64571	-0.63095	-0.56452	-0.2767	0.5057
O	3-Methylpentane	7	1	-0.45381	.	-0.45381	-0.45381	-0.45381	-0.45381	-0.4538	-0.4538
O	3-Methylpentane	8	7	0.09645	0.03828	0.01857	0.08801	0.09976	0.12190	0.1337	0.1337

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	Acetylene	1	21	0.26860	0.05004	0.15418	0.27516	0.28571	0.29193	0.3055	0.3203
O	Acetylene	2	35	-0.22032	0.58422	-0.97995	-0.92619	0.22489	0.25169	0.2778	0.3144
O	Acetylene	3	21	1.30113	0.16984	0.98483	1.16841	1.31251	1.43554	1.5029	1.5713
O	Acetylene	4	1	-0.68905	.	-0.68905	-0.68905	-0.68905	-0.68905	-0.6891	-0.6891
O	Acetylene	5	21	0.04315	0.02217	-0.00806	0.03385	0.04527	0.05076	0.0648	0.0867
O	Acetylene	6	3	-0.85995	0.01498	-0.87607	-0.87607	-0.85730	-0.84648	-0.8465	-0.8465
O	Acetylene	7	14	-0.74482	0.20850	-0.97048	-0.95154	-0.67313	-0.61852	-0.5081	-0.3324
O	Acetylene	8	15	-0.14912	1.18656	-0.88659	-0.83516	-0.70923	-0.20778	2.0738	2.8571
O	Cyclohexane	1	36	0.01584	0.07956	-0.19256	-0.00656	0.05688	0.07527	0.0820	0.0866
O	Cyclohexane	2	36	-0.00185	0.17121	-0.36558	-0.15518	0.01456	0.14209	0.2109	0.3104
O	Cyclohexane	3	36	-0.09050	0.06826	-0.23293	-0.14564	-0.08588	-0.04926	-0.0024	0.0420
O	Cyclohexane	4	36	-0.13402	0.09455	-0.32953	-0.19833	-0.12100	-0.08081	-0.0141	0.0443
O	Cyclohexane	6	111	-0.11265	0.38005	-0.63835	-0.47372	-0.15037	0.16791	0.3332	0.9609
O	Cyclohexane	7	36	0.07501	1.65489	-0.87037	-0.61440	-0.42037	0.04895	0.8744	8.5740
O	Cyclohexane	8	21	0.36956	0.41357	-0.26018	0.07257	0.39046	0.52116	0.5407	1.8116
O	Cyclopentane	1	15	-0.00241	0.01252	-0.01587	-0.00676	-0.00603	0.00381	0.0087	0.0333
O	Cyclopentane	2	15	0.03049	0.02643	-0.01587	0.01037	0.03333	0.04153	0.0661	0.0887
O	Cyclopentane	3	15	-0.01389	0.06726	-0.10198	-0.08476	-0.00403	0.04613	0.0776	0.0796
O	Cyclopentane	4	15	0.17618	0.18897	-0.16349	-0.01587	0.21193	0.30397	0.4393	0.4489
O	Cyclopentane	5	15	1.16720	0.70681	0.39313	0.61333	0.88879	1.96911	2.2604	2.6073
O	Cyclopentane	6	41	-0.21069	0.49811	-0.55350	-0.40952	-0.38492	-0.27421	0.2056	1.5095
O	Cyclopentane	7	15	-0.59831	0.32512	-0.91389	-0.89175	-0.65556	-0.45873	-0.1635	0.2794
O	Cyclopentane	8	2	-0.46488	0.30445	-0.68016	-0.68016	-0.46488	-0.24960	-0.2496	-0.2496
O	Isopropylbenzene	1	36	0.07416	0.02773	0.01611	0.05788	0.08294	0.09009	0.1052	0.1160
O	Isopropylbenzene	2	36	0.12883	0.04460	0.03333	0.08839	0.14159	0.16376	0.1784	0.1877
O	Isopropylbenzene	3	36	-0.02774	0.07305	-0.17075	-0.07515	-0.03234	0.00101	0.0370	0.2137
O	Isopropylbenzene	4	36	0.29809	0.15708	-0.03280	0.19143	0.34850	0.43706	0.4585	0.5160
O	Isopropylbenzene	5	36	0.39905	0.18399	0.15518	0.26218	0.35450	0.52164	0.6934	0.7981
O	Isopropylbenzene	6	111	-0.11337	0.32914	-0.57944	-0.37690	-0.22113	0.07423	0.3004	1.0460
O	Isopropylbenzene	7	34	-0.29846	0.53934	-0.97549	-0.84776	-0.31491	0.04194	0.3950	0.9530
O	Isopropylbenzene	8	23	1.03463	0.82776	0.08000	0.49963	0.84206	1.15278	2.0458	3.6733
O	Isopropylbenzene	9	35	0.00200	1.11425	-0.77770	-0.20675	-0.10445	-0.03668	0.0612	6.2469
O	Methylcyclohexane	1	15	-0.18962	0.27196	-0.72875	-0.29927	-0.19630	0.01267	0.1845	0.2545
O	Methylcyclohexane	2	15	-0.07831	0.03608	-0.16365	-0.09583	-0.06235	-0.05967	-0.0414	-0.0393
O	Methylcyclohexane	3	15	-0.23285	0.17876	-0.63381	-0.31283	-0.18625	-0.12430	-0.0506	0.0244
O	Methylcyclohexane	4	13	0.48688	1.13202	-0.32188	-0.11844	-0.00542	0.46508	2.4358	3.4304
O	Methylcyclohexane	5	15	0.15900	0.29318	-0.03453	0.06443	0.09639	0.11416	0.1768	1.2053
O	Methylcyclohexane	6	40	0.02399	0.59133	-0.60443	-0.26997	-0.09922	0.06240	0.5427	2.7975
O	Methylcyclohexane	7	12	0.04941	0.70717	-0.93671	-0.12974	-0.00458	0.15135	0.5145	1.8481
O	Methylcyclohexane	9	14	-0.00357	0.45018	-0.47802	-0.16392	-0.09784	-0.04270	0.0448	1.4978

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	Methylcyclopentane	1	15	-0.00284	0.04089	-0.09385	-0.02231	0.01346	0.02062	0.0245	0.0492
O	Methylcyclopentane	2	3	1.55101	0.04222	1.50226	1.50226	1.57538	1.57538	1.5754	1.5754
O	Methylcyclopentane	3	15	-0.03844	0.08307	-0.18923	-0.09385	-0.02231	0.02920	0.0359	0.1065
O	Methylcyclopentane	4	15	-0.22582	0.10120	-0.43962	-0.30846	-0.22738	-0.12564	-0.1058	-0.0938
O	Methylcyclopentane	6	41	-0.47473	0.26136	-0.73292	-0.59462	-0.54692	-0.47538	-0.2846	0.4785
O	Methylcyclopentane	7	4	-0.69000	0.18455	-0.88554	-0.84738	-0.67569	-0.53262	-0.5231	-0.5231
O	cis-2-Pentene	1	36	0.10894	0.06524	0.03333	0.05548	0.10292	0.11726	0.2192	0.2797
O	cis-2-Pentene	2	36	0.06615	0.14888	-0.05779	-0.02571	0.01491	0.04956	0.3789	0.4009
O	cis-2-Pentene	3	36	-0.11935	0.19311	-0.52171	-0.29907	-0.04171	0.05365	0.0884	0.1262
O	cis-2-Pentene	4	19	0.37536	0.22929	0.06286	0.20310	0.30643	0.50571	0.7092	0.8319
O	cis-2-Pentene	6	41	-0.52641	0.29887	-0.73210	-0.64571	-0.63095	-0.56452	-0.2767	0.5057
O	cis-2-Pentene	7	31	0.15764	1.64125	-0.96264	-0.84691	-0.47019	0.25321	1.9745	6.1743
O	cis-2-Pentene	8	12	-0.03291	0.24900	-0.36524	-0.13356	-0.10690	0.04810	0.3368	0.5140
O	m-Diethylbenzene	1	15	0.00204	0.03391	-0.04788	-0.03220	0.00813	0.01746	0.0585	0.0585
O	m-Diethylbenzene	2	15	-0.09719	0.10528	-0.31951	-0.21590	-0.06748	-0.01054	0.0018	0.0149
O	m-Diethylbenzene	3	15	0.00090	0.07861	-0.15989	-0.02841	-0.00699	0.04421	0.0989	0.1493
O	m-Diethylbenzene	4	15	0.07073	0.21163	-0.25398	-0.14309	0.07870	0.22992	0.3610	0.3610
O	m-Diethylbenzene	6	40	-0.19358	0.29762	-0.42537	-0.35662	-0.28801	-0.22500	0.1846	1.0667
O	m-Diethylbenzene	7	10	-0.10213	0.12321	-0.26911	-0.24390	-0.08764	-0.04228	0.0711	0.0837
O	m-Diethylbenzene	8	5	1.29956	3.36635	-0.39512	-0.23130	-0.15056	-0.04228	7.3171	7.3171
O	n-Decane	1	36	0.34811	0.29623	-0.12693	0.03333	0.54350	0.59958	0.6156	0.6500
O	n-Decane	2	36	0.65575	0.34785	-0.01929	0.32396	0.79042	0.90650	0.9861	1.0575
O	n-Decane	3	36	-0.04730	0.10370	-0.39292	-0.09444	-0.02404	0.02621	0.0582	0.0768
O	n-Decane	4	36	0.19648	0.19437	-0.28958	0.07444	0.26135	0.34033	0.3920	0.4854
O	n-Decane	5	36	1.97458	0.85473	0.47118	1.25033	2.17010	2.64651	2.9213	3.2148
O	n-Decane	6	111	-0.18550	0.32476	-0.62924	-0.45104	-0.26500	0.06222	0.2067	0.8729
O	n-Decane	7	30	0.85479	1.10143	-0.93429	0.05917	1.20278	1.47031	1.9598	3.1979
O	n-Decane	8	22	2.21865	2.02542	-0.12813	0.45313	2.01194	3.00000	4.7075	7.7833
O	n-Decane	9	35	0.45863	3.88392	-0.93950	-0.65538	-0.32426	-0.03571	1.1628	22.3860
O	n-Heptane	1	36	-0.02002	0.02807	-0.06731	-0.04821	-0.00398	0.00437	0.0073	0.0156
O	n-Heptane	2	36	0.14412	0.17457	-0.12843	0.00279	0.17901	0.21291	0.3789	0.5538
O	n-Heptane	3	33	-0.20853	0.25704	-0.87141	-0.33560	-0.09449	-0.02106	0.0153	0.0362
O	n-Heptane	4	36	0.05176	0.14024	-0.29006	0.00679	0.07160	0.16505	0.2047	0.2742
O	n-Heptane	5	36	0.56183	0.14314	0.41430	0.47678	0.51609	0.55490	0.8568	0.9052
O	n-Heptane	6	47	0.18764	0.63088	-0.45080	-0.14272	0.07160	0.27817	0.7681	3.3936
O	n-Heptane	7	29	-0.44216	0.30124	-0.97028	-0.53651	-0.45339	-0.20701	-0.0490	0.0716
O	n-Heptane	8	8	-0.18305	0.51063	-0.86789	-0.67869	-0.09518	0.28444	0.3824	0.3824
O	n-Nonane	1	36	0.06065	0.11783	-0.01966	0.02329	0.04780	0.05743	0.0734	0.7169
O	n-Nonane	2	36	0.10265	0.04425	0.00869	0.08202	0.10763	0.12710	0.1625	0.1804
O	n-Nonane	3	36	-0.07778	0.10125	-0.44915	-0.10387	-0.06245	-0.01151	0.0233	0.0491

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	n-Nonane	4	36	0.21257	0.16539	-0.15942	0.07463	0.24119	0.35998	0.3822	0.4136
O	n-Nonane	5	36	0.68721	0.31037	0.21737	0.41920	0.63908	0.90972	1.1386	1.2349
O	n-Nonane	6	111	0.01891	0.44258	-0.54917	-0.20734	0.05771	0.16250	0.3417	2.1477
O	n-Nonane	7	29	-0.26327	0.48077	-0.96037	-0.45174	-0.38899	0.03731	0.5738	0.7527
O	n-Nonane	8	23	1.58028	1.94338	0.05358	0.51596	1.10716	1.28923	3.8646	7.7277
O	n-Octane	1	36	0.02659	0.02377	-0.02222	0.01333	0.03458	0.04722	0.0500	0.0625
O	n-Octane	2	36	0.19315	0.18900	-0.05778	-0.02716	0.32833	0.35800	0.3722	0.3844
O	n-Octane	3	36	-0.06869	0.08198	-0.30667	-0.10943	-0.05213	0.00077	0.0150	0.0550
O	n-Octane	4	36	0.11429	0.14136	-0.13000	-0.02500	0.17432	0.23294	0.2586	0.3080
O	n-Octane	5	36	0.27460	0.09521	0.07484	0.21015	0.28395	0.35280	0.3950	0.4304
O	n-Octane	6	111	-0.06583	0.29179	-0.57000	-0.37000	0.04250	0.15500	0.2800	0.6000
O	n-Octane	7	28	-0.40736	0.49521	-0.94714	-0.77708	-0.56717	0.05106	0.4133	0.7600
O	n-Octane	8	22	0.10128	0.78657	-0.67333	-0.39000	-0.29806	0.65333	0.8765	2.1467
O	n-Propylbenzene	1	36	0.10493	0.04822	0.01037	0.07055	0.12619	0.13986	0.1484	0.1780
O	n-Propylbenzene	2	36	0.18413	0.12662	-0.08531	0.10050	0.23640	0.28368	0.3020	0.3322
O	n-Propylbenzene	3	36	-0.01756	0.07214	-0.23740	-0.04689	-0.00344	0.02317	0.0627	0.1036
O	n-Propylbenzene	4	36	0.27586	0.18335	-0.15680	0.15811	0.34065	0.41954	0.4765	0.4880
O	n-Propylbenzene	5	36	1.46167	0.70117	0.44212	0.59392	1.96907	2.05646	2.0798	2.1061
O	n-Propylbenzene	6	111	-0.06619	0.33083	-0.56189	-0.29320	-0.08550	0.05400	0.2549	1.4800
O	n-Propylbenzene	7	33	-0.24881	0.65029	-0.98544	-0.85991	-0.34623	0.05400	0.5190	1.4180
O	n-Propylbenzene	8	23	0.33824	1.23689	-0.47892	-0.27660	-0.13962	0.57633	1.3560	5.3240
O	n-Undecane	1	36	0.32442	0.12968	0.13539	0.26925	0.30121	0.32154	0.4639	0.7911
O	n-Undecane	2	36	0.28817	0.26797	-0.00111	0.14374	0.18241	0.27311	0.9059	1.1011
O	n-Undecane	3	36	-0.01803	0.10148	-0.30422	-0.07341	0.00464	0.04116	0.0750	0.2469
O	n-Undecane	4	33	0.18553	0.23960	-0.44889	0.02785	0.15065	0.35050	0.4294	0.7222
O	n-Undecane	5	36	1.58160	0.45197	0.77210	1.25540	1.62138	1.89104	2.2134	2.3510
O	n-Undecane	6	111	-0.25301	0.43835	-0.71991	-0.52561	-0.29389	-0.20486	0.3433	1.5489
O	n-Undecane	7	25	0.15436	0.67028	-0.97477	-0.17907	-0.02178	0.19918	1.0839	1.7556
O	n-Undecane	8	22	1.86786	4.27148	-0.71738	-0.05554	0.19901	1.63439	3.3951	19.1500
O	p-Diethylbenzene	1	15	0.01906	0.06445	-0.08737	-0.04321	0.03333	0.07308	0.1128	0.1128
O	p-Diethylbenzene	2	15	0.51608	0.36902	-0.05302	0.25192	0.33951	0.75865	1.0667	1.2455
O	p-Diethylbenzene	3	15	0.60834	0.23249	0.31743	0.43872	0.58179	0.65810	0.7249	1.3369
O	p-Diethylbenzene	4	15	0.09911	0.30146	-0.44359	-0.12564	-0.02628	0.31154	0.5103	0.5897
O	p-Diethylbenzene	6	41	-0.01009	0.31840	-0.39649	-0.26401	-0.04615	0.05321	0.5897	0.9077
O	p-Diethylbenzene	7	4	0.05670	0.43299	-0.28462	-0.20807	-0.08884	0.32147	0.6891	0.6891
O	trans-2-Pentene	1	36	0.02755	0.05848	-0.04321	-0.02886	0.04359	0.05364	0.1080	0.1534
O	trans-2-Pentene	2	36	0.10523	0.21072	-0.08148	-0.05033	-0.00248	0.25942	0.5134	0.5361
O	trans-2-Pentene	3	36	-0.15119	0.21974	-0.57901	-0.30597	-0.18338	0.06802	0.0998	0.1314
O	trans-2-Pentene	4	36	0.50021	0.24377	-0.00494	0.27636	0.59772	0.67598	0.7720	0.8727
O	trans-2-Pentene	5	35	0.18363	0.11923	-0.01902	0.04969	0.23536	0.29170	0.3102	0.3367

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
O	trans-2-Pentene	6	111	-0.23987	0.30507	-0.65272	-0.44506	-0.36788	-0.02223	0.0737	0.9519
O	trans-2-Pentene	7	31	0.08603	1.77465	-0.97704	-0.86534	-0.65556	0.09854	1.3728	5.8315
O	trans-2-Pentene	8	23	0.20088	0.47908	-0.36505	-0.08327	0.17903	0.35874	0.3883	2.1383
P	1,2,3-Trimethylbenzene	1	15	0.08441	0.15732	-0.08148	-0.03045	0.03333	0.13667	0.3778	0.4467
P	1,2,3-Trimethylbenzene	2	15	0.15502	0.22307	-0.13251	-0.04321	0.13667	0.41222	0.4639	0.5500
P	1,2,3-Trimethylbenzene	3	14	0.03765	0.14710	-0.13123	-0.07000	0.02024	0.07639	0.2676	0.4122
P	1,2,3-Trimethylbenzene	4	15	0.02732	0.23947	-0.32489	-0.13251	-0.03556	0.17111	0.4467	0.4467
P	1,2,3-Trimethylbenzene	5	15	0.92538	0.78970	0.11141	0.38658	0.58737	1.47242	2.1792	2.8950
P	1,2,3-Trimethylbenzene	6	41	-0.49065	0.18905	-0.80711	-0.58667	-0.55222	-0.47644	-0.3111	0.1711
P	1,2,3-Trimethylbenzene	7	10	-0.09446	0.23813	-0.44889	-0.38000	0.00042	0.07467	0.1281	0.1711
P	1,2,3-Trimethylbenzene	8	8	1.83337	3.04139	-0.48333	-0.19247	0.19152	3.65000	7.8522	7.8522
P	1,2,4-Trimethylbenzene	1	36	0.76108	0.63032	-0.07328	0.04071	1.25084	1.29860	1.3136	1.3442
P	1,2,4-Trimethylbenzene	2	36	0.92717	0.62627	-0.11155	0.25476	1.37449	1.44472	1.4903	1.5410
P	1,2,4-Trimethylbenzene	3	36	-0.09993	0.09205	-0.32997	-0.17274	-0.08419	-0.02166	-0.0037	0.0464
P	1,2,4-Trimethylbenzene	4	36	0.21536	0.45672	-0.64961	0.09484	0.22111	0.37657	0.8108	1.3089
P	1,2,4-Trimethylbenzene	5	36	1.97371	1.40380	-0.05811	0.36909	2.89482	3.14871	3.2996	3.4060
P	1,2,4-Trimethylbenzene	6	111	-0.14264	0.28867	-0.75271	-0.35150	-0.22500	-0.05626	0.3200	0.8600
P	1,2,4-Trimethylbenzene	7	10	0.78781	0.76066	0.06286	0.13995	0.61089	1.23643	2.0336	2.1443
P	1,2,4-Trimethylbenzene	8	23	0.76402	1.25350	-0.58364	-0.06508	0.46804	1.37196	2.0779	5.1114
P	1-Butene	1	36	0.04367	0.05041	-0.03776	0.02452	0.03290	0.04636	0.1200	0.2000
P	1-Butene	2	36	0.03342	0.04730	-0.03704	0.00131	0.01972	0.08865	0.1024	0.1204
P	1-Butene	3	36	-0.08134	0.22730	-0.97867	-0.12967	-0.01298	0.06859	0.1077	0.1836
P	1-Butene	4	36	0.57284	0.50324	-0.04198	0.30752	0.42234	0.68669	0.9893	2.7333
P	1-Butene	5	36	0.17841	0.40264	-0.31093	-0.28560	0.41504	0.53193	0.5797	0.5973
P	1-Butene	6	111	-0.19069	0.42695	-0.85185	-0.46908	-0.33333	0.21121	0.3399	0.9733
P	1-Butene	7	36	-0.39711	0.41672	-0.97308	-0.83262	-0.36125	-0.18743	0.2000	0.6800
P	1-Butene	8	23	0.17248	0.28805	-0.41346	0.09136	0.17805	0.22667	0.2642	1.2800
P	2,2,4-Trimethylpentane	1	36	0.00687	0.03707	-0.06173	-0.02133	0.01344	0.02016	0.0400	0.1200
P	2,2,4-Trimethylpentane	2	36	0.19715	0.22587	-0.16444	-0.04530	0.35961	0.39398	0.4030	0.4392
P	2,2,4-Trimethylpentane	3	36	-0.04835	0.09182	-0.32800	-0.09886	-0.04297	0.02036	0.0494	0.0713
P	2,2,4-Trimethylpentane	4	25	0.16084	0.20006	-0.59049	0.06667	0.21458	0.27407	0.3424	0.4400
P	2,2,4-Trimethylpentane	5	36	0.49010	0.07477	0.42059	0.44497	0.46707	0.49809	0.5800	0.7424
P	2,2,4-Trimethylpentane	6	111	-0.10988	0.31929	-0.62234	-0.35402	-0.14458	0.06879	0.1888	1.5600
P	2,2,4-Trimethylpentane	7	30	-0.49062	0.39657	-0.97116	-0.81226	-0.61140	-0.14667	0.1412	0.2053
P	2,2,4-Trimethylpentane	8	11	0.21752	0.36068	-0.31925	-0.20262	0.29383	0.58916	0.6000	0.6127
P	Benzene	1	36	0.05279	0.02826	0.00000	0.02500	0.06708	0.07333	0.0800	0.1000
P	Benzene	2	36	-0.00280	0.03735	-0.08000	-0.03167	0.00333	0.01796	0.0300	0.1062
P	Benzene	3	36	-0.05952	0.07592	-0.28000	-0.10285	-0.04580	0.00140	0.0203	0.0610
P	Benzene	4	36	-0.08891	0.10768	-0.33000	-0.17238	-0.08056	-0.01250	0.0400	0.1600
P	Benzene	5	36	0.17495	0.19488	-0.09280	0.06088	0.11966	0.24559	0.4929	0.8660

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
P	Benzene	6	110	0.01050	0.46212	-0.64000	-0.32000	-0.01714	0.22250	0.6850	1.7200
P	Benzene	7	35	-0.32970	0.47915	-0.99000	-0.86000	-0.29778	0.03200	0.2400	0.7200
P	Benzene	8	23	1.49624	2.10138	-0.00222	0.31500	0.59000	1.74815	4.5600	9.0400
P	Benzene	9	34	-0.05096	0.28227	-0.33722	-0.18753	-0.08949	-0.00022	0.1547	1.3142
P	Ethane	1	36	0.21468	0.11958	0.07749	0.15042	0.19907	0.23425	0.2956	0.5738
P	Ethane	2	36	0.08664	0.17956	-0.26077	-0.00618	0.09213	0.16035	0.2034	0.8918
P	Ethane	3	36	1.07808	0.20280	0.53887	0.97314	1.11616	1.22781	1.3298	1.3899
P	Ethane	4	36	-0.30682	0.08661	-0.47538	-0.37459	-0.31386	-0.23949	-0.1936	-0.1146
P	Ethane	5	36	-0.56658	0.04685	-0.66011	-0.59057	-0.57439	-0.54678	-0.5258	-0.3672
P	Ethane	6	3	-0.77377	0.02419	-0.79981	-0.79981	-0.76949	-0.75200	-0.7520	-0.7520
P	Ethane	7	33	-0.41622	0.32388	-0.95417	-0.85119	-0.29307	-0.21727	-0.1247	0.0800
P	Ethane	8	23	-0.50635	0.13366	-0.80141	-0.55252	-0.50718	-0.46535	-0.4359	-0.0621
P	Ethylbenzene	1	36	0.01580	0.01882	-0.03745	0.01209	0.01888	0.02682	0.0333	0.0492
P	Ethylbenzene	2	36	0.08332	0.03818	0.00487	0.05453	0.09207	0.10749	0.1205	0.1764
P	Ethylbenzene	3	36	-0.12518	0.13755	-0.62482	-0.15984	-0.08957	-0.03478	-0.0165	0.0173
P	Ethylbenzene	4	36	0.09652	0.15375	-0.20513	-0.06312	0.17589	0.21827	0.2480	0.2999
P	Ethylbenzene	5	36	0.55790	0.26339	0.24302	0.34328	0.45628	0.76668	1.0171	1.2167
P	Ethylbenzene	6	111	-0.17913	0.35611	-0.68091	-0.38931	-0.23418	0.01744	0.2840	1.1621
P	Ethylbenzene	7	35	-0.31749	0.60317	-0.98036	-0.85692	-0.45345	0.08103	0.4308	1.3528
P	Ethylbenzene	8	20	0.97023	1.12583	-0.05184	0.33527	0.57070	1.15086	2.7995	4.3733
P	Ethylbenzene	9	35	-0.09383	0.48276	-0.71859	-0.22783	-0.11062	-0.03818	0.0670	2.3894
P	Ethylene	1	36	-0.01807	0.04154	-0.10864	-0.04921	-0.03522	0.02349	0.0383	0.0629
P	Ethylene	2	36	0.58201	0.55096	0.12978	0.23511	0.37361	0.73111	1.3422	2.6216
P	Ethylene	3	36	1.00093	0.41865	-0.48629	0.91787	1.09107	1.27840	1.3377	1.3900
P	Ethylene	4	36	-0.37976	0.05444	-0.48825	-0.42035	-0.38000	-0.34356	-0.3111	-0.2422
P	Ethylene	5	36	-0.51369	0.06721	-0.58011	-0.55726	-0.53214	-0.49450	-0.4487	-0.2065
P	Ethylene	6	111	-0.20119	0.46745	-0.89065	-0.54238	-0.37016	0.28079	0.4079	0.5719
P	Ethylene	7	34	-0.50183	0.29640	-0.96487	-0.90020	-0.38114	-0.27644	-0.2016	-0.0946
P	Ethylene	8	23	-0.11579	0.52510	-0.75215	-0.64571	-0.09703	0.20297	0.3981	1.2635
P	Isobutane	1	36	0.07717	0.02599	0.00689	0.06415	0.07467	0.09079	0.0982	0.1573
P	Isobutane	2	36	0.03615	0.02093	-0.00654	0.02484	0.03653	0.04556	0.0636	0.0978
P	Isobutane	3	36	-0.05904	0.18262	-0.63957	-0.09985	-0.00831	0.06512	0.1020	0.1283
P	Isobutane	4	15	0.06844	0.12922	-0.14027	0.00027	0.07160	0.19040	0.2565	0.2614
P	Isobutane	5	36	-0.09858	0.05001	-0.13639	-0.12643	-0.11672	-0.09977	-0.0214	0.0823
P	Isobutane	6	41	-0.38795	0.48046	-0.81630	-0.72720	-0.58360	-0.17333	-0.0741	1.4469
P	Isobutane	7	32	-0.36803	0.35643	-0.97775	-0.65280	-0.31628	-0.16857	0.1573	0.2069
P	Isobutane	8	23	0.02342	0.26883	-0.48769	-0.04254	0.01077	0.05813	0.0956	1.0832
P	Isopentane	1	15	-0.01643	0.01791	-0.04321	-0.02986	-0.01473	0.00329	0.0093	0.0093
P	Isopentane	2	15	-0.03306	0.01523	-0.05558	-0.05078	-0.03275	-0.01713	-0.0147	-0.0147
P	Isopentane	3	15	-0.09378	0.09302	-0.32713	-0.14707	-0.09884	-0.02242	0.0117	0.0530

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
P	Isopentane	4	15	0.31927	0.14349	0.10543	0.21357	0.30729	0.50194	0.5220	0.5320
P	Isopentane	5	15	-0.34443	0.10520	-0.70754	-0.33919	-0.32731	-0.32016	-0.2913	-0.2198
P	Isopentane	6	41	-0.55055	0.27677	-0.78194	-0.65155	-0.64554	-0.57345	-0.4112	0.4659
P	Isopentane	7	13	-0.07688	0.51181	-0.69739	-0.52383	-0.21899	0.23159	0.6101	0.6822
P	Isopentane	8	9	0.00084	0.25006	-0.17093	-0.07881	-0.06279	-0.05078	0.6581	0.6581
P	Isoprene	1	36	0.22240	0.16891	-0.03220	0.03018	0.34300	0.37033	0.3740	0.3890
P	Isoprene	2	36	-0.02504	0.15301	-0.24390	-0.20452	0.03500	0.08350	0.1745	0.2035
P	Isoprene	3	36	0.10699	0.14043	-0.18603	-0.02703	0.14192	0.21855	0.2718	0.2954
P	Isoprene	4	36	0.34012	0.35311	-0.45040	0.03959	0.43733	0.59667	0.7390	0.9343
P	Isoprene	5	36	-0.10810	0.19075	-0.36891	-0.32748	-0.03984	0.04481	0.1235	0.1747
P	Isoprene	6	111	-0.24026	0.36360	-0.77130	-0.63455	-0.28000	0.11600	0.2288	0.4067
P	Isoprene	7	33	0.89033	1.90117	-0.58900	-0.09200	0.12080	0.96800	3.7382	8.8293
P	Isoprene	8	21	-0.71189	0.13832	-0.96800	-0.78640	-0.76600	-0.54727	-0.5363	-0.4581
P	Propane	1	36	0.13826	0.05005	0.05056	0.08201	0.14412	0.18202	0.1859	0.2400
P	Propane	2	36	0.01108	0.06709	-0.13200	-0.04740	0.01824	0.06659	0.0906	0.1197
P	Propane	3	36	1.00294	0.18203	0.64843	0.89733	1.02038	1.16061	1.2502	1.2962
P	Propane	4	36	-0.00380	0.09794	-0.25600	-0.07000	-0.02045	0.07382	0.1178	0.2028
P	Propane	5	36	-0.55395	0.02956	-0.59178	-0.57415	-0.56234	-0.54014	-0.5183	-0.4320
P	Propane	6	3	-0.77942	0.02359	-0.80481	-0.80481	-0.77525	-0.75820	-0.7582	-0.7582
P	Propane	7	33	-0.43517	0.34104	-0.96672	-0.88118	-0.29059	-0.19400	-0.1010	0.0835
P	Propane	8	23	-0.01121	0.14151	-0.44353	-0.05647	0.00440	0.09694	0.1144	0.2013
P	Propylene	1	36	0.10300	0.03957	0.02874	0.06144	0.11469	0.13302	0.1403	0.1656
P	Propylene	2	36	0.60989	0.83899	0.01018	0.14662	0.29845	0.63091	1.5172	3.8443
P	Propylene	3	33	0.68347	0.44733	-0.48292	0.48800	0.77439	1.04393	1.1389	1.1904
P	Propylene	4	36	-0.21921	0.10305	-0.50400	-0.29455	-0.19609	-0.13911	-0.1082	-0.0555
P	Propylene	5	36	-0.45248	0.08137	-0.51190	-0.49816	-0.48425	-0.45493	-0.3130	-0.1511
P	Propylene	6	111	-0.22055	0.41590	-0.86222	-0.48540	-0.37380	0.17818	0.3034	0.8352
P	Propylene	7	35	-0.40176	0.41585	-0.97520	-0.88545	-0.37491	-0.04327	0.0416	0.2400
P	Propylene	8	23	0.38460	0.40896	-0.17309	-0.01420	0.38436	0.59791	0.7231	1.5420
P	Styrene	1	36	0.07608	0.06700	-0.06690	0.00873	0.10536	0.12745	0.1375	0.1585
P	Styrene	2	36	-0.10474	0.09767	-0.35364	-0.16356	-0.08065	-0.02862	-0.0059	0.0333
P	Styrene	3	36	-0.09125	0.07263	-0.30091	-0.14027	-0.08617	-0.03358	-0.0168	0.0629
P	Styrene	4	36	-0.12089	0.18217	-0.55911	-0.26678	-0.06016	0.03091	0.0825	0.1416
P	Styrene	5	36	0.51815	0.48330	-0.18128	0.17669	0.36413	0.78947	1.2621	1.5769
P	Styrene	6	111	-0.30302	0.33947	-0.73491	-0.55714	-0.38000	-0.05091	0.1564	0.6140
P	Styrene	7	30	-0.20739	0.60738	-0.99299	-0.46327	-0.31543	0.05498	0.6976	1.4013
P	Styrene	8	23	0.47460	0.62122	-0.51778	-0.04503	0.42609	0.98794	1.0470	1.7949
P	Styrene	9	35	-0.05724	0.98451	-0.83987	-0.29384	-0.14588	-0.04085	0.0745	5.3897
P	Toluene	1	36	0.00292	0.02341	-0.05728	-0.01052	0.00157	0.00882	0.0333	0.0678
P	Toluene	2	36	0.05262	0.02498	0.01037	0.03376	0.05232	0.06751	0.0816	0.1108

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
P	Toluene	3	36	-0.12690	0.13330	-0.62456	-0.16568	-0.09728	-0.03804	-0.0201	0.0123
P	Toluene	4	36	0.03017	0.11710	-0.20778	-0.08592	0.07088	0.12213	0.1539	0.2400
P	Toluene	5	36	-0.10900	0.30586	-0.33770	-0.28403	-0.21636	-0.13443	0.1787	0.8453
P	Toluene	6	47	0.22834	0.48168	-0.46267	-0.31111	0.15389	0.65333	0.8858	0.9892
P	Toluene	7	34	-0.30884	0.50903	-0.96213	-0.84455	-0.31203	0.02058	0.3175	0.9633
P	Toluene	8	22	1.04634	0.62243	0.08982	0.74774	1.00122	1.15345	1.4800	3.0128
P	Toluene	9	35	0.03283	0.42140	-0.44919	-0.17448	-0.05975	0.09038	0.3499	1.2824
P	cis-2-Butene	1	36	0.04828	0.02907	-0.00494	0.02007	0.06323	0.07225	0.0775	0.0874
P	cis-2-Butene	2	36	0.01799	0.02120	-0.02407	0.00310	0.01792	0.03766	0.0429	0.0604
P	cis-2-Butene	3	36	-0.10816	0.16321	-0.61422	-0.15924	-0.06055	0.01025	0.0362	0.0694
P	cis-2-Butene	4	36	0.15667	0.15835	-0.13889	0.02661	0.18629	0.25305	0.3696	0.4551
P	cis-2-Butene	5	36	-0.29468	0.14616	-0.71618	-0.41190	-0.32918	-0.16102	-0.0858	-0.0706
P	cis-2-Butene	6	111	-0.23311	0.41789	-0.87243	-0.52352	-0.40870	0.17709	0.3034	0.6993
P	cis-2-Butene	7	36	-0.38714	0.45536	-0.98691	-0.85394	-0.36373	-0.17897	0.2630	0.7911
P	cis-2-Butene	8	22	-0.15599	0.25009	-0.80527	-0.21926	-0.15666	-0.08527	0.0548	0.5156
P	m,p-Xylene	1	36	0.07538	0.05473	-0.03774	0.03825	0.10161	0.12226	0.1261	0.1289
P	m,p-Xylene	2	36	0.17090	0.08777	-0.01101	0.11762	0.20117	0.22963	0.2656	0.3187
P	m,p-Xylene	3	34	-0.19685	0.23520	-0.94489	-0.28985	-0.09736	-0.02367	0.0018	0.0395
P	m,p-Xylene	4	36	0.15625	0.16636	-0.13397	0.02292	0.20556	0.30192	0.3457	0.3640
P	m,p-Xylene	5	36	0.88653	0.74990	0.26404	0.34124	0.50810	1.20072	2.1207	2.9940
P	m,p-Xylene	6	111	-0.11323	0.78725	-0.76667	-0.40223	-0.17333	-0.03556	0.2678	4.9835
P	m,p-Xylene	7	10	0.88629	0.88720	0.14450	0.27937	0.46635	1.04698	2.4641	2.6216
P	m,p-Xylene	8	23	0.90836	1.20244	0.00000	0.29714	0.63500	0.92556	1.7752	5.8298
P	m,p-Xylene	9	35	0.00488	1.10139	-0.82853	-0.23835	-0.11398	-0.01351	0.1929	6.1413
P	m-Ethyltoluene	1	15	-0.03597	0.07684	-0.10444	-0.09232	-0.06256	0.04160	0.0565	0.1532
P	m-Ethyltoluene	3	15	0.04459	0.10961	-0.11547	-0.02536	0.02523	0.07880	0.2425	0.3020
P	m-Ethyltoluene	4	15	0.02667	0.23277	-0.36016	-0.18160	-0.03280	0.26480	0.2648	0.3392
P	m-Ethyltoluene	6	40	-0.30045	0.11630	-0.55360	-0.38620	-0.27460	-0.21880	-0.1723	-0.0631
P	m-Ethyltoluene	7	9	0.22285	0.15495	0.00440	0.16064	0.20900	0.22016	0.5252	0.5252
P	n-Butane	1	36	0.06570	0.02100	-0.00481	0.05619	0.06508	0.07267	0.0850	0.1367
P	n-Butane	2	36	0.00405	0.01884	-0.04933	-0.00611	0.00611	0.01362	0.0230	0.0574
P	n-Butane	3	36	-0.05034	0.12002	-0.44200	-0.09478	-0.02107	0.03607	0.0664	0.0947
P	n-Butane	4	36	0.17258	0.14360	-0.10100	0.07107	0.19518	0.26165	0.3667	0.4540
P	n-Butane	5	36	-0.33068	0.14926	-0.46473	-0.45566	-0.41932	-0.20507	-0.0968	-0.0376
P	n-Butane	6	111	-0.23752	0.43084	-0.88519	-0.52667	-0.40750	0.19889	0.3167	0.5293
P	n-Butane	7	34	-0.32022	0.41352	-0.86714	-0.74741	-0.33036	-0.08033	0.2193	0.7153
P	n-Butane	8	23	-0.01719	0.18552	-0.50000	-0.07000	0.00233	0.04160	0.0747	0.5707
P	n-Hexane	1	36	0.08104	0.07037	-0.04000	0.00741	0.12418	0.14347	0.1512	0.1571
P	n-Hexane	2	36	0.02043	0.03194	-0.07505	0.00323	0.01745	0.04000	0.0562	0.1168
P	n-Hexane	3	34	-0.15462	0.20600	-0.94400	-0.18889	-0.09562	-0.02113	0.0162	0.0283

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
P	n-Hexane	4	36	-0.00545	0.10470	-0.22000	-0.05950	0.01932	0.06609	0.1193	0.1959
P	n-Hexane	5	36	0.07283	0.11292	-0.08820	-0.00429	0.04469	0.10909	0.2400	0.3952
P	n-Hexane	6	111	-0.36998	0.26306	-0.78400	-0.57000	-0.39373	-0.28982	0.0396	0.3145
P	n-Hexane	7	32	3.07062	6.93398	-0.80855	-0.47833	0.32803	3.03200	10.3800	35.2400
P	n-Hexane	8	13	-0.60069	0.16188	-0.90673	-0.69003	-0.60000	-0.47745	-0.4044	-0.3913
P	n-Hexane	9	35	-0.01422	0.33291	-0.34002	-0.16807	-0.07584	0.01271	0.2123	1.4809
P	n-Pentane	1	36	0.09384	0.04071	0.03333	0.05193	0.11876	0.12880	0.1335	0.1468
P	n-Pentane	2	36	0.09131	0.03808	0.01802	0.06261	0.09723	0.11265	0.1321	0.2124
P	n-Pentane	3	36	1.05367	0.13633	0.72988	0.96648	1.05217	1.17406	1.2104	1.2493
P	n-Pentane	4	36	0.62171	0.23867	0.15733	0.43737	0.65984	0.77517	0.9366	1.0509
P	n-Pentane	5	36	0.06860	0.02997	0.01735	0.04938	0.06549	0.08215	0.1035	0.1673
P	n-Pentane	6	111	-0.21117	0.31607	-0.62494	-0.41455	-0.35536	-0.00287	0.0966	1.1080
P	n-Pentane	7	36	0.29015	1.40325	-0.80485	-0.58520	-0.27335	0.27246	2.6580	4.2080
P	n-Pentane	8	23	0.01929	0.36604	-0.50812	-0.08681	0.00515	0.03333	0.0390	1.5833
P	o-Ethyltoluene	1	15	0.22575	0.05781	0.11600	0.15963	0.24000	0.27100	0.3020	0.3020
P	o-Ethyltoluene	2	15	0.02223	0.04072	-0.07000	-0.00800	0.03850	0.05400	0.0618	0.0850
P	o-Ethyltoluene	3	15	0.08605	0.15156	-0.13200	-0.01030	0.07415	0.12220	0.3702	0.4136
P	o-Ethyltoluene	4	15	0.16455	0.12194	-0.02350	0.05400	0.24000	0.27100	0.3020	0.3020
P	o-Ethyltoluene	5	15	0.53177	0.16373	0.03044	0.50548	0.53621	0.57139	0.7273	0.7695
P	o-Ethyltoluene	6	41	-0.17022	0.18576	-0.50400	-0.28700	-0.24050	0.00750	0.0540	0.3392
P	o-Ethyltoluene	7	15	0.38098	0.72226	-0.34556	-0.05852	0.09120	0.79800	0.8600	2.5960
P	o-Ethyltoluene	8	9	0.71675	1.96539	-0.50400	-0.26519	-0.07000	0.15963	5.5720	5.5720
P	o-Xylene	1	36	0.17125	0.12667	-0.03438	0.04923	0.25575	0.28162	0.2895	0.3034
P	o-Xylene	2	36	0.34049	0.12273	0.09516	0.23470	0.40114	0.44000	0.4635	0.4801
P	o-Xylene	3	36	-0.04778	0.14494	-0.31959	-0.11113	-0.05929	-0.01914	0.0333	0.6724
P	o-Xylene	4	36	-0.02625	0.23819	-0.47093	-0.19884	-0.00795	0.14423	0.2718	0.5002
P	o-Xylene	5	36	0.75620	0.17789	0.20884	0.63505	0.83853	0.85618	0.8682	1.0431
P	o-Xylene	6	111	-0.08850	0.38925	-0.64491	-0.30618	-0.12564	0.11282	0.2698	1.6708
P	o-Xylene	7	35	-0.29564	0.74960	-0.96634	-0.74964	-0.64262	0.20821	0.7169	1.9251
P	o-Xylene	8	23	0.94243	1.11452	-0.00509	0.31809	0.70421	0.90036	2.7200	4.4687
P	o-Xylene	9	35	-0.10013	0.62246	-0.82101	-0.21916	-0.13507	-0.02755	0.0734	3.1550
P	p-Ethyltoluene	1	15	-0.02773	0.03394	-0.07881	-0.06279	-0.02674	-0.00512	0.0165	0.0381
P	p-Ethyltoluene	2	15	0.43549	0.09778	0.28165	0.35174	0.42744	0.52477	0.5302	0.6545
P	p-Ethyltoluene	3	15	0.00408	0.10759	-0.19176	-0.05638	0.00180	0.05652	0.1506	0.2328
P	p-Ethyltoluene	4	15	0.08785	0.15464	-0.16084	-0.02674	0.02949	0.20035	0.2977	0.3842
P	p-Ethyltoluene	6	40	-0.59303	0.06640	-0.74047	-0.64314	-0.57826	-0.54581	-0.5242	-0.4553
P	p-Ethyltoluene	7	15	0.03739	0.82178	-0.96796	-0.93512	0.09005	0.48151	1.2926	1.4223
P	p-Ethyltoluene	8	5	1.24386	3.09535	-0.61070	-0.37279	-0.11886	0.60047	6.7212	6.7212
P	trans-2-Butene	1	36	0.07949	0.02184	0.02082	0.06980	0.08259	0.09142	0.1029	0.1243
P	trans-2-Butene	2	36	0.17792	0.14737	-0.01821	0.02576	0.28356	0.31335	0.3250	0.3487

TARGET	CMPDNAME	VENDORID	n	mean	stddev	min	p25	median	p75	p90	max
P	trans-2-Butene	3	36	-0.00425	0.14288	-0.50731	-0.03164	0.02913	0.07296	0.1301	0.1930
P	trans-2-Butene	4	36	0.14145	0.16942	-0.20640	0.01971	0.17151	0.24599	0.3602	0.4488
P	trans-2-Butene	5	36	-0.09078	0.07562	-0.17869	-0.14151	-0.11032	-0.05943	-0.0017	0.1342
P	trans-2-Butene	6	111	-0.14252	0.43496	-0.81630	-0.46408	-0.17333	0.22151	0.3664	1.4469
P	trans-2-Butene	7	36	-0.35092	0.54358	-0.98642	-0.84466	-0.41483	-0.18023	0.5541	1.2485
P	trans-2-Butene	8	23	0.06928	0.34079	-0.48491	-0.03004	0.05813	0.09019	0.1573	1.4800