# A0344 Sage User Manual

Gas Autosampler

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## **Revision History**

Revision	Date	Notes	
А	December 2024	Initial release	
В	December 2024	Page 21. Number of shipped needles updated to 5. Note added regarding autosampler requires installation of needle for first time use.	
С	June 2025	Pre-installation requirements and compatible analyzers have been updated, and the Sage autosampler setup diagram and procedure have been revised. Additional instructions are now included for unboxing the autosampler and evacuating vials using an external vacuum pump. Appendix A (Evacuate Vials) and Appendix B (Offset Calibration) have also been added.	

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## 1 Introduction

The Picarro A0344 Sage gas autosampler is an advanced solution designed to automate the measurement of greenhouse gas (GHG) concentrations and stable isotope ratios in small discrete gas samples. It addresses the need for high-precision, low-maintenance systems in GHG and isotope analysis, making it the ideal tool for researchers who require efficiency and reliability.

This autosampler offers automated operation, working seamlessly with a variety of Picarro gas analyzers to ensure accurate, high-quality results. The 150-position vial rack, compatible with 12 mL head-space vials, allows for high throughput sample analysis, making it a practical choice for labs handling large volumes of samples.

The A0344 Sage gas autosampler is fully integrated with Picarro's suite of analyzers, creating a seamless workflow from sample introduction to data acquisition. The system's intuitive software allows for automated data analysis and easy export of results, accelerating the data review process. Additionally, the real-time preview feature provides immediate visualization of processed data, enabling researchers to quickly assess the results and make informed decisions.

By simplifying the entire workflow, from sample handling to data analysis, the A0344 Sage gas autosampler enhances lab efficiency while maintaining the precision required for advanced GHG and isotope measurements.

## 1.1 Intended Use

The Picarro A0344 Sage gas autosampler pairs with several of Picarro analyzers. The autosampler is a XYZ sampler system and can prepare, move, and inject samples into Picarro analyzers.

During normal operation of the analyzer, the autosampler is controlled by software running on the computer installed on the Picarro analyzer. This software coordinates sample injections with the Picarro instrument and eliminates the need for user intervention during automated multiple-sample runs. However, there are some one-time set up and once-perrun operations which need to be performed directly with the autosampler software. These are described in this document.

## 1.2 Hardware Overview

### 1.2.1 Front Panel

The front panel of the A0344 Sage gas autosampler has a cover, two LED status lights, a power switch that illuminates when the power is on, a drawer to access the tray, and a lever to open the drawer.

- The orange status light (top) illuminates if the cover is open.
- The red status light (bottom) illuminates if the drawer is open. The A0344 Sage gas autosampler will stop sampling and the arm will return to its home position.
- The power button illuminates when the power is on.
- You can lift the clear cover manually. This provides access to replace the needle, for example.
- The drawer contains the tray of samples. You open it by sliding the opening lever to the right.



Figure 1 - Front view of the A0344 Sage gas autosampler

### 1.2.2 Back Panel

The back panel of the gas autosampler contains a sample inlet port, a flush port, USB communications, and the power connection.



Figure 2 - Back panel of the A0344 Sage gas autosampler



Figure 3 - Back panel connections

## 1.3 Specifications

Parameter	Specifications	
Maximum Number of Vials	150	
Needle	Picarro recommends BD PrecisionGlide™ 22 G X 1" Hypodermic Needles. Equivalent syringes from other manufacturers may be used.	
Vials	Double wadded Labco 12 mL Exetainer vials	
Software	On board software ensures seamless operation, automated data analysis, and real-time preview	
Operating system	Compatible with Windows 10, Windows 11, and Linux Ubuntu 20.04	
	17" w X 13" h X 12.2" d (43.3 x 33.2 x 30 cm) not including 0.25" feet	
Dimensions	Back clearance: 2.5" (65 mm)	
Weight	24.5 lb. (11.1 kg)	
Flootrical	Voltage: 24 VDC	
Electrical	Current: 1.5 A	
Power	110 - 230 VAC, 50/60 Hz	
Requirement	Note: Use only the power adapter supplied by Picarro	
Operating Temperature	4 °C (40 °F) to 40 °C (104 °F)	
Storage Temperature	4 °C (40 °F ) to 50 °C (122 °F)	
Relative Humidity	10% to 75% non-condensing	

Table 1 - Specifications for the A0344 Sage gas autosampler

## 1.4 Compatible Analyzers

Table 2 - Analyzers compatible with the A0344 Sage gas autosampler

NOTE

Existing analyzers require Windows 10 or above.

Model Number	Gases Measured	
G2131- <i>i</i>	$\delta^{13}$ C in CO <sub>2</sub>	
G2201-i	$\delta^{13}$ C in CO <sub>2</sub> and CH <sub>4</sub>	
G2210-i	$\delta^{13}$ C in CH <sub>4</sub> , CH <sub>4</sub> and C <sub>2</sub> H <sub>6</sub>	
G2301 CO <sub>2</sub> , CH <sub>4</sub> , H <sub>2</sub> O		
G2401 CO <sub>2</sub> , CO, CH <sub>4</sub> , H <sub>2</sub> O		
G2508	$N_2O$ , $CH_4$ , $CO_2$ , $NH_3$ , $H_2O$	
G5131- <i>i</i>	$\delta^{15}N,\delta^{15}N\alpha,\delta^{15}N\beta,and\delta^{18}O$ in $N_2O$	
PI5131- <i>i</i>	$\delta^{15}N,\delta^{15}N\alpha,\delta^{15}N\beta,and\delta^{18}O$ in $N_2O$	
G5310 N <sub>2</sub> O, CO, H <sub>2</sub> O		
PI5310	N <sub>2</sub> O, CO, H <sub>2</sub> O	

## 2 Safety

The following chapter provides an overview of warning symbols used in this document, general safety guidelines for using the A0344 Sage gas autosampler, and acquired certifications.

## 2.1 Warning Symbols

The purpose of these icons is to provide a visual convention to alert you of important information. They indicate dangers to either the operator or to the product, and other important information. The following symbols are used in this manual.

WARNING indicates a potentially hazardous situation which, if not avoided, could result in death or severe injury.

#### 

PINCH POINT alerts the user of a potential pinch point.

CAUTION alerts user of a potential danger to equipment or to the user.



HOT SURFACE alerts user to potential injury from hot surfaces.

### 

The NOTE is important information to be aware of before proceeding.

## 2.2 General Safety

This section describes the CE certifications for regulatory conformity for the European Union.

### 2.2.1 CE Certification

This Picarro analyzer complies with the European standards and the instrument is affixed with a CE label. This CE label is located on the rear of the instrument.

### 

Using the A0344 Sagein a manner not specified by Picarro may result in damage to the Sage and render it unsafe to operate.



The A0344 Sage is for indoor use only and has an ingress protection rating of IPx-0. It is NOT protected against exposure to water including dripping, spraying, splashing or immersion.

#### 

Do not operate in an explosive atmosphere! Do not operate in the presence of flammable gases or fumes.

### 

When using compressed gases, follow all appropriate safety conventions, including use of eye protection, physical restraint of cylinders, etc.

### 

Do not replace the mains supply power cord with an inadequately rated cord.

### 

The A0344 Sage contains no user-serviceable components except those specified in the Maintenance chapter of this user manual.

Do not attempt repairs; instead, report all problems to Picarro Customer Support or your local distributor. Please contact Picarro if you have any questions regarding the safe operation of this equipment.

### 

Equipment Damage: Exceeding gas inlet pressure or temperature specifications could result in damage to the instrument. In the case of higher input pressure or flow, configuring a sampling bypass manifold system is recommended. Use a 'tee' at the gas inlet and exhaust the remainder of the gas stream appropriately.

### HOT SURFACE

The inlet gas connector on the back panel of the A0344 Sage, and its immediate vicinity, run hot during operation of the A0344 Sage. Take care when connecting gas lines or working at the rear of the instrument to wear protective gloves or avoid contact with these surfaces.

### 

The A0344 Sage uses needles to sample gas from vials. Used needles are a biohazard and must be disposed of according to local or national regulations.

#### 

Pinch Point Danger: The A0344 Sage has automatically moving parts which may suddenly and unexpectedly change position. Please keep the cover closed and your hands away from the unit during operation.

## 3 Pre-Installation Requirements

The A0344 Sage gas autosampler is intended to be used as an accessory to compatible Picarro analyzers (for a list of analyzers that are compatible with the A0344 Sage, see section 1.4 Compatible Analyzers). It cannot function as a stand-alone device. The following preinstallation requirements are divided into two segments: requirements, and optional aspects a user may wish to prepare prior to installation. The accessory kit contains the required connectors and fittings to install and operate the A0344 Sage gas autosampler.

#### **Required:**

- Picarro analyzer
- A0344 Sage autosampler
- Flush gas tank (refer to section 3.3 Gas Line Connections).

#### Optional:

- A0346 Sage Sample Preparation Kit
- Additional A2000 pump
- A minimum of two reference gases are needed for automated calibrations.
- Double Wadded 12 mL Labco vials (100 vials included in the A0346 kit)

#### NOTE

If users do not have A0346 kit or the additional external pump for vial evacuation and preparation, they can consult Picarro for alternative methods."

## 3.1 QuickStart

Before connecting gas lines, connect your A0344 Sage gas autosampler to the analyzer by using a USB cable. Power on both the A0344 Sage gas autosampler and the CRDS analyzer to verify that they function properly and communicate with each other.

#### To test the connection:

- 1. Connect the USB cable from the A0344 Sage gas autosampler to any USB port on the CRDS analyzer.
- 2. Remove the port caps on the Sample and the Flush ports.
- 3. Connect the power cable to the A0344 Sage gas autosampler.
- 4. Press the power switch on the front of the autosampler.

The green LED on the power switch illuminates to indicate that the power is on.

## 3.2 Installing the Software from a USB flash drive

If you purchased the A0344 Sage gas autosampler separately and already own an analyzer, you must install the Sage software on your analyzer.

#### To install the software from the included USB flash drive:

- 1. Insert the USB drive included in the installation kit into any USB port on your Picarro analyzer.
- 2. Run the included software installation program.
- 3. Open the Sage software interface by double-clicking the icon on the analyzer desktop.

## 3.3 Gas Line Connections

Flush gas connections on the A0344 Sage gas autosampler are 1/8" Swagelok fittings and 1/8" tubing.

- Fittings can be tightened with a 7/16" wrench. Initially hand-tighten the connector onto the port, and then tighten the connector an additional 1/4 turn using a 7/16" wrench.
- Gas output from the A0344 Sage gas autosampler to CRDS inlet is 1/16" OD tubing with 1/16" Swagelok fittings on the A0344 Sage input port and connected via an adapter to 1/4" inlet port of the CRDS analyzer.

Use this tightening procedure for all following Swagelok connections.

For an illustration of gas connections between the A0344 Sage gas autosampler and the Picarro analyzer, see 5.3 A0344 Sage Startup and Setup.

#### To connect a gas line:

1. Connect your flush gas line to the A0344 Sage gas autosampler "Flush" port.

There is a 1/8" gas line in the installation kit. Ensure the ultra high purity zero air or  $N_2$  tank being used for flush is connected with a 2-stage regulator, whose delivery pressure is adjusted to 2.5 psi units. Exceeding the maximum of 5 psi pressure can cause damage to the CRDS analyzer.

Refer to the CRDS analyzer user manual for further information.

2. Connect the 1/16" green tubing from the input port on the A0344 Sage gas autosampler to the analyzer's sample inlet. Use 5/16 wrench to tighten the 1/16" compression fitting on the Sage gas output and 9/16" wrench to tighten the 1/4" compression fitting on analyzer inlet.

## 4 Unpacking

Picarro products are inspected and tested before leaving the factory. Their packing containers have been designed to keep the equipment safe from damage during transit.

## 4.1 Inspect the Shipping Boxes

Inspect the condition of all boxes upon arrival. Even if the outer box shows damage, the inner box holding the analyzer will protect the instrument under most circumstances.

If the equipment does appear to be damaged, photograph the damage and contact Picarro (email pictures) as soon as possible.



Keep all packing materials so the instrument can easily be returned Picarro if necessary or transported to another location.

## 4.2 Unboxing Contents

Use caution when unboxing the autosampler. The unit contains delicate components that may be damaged by improper handling. To ensure safe setup and protect the integrity of the equipment, please follow the steps in this procedure exactly as outlined.

### 

Failure to follow the recommended unboxing procedure may result in equipment damage and void warranty coverage.

- 1. Make sure the box is on a stable and flat surface that can properly support the autosamplers box and contents.
- 2. Using a box cutter or scissors carefully cut along the tape seams and gently open the flaps.
- 3. Remove the documentation and parts packet as shown in the following figure.



Documentation and supplied parts

Figure 4 - Shipping Packet

4. With two people, carefully lift the autosampler unit from the box. Use the grab handles to lift from the bottom of the autosampler while another person holds the cardboard box. Set the autosampler on a flat and stable surface.





Figure 5 - Foam Grab Handles

5. Remove the outer foam inserts and open the autosampler cover to access the internal foam components.



Figure 6 - Autosampler Internal Foam Inserts

6. Remove the inner foam inserts in the following order.





1 Remove the center horizontal foam insert by carefully pulling and turning at an angle until the flange is removed from the notch of the vertical foam insert.

Remove the vertical foam insert

Figure 7 - Internal Foam Inserts Removal

## NOTE

Save all packaging materials in case of return or service needs.

- 7. Check the autosampler for any shipping-related damage before setup.
- 8. If the equipment does appear to be damaged, photograph the damage and contact Picarro (email pictures) as soon as possible.

### 4.3 Box Contents

The following items are included in the gas autosampler box:

- A0344 Sage gas autosampler
- Tray for 150 vials
- Power adapter
- USB 2.0 (Type A)-to-USB cable (Type B), 3 ft (1 meter) in length
- 1/16" tubing for the sample line, preassembled with a Swagelok fitting and an adapter, 4 ft (1.3 m) in length

One end connects to the gas autosampler sample outlet, the other connects to the analyzer sample inlet

- for zero air:
  - 1/8" tubing for zero air, 12 ft (4 m) in length
  - Swagelok set (including nuts, ferrules, and an adapter) to connect to the zero-air cylinder
  - Swagelok set to connect to the flush port on the gas autosampler
- 4 nuts and ferrules for 1/16"
- 4 nuts and ferrules for 1/8"
- Protective covers for the sample outlet and flush inlet
- Plastic bag containing accessories
- USB Flash Drive
- User Manual
- A set of 5 Needles

The Sage gas auto sampler does not come with a pre-installed needle to avoid breakage. It is required to install a needle for first time setup and use. For more information about installing a needle, see section 9.1 Replace the Needle.

Table 3 - Options and recommendations for tubing and connections

Tubing and Accessories (A0344 Box)	Part Number
1/16" nut + ferrules on gas autosampler's side	SS-100-NFSET
1/16" nut and ferrule on analyzer side	Swagelok SS-100-NFSET

Tubing and Accessories (A0344 Box)	Part Number
1/6" to 1/4" adapter	Swagelok SS-100-R-4
1/4" ferrule set	Swagelok SS-400-NFSET

## 5 Hardware Installation and Setup

Follow the steps described in this section to make the proper gas and electrical connections.

## 5.1 Setup Safety

#### \Lambda WARNING

When using compressed gases, follow all appropriate safety conventions, including use of eye protection, physical restraint of cylinders, etc.

#### 

When the A0344 Sage gas autosampler and the analyzer are being integrated to an external system, the safety of that system is the responsibility of the assembler of that system.

#### NOTE

It is imperative that all gas connections be free of leaks to achieve proper measurement of a sample and ensure performance of the system. All gas connections should be made with stainless steel tubing and Swagelok connectors.

### A HOT SURFACE

The inlet gas connector on the back panel of the analyzer, and its immediate vicinity, runs hot during operation of the analyzer. Take care when connecting gas lines or working at the rear of the instrument to wear protective gloves or avoid contact with these surfaces.

## 5.2 Required Analyzer Setup

A Picarro analyzer is required to run the A0344 Sage gas autosampler and its software. The basic gas analyzer setup (CRDS analyzer and external vacuum pump) can be found in its user manual.



Figure 8 - Basic analyzer setup

### 5.2.1 Instrument Dimensions and Placement

The A0344 Sage gas autosampler is 17" w X 13" h X 12.2" d (43.3 x 33.2 x 30 cm) and weighs 24.15 lb. (11.1 kg). It can be placed directly on top of a Picarro analyzer.



It is imperative that the A0344 Sage gas autosampler, analyzer, and other peripherals have adequate ventilation and cooling to maintain the ambient temperature below 35 °C (95 °F) when operating.

Failure to provide adequate airflow, especially clearance at the front and rear panels, to ensure proper airflow and cooling to the equipment will result in overheating the analyzer, causing a shutdown and potential damage.

There should be 2" (5 cm) of clearance in the front and back of the equipment.

Thermal Specifications	Min	Max	Description
Ambient Operating	4 °C	40 °C	Worst-case environmental limits
Temperature	(40 °F)	(104 °F)	(unless otherwise specified)

## 5.3 A0344 Sage Startup and Setup



Figure 9 - A0344 Sage gas autosampler to analyzer connections



Before you begin, ensure all pre-installation requirements have been met. For information, see section 1 Pre-Installation Requirements.

- 1. Place the A0344 Sage gas autosampler on top or to the side of the analyzer.
- 2. Remove all gas port caps.
- 3. Install one needle after removing the luer lock cap in the autosampler's arm. Refer to the following image.



2 Remove zip ties by pulling from specified location (top end)

Twist to remove plastic cap for needle installation

Figure 10 - Autosampler Needle Installation - Initial Setup

4. Plug in the communication cable and power cable to power-on the A0344 Sage gas autosampler.



To ensure the best precision measurements, the companion analyzer should be allowed to run for at least 2 hrs prior to making the final gas connection from the A0344 Sage gas autosampler to the analyzer (the analyzer must be stabilized). There should be no gas connection between the A0344 Sage gas autosampler and analyzer as the analyzer is starting up.



All gas connection ports on the A0344 Sage gas autosampler accept 1/4" Swagelok female connectors. When connecting gas lines to the ports, initially finger tighten the Swagelok fittings and then tighten the fittings another 1/4 turn using the provided 9/16" wrench.

5. Once all hardware connections have been made, you can run the Sage software. Refer to Chapter 6, Softwarein the manual.

NOTE

The autosampler may require calibration before running an experiment due to the offset of the autosampler's arm caused during shipping. For more information, see Appendix B, Offset Calibration.

## 6 Software

The Picarro Sage Gas Autosampler software automates sample measurement and streamlines data analysis of the results. Powerful new tools generate real-time data visualizations, calibration curves, and other actionable data for faster, easier sample analysis and interpretation.

The Sage software has the following pages:

- <u>Method</u>
- <u>Run</u>
- Results
- Settings

You'll use those pages to:

- Run an experiment
- View the results of an experiment

## 6.1 About the Pages

All pages share common elements that you'll use as you work with them. These include:



Figure 11 - Common elements of Sage pages

## 6.2 Information on the Status Bar

The status bar at the bottom of the application provides information about the current status of the application, its connection to an analyzer, and information logged by the application.

## ΡΙСΔ R R O





You can view the logs by clicking **Show Logs**. The logs appear above the status bar and the button changes to *Hide Logs*. Click **Hide Logs** to hide the logs.

		1		2
	20: 14/11/2024 10:12:57:			
	20. 14/11/2024 10.12.30.			
20: 14/11/2024 10:12:57: 1000000000000000000000000000000000000		Connected to Sage	Instrument type:	Hide Logs



The log items appear in a panel above the status bar.

The button changes names to Hide Logs.

Figure 13 - Status bar example with the logs shown

## 6.3 The Method Page

The *Method* page shows the currently defined sampling methods available for your experiments. You can also create and define new sampling methods.



Figure 14 - The Method page

### 6.3.1 About Method Timing

The sampling methods determine how long each phase of the sampling takes. There are two primary phases:

**Flush**, which is the time specified to flush the lines so that the analyzer is ready to sample the gas in a vial. Gases for flushing could be zero air or  $N_2$  depending on the installed modes on the CRDS analyzer and the intended application.

**Sample**, which is the time specified for the autosampler to sample each vial. The sample time is divided into three phases, and the total number of seconds indicated for sampling is divided among them:

- Stabilization, where the system begins taking on the gas from the sample but the line is not yet wholly composed of the sample gas, but may still contain the reference gas introduced during flushing. This time is set to ensure that the sample gas fully occupies the sampling lines.
- **Measurement**, where the sampling data is captured. This data is considered to be accurate during this phase.
- **Post Measurement**, where the autosampler has a few seconds to reset and finalize the readings from the sample. This value is the remainder of the difference between the *Sample* time minus the *Stabilization* and *Measurement* time values. You cannot edit this value other than by changing the values for the other three. The value must be more than 5 seconds and is recommended to be less than 30 seconds.

The method phases are color-coded in the plots.



Figure 15 - Method phases and associated colors



The timing of stabilization and measurements should be chosen wisely, as including rise and fall of the peak data within the measurement will deteriorate the standard deviation of the data.

## 6.4 The Run Page

You use the *Run* page to set up and run an experiment, and to monitor the experiment's results, which display in real-time as the experiment commences.

Run pages include:

- The Sample List tab, where you create and set up experiments.
- The **Real Time** tab, where you monitor the currently running experiment.

### 6.4.1 Sample List Tab

In the *Sample List* tab, you set up the experiment. You can create a new experiment or choose from existing experiments, modify settings, or duplicate.

If you're creating a new experiment, you'll first provide a name for the experiment and select the sampling method you want to use. Then you'll add information in the *Sample List* area about your samples that you want to test.

Using the pop-up window, you can indicate the location on the tray for each group of vials you add to the sample group. For each sample group, you can also choose the sample type and standard name.

### 

After you start an experiment, information about the currently running experiment appears at the top of the Sage software page.

## ΡΙΟΔ R R Ο

	1		2		3	
Sample List Real Time						
Experin Experin Exper Samplin Defau	nent Tamplate Settings nent Name ng Method 0	Group Name Vials	Sample Type Standard Name	Im Sampling Meth	Import Export thod Anthod © @	
	New Open Save Save As Copy	Replace Needle	Deter	Al Rous •Ad	Add Row Start	
1	1Experiment Template Settings area, where you can name your experiment and select a sampling method.5			5	<ul><li>Button to <u>replace the needle</u>.</li><li>Removes all rows in the detail area for the selected experiment.</li></ul>	
2	2 The <i>Sample List</i> area—including details, locations, and whether the vial isa standard or quality control sample.			Adds a row to the list of vials in the experiment.		
3	<ul> <li>Buttons to import or export a CSV file</li> <li>of the vial data.</li> </ul>			Starts the experiment.		
4	4 Buttons to create, open, or save experiment data files.					
Figur	Figure 16 - The Run page, Sample List tab					
## 6.4.2 Real Time Tab

The *Real Time* tab displays the current readings in real time. The readings are color coded to show the different stages, such as standby, flush, stabilization, measurement, and post-measurement stages.



Figure 17 - The Run page, Real Time tab

# 6.5 The Results Page

You can view and interpret the results of your experiments on the Results page. The Results page has four tabs:

- Vial Results
- Calibration Curve
- Experiment Results
- Export Data

#### 6.5.1 The Vial Results Tab

The Vial Results tab displays a list of vials, their names, and their status for a selected experiment. You can view two available species measurements in plots and view the mean and standard deviation calculations derived during the measurement period.

The plots let you evaluate the quality of the sampling process - you can see every time point for each variable and determine if there was an issue with a specific measurement, such as a leak, improper pressurization, or the zero air turned off.



List of vials.

3

Data selection box.

Figure 18 - The Results page, Vial Results tab



Calculated mean and standard deviation for the displayed variable.

#### 6.5.2 The Calibration Curve Tab

On the calibration curve page, you can view the already-selected experiment or select a different one from the drop list.

If the experiment measured a series of standards, the Sage Software can use the values to construct a calibration curve. This calibration can then be used to calculate an adjusted or "corrected" result for each vial. You can exclude the results from individual vials if they appear as outliers to ensure that the calibration curve is as accurate as possible.



- Buttons to automatically exclude all flagged vials, or to include all vials regardless of outlier flags
- 4 Vial list, showing which are included, which are outliers, and which are excluded

- - Calculations for the included vials
- The calibration curve

Figure 19 - The Results page, Calibration Curve tab

### **View Calibration Curve Details**

Click a point on the calibration curve to highlight the corresponding vial in the vial list on the left pane.



Figure 20 - Drag to view detailed measurement points

You may need to zoom in to see multiple vial measurements that are closely spaced on the curve. To do so, drag within the calibration curve area around the point of interest.



Figure 21 - Drag to zoom in on tightly grouped points

Double-click within the calibration curve to return to normal zoom.

### Flags on the Calibration Curve Page

Flags indicate results of the automatic outlier calculations, depending on which species (or data key) is selected to view.

- **Pred flag** indicates a pressure outlier.
- Folid black flag indicates a measurement outlier for the selected species or data key.
- **WE** Checkered black flag indicates that there is a measurement outlier for that vial, but not for the selected species or data key.

$= \mathcal{A}$	NOTE

Automatic flags are not a substitute for review by an expert. They are simply an indication of a possible outlier. Sometimes outliers may be missed or non-outliers may be flagged.

Flagged items display details when hovered over.



Figure 22 - Hover over a flag to view details

## **Removing Outliers**

You can exclude outliers and problem vial readings by clearing the check box next to vial number.



- Shows vials individually or by sample groups.
- 3 Excludes all flagged readings or includes all readings.
- are excluded or included.
- Excluded values are shown with a hollow circle.

Figure 23 - Exclude flagged values to correct the data calculations

### View by Sample Groups

You can also view the vial results by the <u>group assigned when creating the sample list.</u> In doing so, you can exclude entire sample groups.

If you select a group, the associated vials appear in the bottom pane, where you can work with them as in the vial view.

v 🔘	Gro	up View	
Flagge	d Val	ues	Include All
•	#	Name	Standard
	1	DCC CUA	DC ( Mathema
	2	BC0 CH4	DC ( Mathana
	2	BC6 CH4	BC 6 Methane
	3	BC6 CH4	BC 6 Methane
	4	BC6 CH4	BC 6 Methane
	5	BC6 CH4	BC 6 Methane
8 <b>&gt;</b>	6	BC6 CH4	BC 6 Methane
	21	DOE COR	DOE Carbon Di
	21	BUSCUZ	BC5 Carbon Di
	22	BC5 CO2	BC5 Carbon Di
	22 23	BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
	22 23 24	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
	21 22 23 24 25	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
•	21 22 23 24 25 26	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
-	21 22 23 24 25 26 31	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC4 Carbon D
•	21 22 23 24 25 26 31 32	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC 4 Carbon D BC 4 Carbon D
•	21 22 23 24 25 26 31 32 33	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2 BC4 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC 4 Carbon D BC 4 Carbon D
•	21 22 23 24 25 26 31 32 33 34	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2 BC4 CO2 BC4 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC 4 Carbon D BC 4 Carbon D BC 4 Carbon D BC 4 Carbon D

Figure 24 - Vial View compared to Group View

## 6.5.3 The Experiment Results Tab

The Experiment Results tab displays the measured and corrected results of the experiment. Like the Calibration tab, you can include or exclude readings from your results.

Measurement values are shown for all sample types on this tab. If a calibration curve has been calculated for the displayed species, both the originally measured value and the corrected value can be displayed here.



You can't include or exclude standards from this page, as doing so would alter the calibration curve without seeing the effect.

0	2	3	4	•	5	6			7					
Vial Res	ults Cali	bration Curve	Experiment	Results Export	Data									
Sele	ect Expe ime otopic Carbor	ent n Experiment A	UG23	<sup>12</sup> CH <sub>4</sub> , High	Precision, dry 0		Me	easured Value:	82.5313 Correc	ted Value: 100.3	780			
	Show Co	orrected easured		100		••••								
In	clude 🕨 🟲	# Name	Standar	80	-	••••								
	** ** *	33      BC4 CO        34      BC4 CO        35      BC4 CO        36      BC4 CO        41      N2        42      N2        43      N2        44      N2        45      N2        46      N2        51      SAMPLI        52      SAMPLI        54      SAMPLI        55      SAMPLI        56      SAMPLI	2 BC 4 Carbon I 2 BC 4 Carbon I Empty Standa Empty Standa Empty Standa Empty Standa E E E E E E E	C (mdd)	<b>*****</b> •	10	•••••• 20 3 Vial	••••••• 30 #	40	50				
1	The	select	ed exp	periment			5	Thes	selecte	ed spec	cies.			
2	Sho	ws inc	lividua	l or grou	ps of vi	als.	6	Corre	ected sured s	values	are s are ir	hown i vellov	n greer	1;
3	Sho valu	w or h es.	ides co	prrected	or mea	sured	7	Calc	ulated	values	5.	. ,		
4	Vial: a se	s inclu lected	ded in I check	the resu box.	llts shov	w with								

Figure 25 - The Results page, Experiment Results tab

### View by Sample Groups

You can also view the vial results by the <u>group assigned when creating the sample list.</u> In doing so, you can exclude entire sample groups.

If you select a group, the associated vials appear in the bottom pane, where you can work with them as in the vial view.

v 🔘	Gro	up View	
Flagge	d Val	ues	Include All
•	#	Name	Standard
	1	DCC CUA	DC ( Mathema
	2	BC0 CH4	DC ( Mathana
	2	BC6 CH4	BC 6 Methane
	3	BC6 CH4	BC 6 Methane
	4	BC6 CH4	BC 6 Methane
	5	BC6 CH4	BC 6 Methane
8 <b>&gt;</b>	6	BC6 CH4	BC 6 Methane
	21	DOE COR	DOE Carbon Di
	21	BUSCUZ	BC5 Carbon Di
	22	BC5 CO2	BC5 Carbon Di
	22 23	BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
	22 23 24	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
	21 22 23 24 25	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
•	21 22 23 24 25 26	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di
-	21 22 23 24 25 26 31	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC4 Carbon D
•	21 22 23 24 25 26 31 32	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC 4 Carbon D BC 4 Carbon D
•	21 22 23 24 25 26 31 32 33	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2 BC4 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC 4 Carbon D BC 4 Carbon D BC 4 Carbon D
•	21 22 23 24 25 26 31 32 33 34	BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC5 CO2 BC4 CO2 BC4 CO2 BC4 CO2 BC4 CO2	BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC5 Carbon Di BC 4 Carbon D BC 4 Carbon D BC 4 Carbon D BC 4 Carbon D

Figure 26 - Vial View compared to Group View

## 6.5.4 The Export Data Tab

Once you are satisfied with the results, you can export the data to csv file format. They can then continue data analysis according to your individual research needs.



The modifications you make, such as excluding vials, are not saved within the software. Instead, you must export the data in order to have a record of the results.

# ΡΙCΔRRΟ

The experiment that you selected on the previous *Results* page tab is automatically selected here for data export. You can select the type of export file or type of data. Each check box corresponds to a different kind of export file with different information.

You can also export Quality Control (QC) sample measurements that may carry across several months of experiments. You can select a date range for the QC data.

Exported data is saved on your local disk in this location:

2 Export Data Calibration C ent Results (Updated) QCs Export Experiment Customize your data export selecting the specific results you need from the expe Select a date range for exporting QC Choose vial-specific data, calibration curves, or full experiment results. Start 2024/08/14 2024/11/12 (2024/08/23 14:15 -08:00) Isotopic Carbon Experiment AUG23 Select Select Reset Reset Include in Export Vial Results Measurement Period Only Calibration Curve Select Date × Experiment Results un Mon Tue Wed Thu Fri 27 28 29 30 31 44 Group Results 4 5 6 11 12 13 18 19 20 45 3 10 7 8 9 46 14 15 16 Standards 47 17 21 22 28 29 23 30 48 24 25 26 27 49 1 2 3 4 5 6 7 OK Cancel The selected experiment. Export a range of QC data. To specify the start or end date range, click Select which data to include from the Select and choose a date on the date experiment. picker.

C:\Users\[User\_Name]\Documents\Picarro Sage

Figure 27 - The Results page, Export Data tab

# 6.6 The Settings Page

You can use the Settings page to set or change the default settings, or when you want to manage standards, or manually control the autosampler. Settings pages include:

The <u>Settings</u> tab, where you can set serial port connection and specify how long that the system keeps data.

The <u>Standards</u> tab, where you can view an existing standard, edit an existing standard, or create a new standard.

The <u>Manual Control</u> tab, where you can control individual components of the autosampler for troubleshooting purposes.

## 6.6.1 The Settings Tab

You use this tab to specify the serial port to connect to and whether the system should connect automatically on startup. You can also set up a data retention duration after which the Sage Software will notify you that data exceeds that time frame and ask whether you wish to delete it. A



The Sage Software will prompt you on startup if data is older than the time period selected for the Data Retention field, but will not automatically delete data. If you choose to wait until later, it will prompt you again the next time you start up the software.



Figure 28 - The Settings page, Settings tab

## 6.6.2 The Standards Tab

On the Standards tab, you define standards that can be used in your experiments. Standards specify a physical tank of gas with specific certified concentrations or deltas (or both).

The page contains a list of standards, and the details defined within it. You can <u>add new</u> <u>standards</u>, <u>edit and save changes you make to standards</u>, and <u>duplicate standards</u> by saving as a new name before editing the copy.

To see the details for a standard, select it from the list to populate the details area.

tings	Standards	Manual Control							
	Standard	Last Updated							Û
1			Name			Manufacturer			
2			Empty Standard						
3			Serial Number			Expiration Date			
4								Select	Clea
5			Created: 2024-08-16	12:05:51		Last Updated: 2024-	08-16 12:05:51		
6			Species	Certified Concentratio	n Units	Certified Delta	Units		
7			CH₄	○ 0	ppm	0	‰	Clear	Û
8	Empty Standard	2024-08-16	CO-			0	9/	Clear	•
10	Empty Standard	2024 00 10	002	Ŭ	ppm	U	/60	Clear	<u> </u>
11									
11									
11 12									
11 12 13	_								
11 12 13 14	_								
11 12 13 14 15	-								
11 12 13 14 15 16	_								
11 12 13 14 15 16 17	-								
11 12 13 14 15 16 17	New Stan	dard	Save Save As				+ A(	dd Row	Cance
11 12 13 14 15 16 17	New Stand	dard	Save Save As				+ Ac	dd Row	Cance
11 12 13 14 15 16 17	New Stan	dard	Save Save As				+ Ac	dd Row	Cance
11 12 13 14 15 16 17	New Stand	dard	Save Save As 5 The selected	4 (	Create	es a standar	+ Ac d.	dd Row	Cance
11 12 13 14 15 16 17 17	New Stand	dard tandards. T	Save As 5 The selected ed.	4 (	Create	es a standar	+ Ad	dd Row	Cance
11 12 13 14 15 16 17 16 17	New Stand 4 Existing standard in Details for	tandards. T is highlight r the standa	Save Save As 5 The selected ed. ard.	4 (	Create Saves standa	es a standar changes yc ard, or saves	+ Ad d. bu make s a copy	dd Row 6 to a	Cance

## 6.6.3 The Manual Control Tab

You can use the Manual Control tab to troubleshoot the autosampler or your sample preparation. This page lets you specify a vial position and move the needle to it, raise and lower the needle, open and close the valve, and change a needle.



- 1 A visual representation of the tray of vials. Select a position to move the needle to that location.
- 2 Click **Find Home** to return the needle to the standby position.
- 3 Click **Insert Needle** to insert the needle into the selected vial. Click **Raise Needle** to withdraw the needle.

Figure 30 - The Settings page, Manual Control tab

- 4 Click **Replace Needle** to pause the system so that you can change the needle.
- 5 Click **Open Valve** to open the valve. Click **Close Valve** to close it.
- 6 Click **Motors Off** to stop the motors from actively maintaining the position of the arm.

# 7 Run an Experiment

Running an experiment on the A0344 Sage gas autosampler occurs in two phases: the work you do setting up the physical sampling vials and trays, and the sampling done automatically by the A0344 Sage gas autosampler using the software settings you choose.

Here's an overview of the process, with links to the detailed procedures you'll follow to conduct the experiment.

## NOTE

The autosampler may require calibration before running an experiment due to the offset of the autosampler's arm caused during shipping. For more information, see Appendix B, Offset Calibration.

#### To run an experiment:

1. Evacuate the vials you will use in your experiment.

Follow your preferred method. You can also evacuate vials <u>using a Picarro pump and the</u> sample preparation kit A0346.

2. Place the vials in the autosampler tray. You'll want to mark and identify the location and contents of each vial, including which are used for calibration.

You can do this downloading a comma-separated value (CSV) file from the Sage software and then using your favorite spreadsheet tool to document them. You can later import the file to quickly populate the experiment data.

## 

Ideally each sample experiment should include a set of 3 standards per variable. A minimum of two standards is a must to be able to use the calibration feature of Sage software. You can also add Quality Control (QC) vials in each experiment. Sage software is enabled with the tracking of QC data over time.

3. <u>Fill the vials with the gas samples from a tank</u> or <u>gas bag or other container</u>.

If using a standard gas tank to fill vials directly, delivery pressure should be 9 psi (no less than 7 psi and no greater than 11 psi).

4. Place the vials in the autosampler and close the cover.

### 🔌 WARNING

The autosampler is designed to operate only with the cover closed. You should never attempt to enter the autosampler chamber while it is running as it can move unexpectedly and cause bodily injury or equipment damage.

- 5. Power on your analyzer and launch the <u>Sage software app</u> once you've completed the physical setup of the experiment.
- 6. <u>Create or select the standards</u> you want to use for the experiment. Ideally, you'll have at least three standards for each experiment, but a minimum of two is required. (You can also create quality control standards.)
- Create or select the method for the experiment. An example for the method timing is given below:
  - Flush 120s
  - Stabilization 180s
  - Measurement 90
  - Post-measurement 10s
- 8. <u>Define your experiment by entering experiment details</u>, including the vial location and contents on the tray.

You can enter vial data values <u>manually</u> or <u>import a CSV file</u> to add the detail rows quickly.

9. Click Start to begin the experiment.

## 7.1 Prepare Vials for an Experiment

As you prepare your vials for an experiment, you must first evacuate the vials, and then fill the evacuated vials with gas from an external source.



Accuracy in concentration measurements may be dependent on how well vials are evacuated and filled with sample gases.

#### 

For information about evacuating vials using a Picarro vacuum pump, see Appendix A, Evacuate Vials.

## 7.1.1 Fill Vials from a Tank

Follow the steps below to transfer calibration gas directly from a gas tank or cylinder into the A0344 Sage exetainer vials.

#### To transfer calibration gas from a tank or cylinder:

1. Evacuate the vials to remove any gasses.

For information on evacuating vials, see Appendix A, Evacuate Vials.

- 2. Use the 1/8" tubing in the A0344 Sage sample preparation kit to connect to the included luer lock using 1/8" compression fitting.
- 3. Connect the included needle to the luer lock and prepare the tubing.
- 4. Prepare the standard gas tank with a 2-stage regulator and connect the prepared tubing to the regulator.
- 5. Ensure the gas tank regulator and tubing connections are leak tight.



Refer to Picarro video tutorial webpage for leak-check tutorials.

6. Once the connections are set, open the valve from the gas tank, and adjust the delivery pressure to less than 9 psi on the delivery stage of the regulator.

When you open the safety cover of the needle, you will feel gas passing through the needle. Use caution around the open end of the needle.

- 7. Place evacuated vials in an external sample preparation holder tray.
- 8. Insert the needle, while the gas flow is on, through the septum of the vial.
- 9. Hold this set-up steady, without bending the needle, for approximately 10 seconds.
- 10. Swiftly lift the needle out of the vial.
- 11. Repeat the previous three steps for each vial you want to fill with the gas.

When you switch to a different gas tank, flush the lines before filling vials to avoid contamination with the previous concentration of standard gas.

## 7.1.2 Fill Vials from a Gas Bag or Other Sources

Follow the steps below to transfer a gas sample from gas bags or other sources into the A0344 Sage exetainer vials.



Figure 31 - Preparing to fill vials from a gas bag

#### To fill vials from a gas bag or other source:

- Evacuate the vials to remove any gasses.
  For information on evacuating vials, see Appendix A, Evacuate Vials.
- Arrange pre-labeled and pre-evacuated vials in the external sample holding tray.
  For each sample, we recommend three replicate vials.
- 3. Use the Teflon tape to make a leak-tight connection of the included syringe and needle.
- 4. Ensure there is a septum through which the syringe with needle can be used to extract gas sample.

# ΡΙΟΔ R R Ο



Figure 32 - Filling a syringe from a gas bag

- 5. Extract at least >20 mL of gas sample from the source.
- 6. Insert the needle of the syringe into the evacuated vial.
- 7. Open the valve.

Pre-evacuated vials take in the gas sample as soon as the needle is inserted and the valve is opened on the syringe.

8. Push the syringe so that at least 20 mL of sample gas is inserted into the vial. Needle pressure-based data quality checks work better when the vial is over-pressured (for example filled up to 30 mL).



Figure 33 - Filling the vial

9. Repeat steps #5-8 to fill replicate vials based on sample availability.

This procedure can also be used to fill gas bags with calibration gases ahead of time.

# 7.2 Download the CSV File

You can download a comma-separated value (CSV) file that you can use to document the location and contents of the vials offline, and then import later to quickly add the information in your experiment.

#### To download a blank sample list as a comma-separated value (CSV) file:

- 1. Click **Run** to load the *Run* page, *Sample List* tab.
- 2. Click Export.
- 3. Locate the destination folder and type a file name for the export file and click **Save**.

The exported file, when opened, resembles the figure below, with column heads and one sample row of data.

	Α	В	С	D	E
1	vials	group_name	standard	group_type	sampling_method
2	1	Sample Group Name		Unknown	Default Sampling Method
3					
4					
5					
-					

Figure 34 - The csv export file opened in a spreadsheet program

# 7.3 Working with Standards

A standard determines the gas species, including concentration and delta, that will be used as the known value to compare against.

## 7.3.1 Create a Standard

You can create one or more standards that specify the certified concentration and/or delta for the species of interest.

#### To create a standard:

- 1. On the *Settings* page, click the **Standards** tab.
- 2. In the left pane, click New Standard.
- 3. In the right pane, in the **Name** field, type a name for the standard.
- 4. (Optional) In the **Manufacturer** field, type a name for the manufacturer of the tank or standard.
- 5. (Optional) In the **Serial Number** field, type the serial number of the tank or standard.
- 6. (Optional) Click **Select** in the *Expiration Date* area to select an expiration date for the sample.
- 7. In the **Species** drop-down, select the species for the sample.
- 8. In the **Certified Concentration** field, enter a value in parts-per-million (ppm) of the species for the sample.
- 9. In the **Certified Delta** field, enter a value as a percentage.

#### 

You can add additional species entries for the sample.

- To add additional species entries, click Add Row and complete the fields.
- To remove rows, click the Delete button at the end of the row you want to remove.

10. Click **Save** to save the standard.

## 7.3.2 Edit a Standard

You can edit an existing standard and then save it under the same name, or save as a new name to duplicate the standard.

#### To edit a standard:

1. On the *Settings* page, click the **Standards** tab.

- 2. In the left pane, click the name of the standard you want to edit.
- 3. Modify the fields you want to change.
- 4. Click **Save** to save the standard.
  - OR

Click **Save As** to save the standard under a different name.

## 7.3.3 Duplicate a Standard

You can open an existing standard and then save it under a new name to duplicate the standard.

#### To duplicate a standard:

- 1. On the *Settings* page, click the **Standards** tab.
- 2. In the left pane, click the name of the standard you want to duplicate.
- 3. (Optional) Modify the fields you want to change.
- 4. Click **Save As** to save the standard under a different name.

## 7.4 Working with Methods

A method determines the timing of the sampling process, from the initial flushing of the analyzer lines to the time to allow for stabilization of the gas within the lines, the actual sampling times, and time between sampling sequences for the system to reset.

You can access methods on the Methods page.

### 7.4.1 View and Select a Method

#### To view details about a defined sampling method:

1. In the *Method* page, select the sampling method you want to view.

The method values appear in the details area.

## 7.4.2 Add a Method

#### To add a new method:

1. In the *Method* page, click **Add New Method**.

The Enter Method Name dialog box appears.

- 2. Enter a name for the sampling method you want to add.
- 3. Click OK.

The new sampling method displays in the Method List and in the details area.

4. In the **Flush** box, enter the number of seconds required to clear the lines of previous gasses. This duration will vary depending on the flow rate and the system volume.

- 5. In the **Sample** box, enter the number of seconds the equipment will take readings from the samples. This value will equal the cumulative value of the *Stabilization*, *Measurement*, and *Post Measurement* boxes.
- 6. In the **Stabilization** box, enter the number of seconds you want to allow the equipment to rest and stabilize after flushing the system of previous gasses.
- 7. In the **Measurement** box, enter the number of seconds for each reading.
- 8. In the **Post Measurement** box, review the number of seconds the equipment should pause after each reading.

The post-measurement duration is calculated automatically as the difference between the *Sample* box and the values in the *Stabilization* and *Measurement* boxes. If the value is outside the optimal range of 5-30 seconds, adjust the values in the other boxes until this value is within the optimal range.

9. Click **Save** to save the method.

## 7.4.3 Edit a Method

#### To edit a method:

- 1. In the *Method* page, select the sampling method you want to edit.
- 2. Adjust the values as appropriate.
- 3. Click Save.

## 7.4.4 Duplicate a Method

#### To duplicate a method:

- 1. In the *Method* page, select the sampling method you want to duplicate.
- 2. Adjust the values as appropriate.
- 3. Click Save As...
- 4. In the Enter Method Name box, enter a name for the revised sampling method and click OK.

## 7.4.5 Delete a Method

#### To delete an existing method:

- 1. In the *Method* page, select the sampling method you want to edit.
- 2. Click **1 Delete**.
- 3. In the *Confirm Deletion* box, click **Yes** to delete it.

## 7.5 Add Experiment Details

Once you've prepared your samples and selected the experiment's standard and method, create the experiment details file, where you enter the location of each vial and its contents on the *Sample List* tab on the *Run* page.

If you created a comma-separated value (CSV) file of the sample list, you can import that file to quickly complete the details about the samples.

Once you've added all details, you can start the experiment.

### 7.5.1 Create a New Experiment

When you create a new experiment, you name it and choose a default sampling method. Then you enter the sample details, including the location of vials, their type (unknown, standard, or QC) and their content, the standard name (if the content type is standard), and the sampling method to use, if different from the experiment's default.

#### To create a new experiment:

- 1. On the *Run* page, click the <u>Sample List</u> tab.
- 2. In the **Experiment Name** field, type a name for the experiment.
- 3. In the **Sampling Method** field, select the desired sampling method for the experiment.
- 4. In the right pane, enter information about each group of samples.

You can enter the sample group information manually or from a CSV import file.

5. Click **Save** to save the experiment file.

## 7.5.2 Add Sample Details to an Experiment

Each experiment lists the specifics of vial location and contents. You do that on the right pane of the *Sample List* tab of the *Run* page.

#### 

Follow these steps to manually add details for your samples. You can also <u>import a CSV</u> <u>file</u> to quickly add this information.

#### To manually add sample details:

1. In the **Group Name** field, type a name that describes the group.

NOTE

Providing a group name allows you to group like samples and to view the measurement results individually or by groups on the Results page.

2. Click 🖉 to see the Vial Selection pop-up.



Figure 35 - The Vial Selection pop-up

3. Click individual vial locations on the tray to specify where this sample group is located. OR

Click and drag a range of locations.

## 

Depending on your planned sampling sequence, there is an option to drag and select a row, which can be assigned to one sample group. For example, if a standard gas will be analyzed in 3 replicate vials, you can drag and select one row (highlighting 3 vial locations) and assign that group to the standard.





NOTE	
You can also specify loca	tions by typing the locations directly in the Vials field.

4. In the **Sample Type** box, select the type of sample for this group.

You can choose from:

- Unknown the vials containing the samples you want to test.
- Standard the vials containing the gas species identified in a standard.
- **QC** vials containing a known version of the species you want to use as a quality control for the experiment.
- 5. If the sample type is *Standard*, in the **Standard Name** box, select the standard to apply.
- 6. In the **Sampling Method** box, select the sampling method, if different from the default.

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## 

The *Sampling Method* box is editable only if the sampling method selected for the experiment in the Experiment Template area (left pane) is *By Row*. Otherwise the selected sampling method applies to all samples in the experiment.

Experiment Template Settings Experiment Name Experiment Name Sampling Method By Row O	Group Name Vials Sample Type Sample 0 1 OC C	Standard Name	Import Sampling Method Default Sampling Method	Export	
1 If you select experiment	t By Row as the 's sampling method		2 yo meth	u mu nod fo	ist select a sampling or each entry.

Figure 37 - The Sampling Method drop-down, with By Row selected.

- 7. To add an additional sample group row, click +Add Row.
- 8. Follow the above steps to complete the information for each sample group row.

## 7.5.3 Import Sample Details for an Experiment

The Sample List provides the details of vial location and contents. You do that on the right pane of the *Sample List* tab of the *Run* page.



Follow these steps to import a CSV file to quickly add this information. You can also manually add details for your samples.

#### To import sample details:

- 1. Click Import.
- 2. In the Open Sample List dialog box, locate the CSV file you want to import.
- 3. Click **Open** to import the file.

# 8 View Results

You can view results as soon as an experiment has completed. You'll do that on the *Results* page.

For the *Vial Results*, *Calibration Curve*, and *Experiment Results* tabs, you'll first need to select an experiment to see the data.

# 8.1 Using the Vial Results Tab

The Vial Results tab provides data for each vial in the experiment. You can select a vial from the list and then choose a variable for each of the upper and lower plots. When you do that, you'll see the measurement data for that vial plotted in graph form.

To quickly compare the two variables against multiple vials, select the vial from the list and press the up and down arrow keys to scroll through the plots for each of the vials. Doing this might enable you to detect vials that produced measurements that are outliers, due perhaps to a leaky septum or under-pressurized vial.

You can also compare multiple variables for an individual vial. Select the vial you want and then select the first variable in the upper plot. Press the up and down arrow keys to scroll through the variables for that vial.

To view the variable data plots with the same time frame and zoom level, select Align Time Axes. When you zoom in on one plot, the other zooms in at the same level.

For additional information on using the Vial Results tab, see 6.5.1 The Vial Results Tab.

# 8.2 Using the Calibration Curve Tab

The Calibration Curve tab calculates a calibration curve based on the vial measurements. You can detect and exclude outliers and problem readings to ensure that your data is accurate.

You can view the list of vials in two ways:

- As individual vials based on their tray location.
- As groups of vials based on how they were grouped when entered into the *Sample List* tab on the *Run* page.

For example, you may have grouped samples based on a commonality such as field work date or location. Viewing by group enables you to view statistics across all vials in a group, include or exclude a group's samples, or exclude all other samples to focus on a single group.

The Sage Software automatically flags measurements with anomalous data so that you can look more closely to determine if they are outliers and should be excluded. You can choose whether to exclude them, and you can also exclude outliers that you detected based on your evaluation of the measurements on the *Vial Results* tab.

As you include or exclude vial measurements, the calibration curve is recalculated in real time.

For additional information on using the *Calibration Curve* tab, see 6.5.2 The Calibration Curve Tab.

# 8.3 Using the Experiment Results Tab

On the Experiment Results tab, you can toggle between corrected (i.e. calibrated against the chosen calibration curve from the section above) and measured (i.e. not calibrated) values.

Like the *Vial Results* tab, you can press the up and down arrow keys to scroll through the vials or the variables. And like the Calibration Curve tab, you can view the list of vials either individually or by groups.

#### 

If you make a change on the Calibration Curve tab, such as by including or excluding a vial reading, the tab name changes to *Experiment Results (Updated)* to indicate that the values on this tab have changed. The tab name reverts back when you visit the *Experiment Results* tab.

For additional information on using the *Experiment Results* tab, see 6.5.3 The Experiment Results Tab.

## 8.4 Using the Export Data Tab

You can customize and download data on the Export Data tab.

You can choose which data measurements or calculations you want to include from the *Include in Export* list. Select a check box to include the corresponding data. The data in this export is limited to the selected experiment.

The exported data can be used offline as spreadsheets on external computers for archiving and further evaluation and processing.

### 

Do not install third-party data processing applications on the Picarro analyzer.

You can also export Quality Control (QC) data for a range of dates. This QC export is not limited to a single experiment.

Exported data is saved on your local disk in this location:

C:\Users\[User\_Name]\Documents\Picarro Sage

For additional information on using the *Export Data* tab, see 6.5.4 The Export Data Tab.

# 8.5 Understanding Results

The Sage software creates graphs of the vial measurements to visually represent the data. An example is shown below.



Figure 38 - A sample view of the *Results* page

Figure 38 displays various stages of sampling a vial.

The blue stage is the *flush* stage, where the lines are being flushed with UZA/N2 and hence the vial result displays a near zero  $CO_2$  value.

As soon as sampling phase begins, the needle punctures the septum, which is generally accompanied by a rise in needle pressure and then a steep fall. This is the *stabilization* stage and it displays the steady rise of  $CO_2$  as the analyzer starts measuring the actual vial's sample gas.

The green phase is the *measurement* phase which is used by the Sage software to calculate individual vial results. Once the measurement is completed, the sampling ends by a *post measurement* phase, as the needle steadily retracts form the vial.



The timing of stabilization and measurements should be chosen wisely, as including rise and fall of the peak data within the measurement will deteriorate the standard deviation of the data.

# 9 Maintenance

To ensure the best performance of your A0344 Sage gas autosampler, follow these guidelines:

- Replace the needle after 2000 injections.
- Follow best practices for maintaining the CRDS analyzer.
- If using the external evacuation pump and 4-way valve system (refer to appendix for evacuation of vials), ensure pump is powered off as soon as evacuation sequence is completed, and 4-way valve turned to A0344 Sage-CRDS direction.

# 9.1 Replace the Needle

The needle should be replaced after 2000 injections.

#### 

After replacing a needle, best practice is to test the needle position and operation by using the Manual Control options on one or more vials.

#### 

Before replacing a needle, ensure that the A0344 Sage is not currently active in an experiment. The XYZ arm can move suddenly and unexpectedly when autosampling and may cause bodily injury and damage to the instrument.

#### To replace the needle:

- 1. Start the Sage software and go to the *Settings* page, *Manual Control* tab.
- 2. Click Replace Needle.

The XYZ arm moves to the needle-change position.

- 3. Open the cover of the A0344 Sage autosampler.
- 4. Disconnect the current needle from the luer lock at the XYZ arm of the A0344 Sage autosampler.



1) The needle in the luer lock.

Figure 39 - The needle inside the autosampler

- 5. Replace with the new needle.
- 6. Ensure the needle is connected and locked into the luer lock of the XYZ arm.
- 7. Close the cover on the A0344 Sage autosampler.
- 8. Click Done.

## 9.2 Replace the Needle During an Experiment

If you must replace a needle during an experiment, you must first pause the experiment.

To replace the needle during an experiment:

While an experiment is in progress, the *Replace Needle* button is disabled.

1. On the *Run* page, press **Pause**.

The instrument completes the sampling of the current vial and then the arm moves to its home position. No further samples will be taken.

2. Click Replace Needle.

The arm moves to a convenient location for needle replacement.

- 3. Open the cover of the A0344 Sage autosampler.
- 4. Disconnect the current needle from the luer lock at the XYZ arm of the A0344 Sage autosampler.
- 5. Replace with the new needle.
- 6. Ensure the needle is connected and locked into the luer lock of the XYZ arm.
- 7. Close the cover.
- 8. Click **Done** when the needle has been replaced.
- 9. Click **Resume** to continue the experiment.

# 10 Troubleshooting

# 10.1 Test the vacuum in the vials: the bubble test

It is important to test the vacuum in the vials that will be used. An easy way of testing the vacuum is the bubble test.

#### To bubble-test vials:

- 1. Take 10 evacuated exetainers.
- 2. Take a needle (no syringe) (22Ga works).
- 3. Hold the exetainer under water, and put the needle in the septum.
- 4. Wait for the vial to fill with water.
- 5. Repeat for the other exetainers.
- 6. Look at the size of the bubble left in the exetainers.

The bubbles should be small (2-3 mm) and equal in size for all exetainers.



Figure 40 - Vials filled with water, showing equal small bubbles, indicating good vials

# 10.2 Leaks

#### **Needle Pressure**

Good injections typically have a higher needle pressure reading as soon as the needle punctures the septum during an injection for sampling. However, lower pressure does not necessarily suggest a bad injection. The image below shows a vial reading as an outlier because it had low needle pressure at the start of sampling. This is likely because of an under-pressurized vial or a leaky septum.

# ΡΙСΔ R R O



Figure 41 - Plots indicating that the needle pressure is faulty

### **Outlet valve**

Outlet valve behavior can also be used to track bad injections.



Figure 42 - A good and bad injection differs in outlet valve behavior

# 10.3 Septum Caps Over-Tightened

Caps should be optimally tightened and too much tightness leads to septum kink and subsequent leaks.

## 

It is very important not to over-tighten the caps. The butyl rubber septum will be pushed into the vial. Holes from previous piercings of the septa will open up. It is likely that the vial will leak. It is also possible that the needle will bend when the caps are too tight.



Figure 43 - Septa caps tightened correctly and over-tightened

# 10.4 Reused Septa

Septa that have been reused and punctured multiple times may have difficulty sealing.

# ΡΙΟΔ R R Ο





A septum with multiple punctures

An unused septum

Figure 44 - Bad and good septa

# 10.5 Outliers on Calibration Curve

Check for outliers. Flagged data points should be reviewed by users and excluded from calibration as appropriate. Some outliers may also exist in concentration or isotope variables, which need to be reviewed and excluded accordingly. Below is an example of how R<sup>2</sup> improves based on inclusion or exclusion of outliers.


Figure 45 - Outliers on the calibration curve

## 10.6 Manual Control of the Sage Gas Autosampler

You can use the <u>Manual Control</u> options, located on the <u>Settings</u> page, to test or troubleshoot the autosampler or your sample preparation setup.

The manual control of the A0344 Sage can help you troubleshoot and perform preventative maintenance.

For example, from this page you can:

- Move the arm to an optimal spot for needle replacement.
- Turn on or off the valve for the flush gas tank valve.
- Move the arm to the home position.
- Test the behaviors of XYZ arm by manually selecting a vial position.
- Export diagnostic data to help your service representative troubleshoot remotely.

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10.7



You can export diagnostic data to help your service representative troubleshoot remotely.

#### To export data remotely:

- 1. In Sage software, click **Settings** and then **Manual Control**.
- 2. On the *Manual Control* page, click **Export Diagnostic Data**.
- 3. Provide a name for the saved data file.
- 4. Click Export.

# A Evacuate Vials

Before filling the vials with the gas you intend to measure, you must first evacuate the vials from any existing gas and ambient air to ensure an accurate reading. Follow the instructions below to evacuate vials using a Picarro A2000 or similar external vacuum pump and the A0346 Sage Sample Preparation Kit.

## A.1 Sage Sample Preparation Kit



Figure 47 - A0346 Sage Sample Preparation Kit Example

ltem	Sage Sample Preparation Kit	Quantity
1	Exetainers with caps & septa	100 (1 box)
2	Nut with ferrule, 1/8" Swagelok	1
3	Valve, manual switching, double diagonal, bulkhead, peek/PTFE, 4- position, 4-port	1
4	Needles, luer lock, metal hub side port	10
5	Syringe 60 mL, single use, sterile	2
6	FTG, 1/16" nut with front-ferrule & back-ferrule set	1

Item	Sage Sample Preparation Kit	Quantity
7	Fitting, luer lock to 1/8" compression, male	1
8	Peek tubing, 1/16" OD, 0.03" ID, opaque green	5
9	Fitting, reducing union, 3/8" tube OD x 1/16 OD	1
12	Tubing 1/8" OD, 1/16" ID	2
1	Gas sample bag, 7" x 7", 82°C max, ~2 psi max, PVF	1
12	Stopcock, one-way with male luer lock	2

## A.2 Evacuating Vials Using an External Vacuum Pump

#### 

Before you begin:

- Use Sage Sample Preparation kit (A0346) as you follow the vial evacuation steps.
- Ensure the A2000 pump's voltage is set as per the local guidelines and connected to power.
- You can also evacuate and prepare the vials using alternative methods if you do not have an A0346 Kit. Consult Picarro for more information.
- 1. Refer to Figure 49 for the complete tubing and component layout before beginning the following steps. Use the parts provided in the A0344 Sage and A0346 kit boxes.

The green 1/16" tubing supplied in the A0346 kit must be cut into three equal lengths using a tubing cutter.

- a. **Piece 1:** Attach the end with the **1/16" nut/ferrule** to the **Sample** port on the Sage device.
- b. Piece 2: Attach the end with the 1/16" to 1/4" adapter to the analyzer's Sample Inlet.
- c. Piece 3: Use the plain tubing (no fittings) to connect to the 3/8" adapter for the external A2000 pump hose.

(pump not included in kits A0346/A0344).

d. Connect the opposite ends of all three tubing pieces to the 4-way valve using the plastic nuts and ferrules provided in the 4-way valve bag.
Ensure all fittings are oriented correctly as shown in Figure 48.



Figure 48 - Plastic Nut/Ferrule



Figure 49 - Evacuation setup using the A0346 Kit



2. Ensure the 4-way valve is turned to evacuation.

Figure 50 - Setup of the four-way valve

## 

This setup ensures that while the external pump is used to evacuate vials using the A0344 Sage gas autosampler, the analyzer's inlet allows ambient air to flow in. Any deviation from this setup may result in overly restricting airflow into the cavity and, over time, cause damage.

- 3. Launch the Sage software application.
- 4. From the main menu, click the **Method** and, if you do not have an existing evacuation method, create one and name it *evacuation*.

For information on creating a method, see 6.3 The Method Page.

Sample evacuation method time settings:

Flush = 5 seconds Sample = 60 seconds Stabilization = 10 seconds Measurement = 45 seconds Post measurement = 5 seconds

- 5. From the main menu, click **Run**, and then the **Sample List** tab.
- 6. In the **Sampling Method** dropdown, select evacuation.
- 7. In the sample area, specify the vial positions to be evacuated in this sequence.

For information on adding vial information and specifying positions, see section **7.5 Add Experiment Details**.

- 8. Power on the external vacuum pump.
- 9. Click Start to begin the evacuation run.

The progress of the evacuation run appears at the top of the Sage software page, including the time remaining until the run is complete.

	NOTE					
	No data from the vials are collected by the analyzer. During this run, the data the appears in the Sage software is the ambient air measured by the analyzer durine vacuation step.					
10. When the evacuation is complete, turn off the power to the external evacuation pump.						
Evacuated vials should be filled up with samples/reference gases as quickly possible after evacuation.						
	If the every stad viele mu	at he stored before filling, use parafilm to sover the conta				

If the evacuated vials must be stored before filling, use parafilm to cover the septa and avoid leaking ambient air into the vials.

# B Offset Calibration

The Sage software has an offset calibration feature if the autosampler's arm gets disoriented during shipping (or other instances). Picarro recommends using this feature after you have evaluated that the needle position has suffered from some offset and is no longer in the accurate position to puncture the vial cap in its central region. In that case, users can follow the steps below to recalibrate the position of the autosampler's arm.

1. Select the Settings Page, Manual Control, and Change XY Offset from the Sage software.



Figure 51 - Change XY Offset tab

2. Select X and Y in + and – directions to move the arm accordingly from the XY Offset Calibration dialog.

XY Offset calibration		×
	Default Offset	X: 1
		Y: 4
	Saved Offset	X: 1
Y-		Y: 4
	Current Offset	X: 1
X- X+		Y: 4
Y+	Calibration position is a	above vial 113
		Restore Default
	Save Cano	cel Exit

- 3. Once the arm is in the correct position to puncture the vial cap centrally, click **Save**.
- 4. If there is a mistake, use the **Restore Default** button to return to the original position.
- 5. Select **Exit** to have the autosampler arm go back to its Home position.

# C Limited Warranty

Limited Warranty for Picarro Products and Peripherals. Picarro warrants that during the Warranty Period the Picarro Products and Peripherals will be free from substantial defects in material and workmanship under normal uses, and will substantially conform to Picarro's published Specifications for the Product. "Specification" means the then current user guide, technical specification or other product documentation prepared by Picarro (and does not include marketing collateral). This limited warranty extends only to the original end-user ("Customer") of the Product.

**Warranty Period**. The Warranty Period commences upon shipment of the Product and the Warranty Period continues for a period of 13 (thirteen) months (for shipments directly to customers) or 15 (fifteen) months (for shipments to a Picarro partner).

**Warranty Remedies**. Customer's sole and exclusive remedy and the entire liability of Picarro and its suppliers under this limited warranty will be, at Picarro's option, repair of the Product; or shipment of a replacement Product within the warranty period and according to Picarro's replacement process; or a refund of the purchase price if the Product is returned to Picarro, freight and insurance prepaid. Picarro replacement parts used in Product replacement may be new or equivalent to new.

In the event Picarro repairs or replaces the Product under this warranty, then the Warranty Period will be extended for the longer of a) ninety (90) days, or b) the period of time during which Customer has been unable to use the Product based upon the date on which the Customer or partner first reported to Picarro the problem giving rise to the warranty claim.

As part of the Limited Warranty, during the Warranty Period Picarro may provide: (1) telephone and email technical support, including remote log-in capabilities during Picarro's regular support hours and (2) software updates that Picarro generally makes available without additional cost. Picarro will provide all parts and services required to repair or replace the Product, provided that repairs will be performed remotely or at Picarro's factory. Picarro reserves the right to use local, authorized partners to assist in providing warranty repairs and/or factory returns and End Customer will cooperate with such local partners.

Picarro's obligations hereunder are conditioned upon the return of the defective Product in accordance with Picarro's then-current Return Material Authorization (RMA) procedures. Customer or partner will pay for shipping of the Product to Picarro, and following repair of the Product Picarro will pay for return shipment to the Customer or partner under Incoterm DDP. Any other costs of shipment will be Customer's or partner's responsibility. Customer must follow instructions provided by Picarro for packaging and shipping the Product.

**Warranty Restrictions**. The above Product warranty does not apply if the Product (a) has been altered, except by Picarro or by Customer with Picarro's prior written approval, (b) has not been installed and used in accordance with Picarro's Specification, (c) has been subjected to abnormal physical or electrical stress, abnormal environmental conditions, misuse, negligence, or accident; (d) is licensed for beta, evaluation, testing or demonstration purposes; and (e) does not extend to recovery or replacement of any data from any medium. The Warranty Periods for spare parts, consumables and RMA repairs are not included in this document and are described under the Support Service Terms document.

**Disclaimer**: <u>Picarro disclaims all other warranties, either express or implied, including</u> warranties of fitness for a particular purpose. Except as set forth in this document, or as otherwise expressly agreed in writing by Picarro, there are no other warranties applicable to Picarro Products.

### **About Picarro**

Picarro is a leading provider of solutions to measure greenhouse gas (GHG) concentrations, trace gases, and stable isotopes across many scientific applications, along with the energy and utilities markets. Our patented Cavity Ring-Down Spectroscopy (CRDS) is at the heart of all Picarro instruments and solutions, enabling the detection of target molecules at part per billion or better resolution.

#### **Product Support**

Utilize Picarro support resources for product support. Join the Picarro community to ask questions and get answers, search the document library for datasheets and user manuals, download software, and purchase products and replacement parts. Access to online community forums and software downloads are available only for registered Picarro customers with login credentials. If you do not have an account, you can register by using the community and software download links below.

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Contact Picarro for questions regarding specific applications and additional information.

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