L21x0 Isotopic Water Analyzer
Installation and Operation Manual

PICARRO

Edition: July 2026, Revision J
Document Number: 40035

Picarro Inc. | 3105 Patrick Henry Drive | Santa Clara, CA 95054 USA
+1 408 982 3900 | www.picarro.com

Revision History

This section summarizes the revision history of this document. It provides a record of updates made across versions, including the revision identifier, publication date, and a brief description of key changes.

Revision	Date	Notes
J	July 2026	Updated the manual to reflect the Windows 11 operating system.

Picarro Notices

Thank you for purchasing a Picarro product. Your Picarro system is a quality product that was designed and manufactured to provide reliable performance.

This User Manual is an important part of your purchase as it will help familiarize you with the system and explain the numerous features that have been designed into it. Please read this manual thoroughly before using your Picarro system.

Please contact Picarro or your authorized Picarro distributor should you have questions regarding specific applications or if you require additional information.

DISCLAIMER AND RESERVATION OF RIGHTS

Picarro has prepared this manual solely for the information and use by its customers as a guide for the selection, installation, operation, and maintenance of the products described.

EXCEPT AS PROVIDED IN THE TERMS AND CONDITIONS OF SALE FOR PICARRO PRODUCTS, PICARRO ASSUMES NO LIABILITY WHATSOEVER, AND PICARRO DISCLAIMS ANY EXPRESS OR IMPLIED WARRANTY, RELATING TO SALE OR USE OF PICARRO PRODUCTS, INCLUDING LIABILITY OR WARRANTIES RELATING TO MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE.

Picarro reserves the right to change or update the contents of this manual and the specifications of its products at any time, without notice. Picarro has endeavored to include information that is current and accurate as of the date of the publication or revision of this document, but Picarro does not guarantee that this document is error free or that it is accurate regarding any particular specification.

Picarro expressly reserves all intellectual property rights, including all intellectual property rights relating to any product described in this manual. This document does not grant any license, express or implied, by estoppel or otherwise, to any intellectual property rights of Picarro or any third party.

PATENTS

The products described in this manual are subject to Picarro patents and patents pending. Information about Picarro patents applicable to these products is available at www.picarro.com/company/patents

TRADEMARKS

Picarro and the Picarro logo are trademarks of Picarro, Inc.
ChemCorrect™ is a trademark of Picarro, Inc.
Snoop® is a registered trademark of Swagelok Company.
Swagelok® is a trademark of Swagelok Company.
Windows® is a trademark of Microsoft Corporation.

Table of Contents

List of Figures

List of Tables

1 Read Before Using this Manual

This manual includes information on how to install the water analyzer in its most common configuration (analyzer with vaporizer). For other configurations (autosampler, SDM, IM, MCM, CWS), please refer to those manuals directly:

- **A0340 Autosampler User Manual** (PN 40-0094)
- **A0325 Autosampler User Manual** (PN 40025)
- **A0211 High-Precision Vaporizer User Manual** (PN 40-0044)
- **A0214 MCM User Manual** (PN 40022)
- **A0213 Induction Module-CRDS Setup User Manual** (PN 40033)
- **A0101 SDM User Manual** (PN 40-0005)
- **A0217 Continuous Water Sampler Installation and User Manual** (PN 40-0003)

NOTE

The High Throughput Vaporizer was discontinued in December 2013.

For information on Picarro's measurement technology, see Appendix C Introduction to Technology.

Be selective when following the manual by only referring to the sections relevant to your configuration of interest. To start, choose one of the setups in the table below based on your configuration.

Refer to Table of Contents to find the location of any of the chapters described below.

Table 1 - L21x0-i Setups & Configurations

Setup	Use Case	Setup Chapter
Basic Water Analyzer	This mode is used to measure ambient vapor which does not require any calibration with liquid standards.	See section 5 Hardware Installation and Setup. This setup requires a CRDS analyzer.

Setup	Use Case	Setup Chapter
Dual Mode	This mode is used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. The measurement mode alternates between analyzing ambient vapor and liquid standards based on a user defined sequence.	See section 5 Hardware Installation and Setup. This setup requires A0211 High Precision Vaporizer, A0912 Dual Mode Configuration hardware and software for vapor calibration and an Autosampler. This mode uses high precision method for liquid calibration. Each injection cycle takes 9 minutes.
Manual Mode	This mode is used for semi-automated measurement of liquid water samples with maximum precision.	See section 5 Hardware Installation and Setup. The setup requires an A0211 High Precision Vaporizer. User manually injects samples after prompt. The control of the vaporizer and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.

Setup	Use Case	Setup Chapter
Picarro Autosampler and High Precision Vaporizer (A0211)	This setup is used for automated injection of liquid waters. It consists of two modes that utilize the same hardware: High Precision Mode and High Throughput Mode.	See section 5 Hardware Installation and Setup. The setup can operate in five measurement modes: High Precision*, High Throughput*, Standard**, Express**, and Survey**. **High Precision* (same as Standard Mode):** Measures liquid water samples with maximum precision. Liquid samples are automatically injected and analyzed. Each injection cycle takes 9 minutes. **High Throughput*:** Used for faster measurement of liquid water samples with good precision. Liquid samples are automatically injected and analyzed. Each injection cycle takes 4 minutes. High Precision and High Throughput Coordinator Modes operate in the exact same fashion except that the steps of sample preparation and analysis are faster in the high throughput coordinator mode. **Standard** (same as High Precision Mode):** Used to measure liquid water samples with maximum precision. Automatically injects and analyzes liquid samples. Each injection cycle takes 9 minutes. **Express**:** Used for faster measurement of liquid water samples with good precision. Automatically injects and analyzes liquid water samples. when using the Express coordinator, we recommend 10 injections, the first 6 injections take 1.5 minutes each, while the last 4 injections take 5 minutes each. The first 7 injections will be discarded to achieve the optimal memory reduction.

Setup	Use Case	Setup Chapter
		Survey:** Used for super-fast measurements of large sample batches at moderate precision and enables more efficient sample sorting. By manually rearranging samples accordingly, one can reduce the memory effect between adjacent sample. Automatically injects and measures liquid samples. *Only available without Coordinator software upgrade **Only available with Coordinator software upgrade

2 Introduction

This user manual provides information for the installation, operation, and maintenance of the L2130-*i* and L2140-*i* isotopic water analyzers. These instruments are high-precision analytical systems designed to measure stable water isotope ratios using Picarro's patented Cavity Ring-Down Spectroscopy (CRDS) technology.

The L2130-*i* and L2140-*i* analyzers are intended for use by trained personnel in laboratory or field environments and support a wide range of scientific, industrial, and environmental monitoring applications. This manual describes the intended use of the analyzers, provides an overview of system components, and outlines essential operating and safety information required for reliable performance.

Unless otherwise noted, the information in this manual applies to both analyzers. Model-specific capabilities and differences are identified where applicable.

This section also includes intended use, system overview, analyzer specifications, a list of acronyms used throughout this manual, and an explanation of text conventions.

2.1 Intended Use

The L2140-*i* isotopic water analyzer measures concentrations of $\delta^{18}O$, $\delta^{17}O$, $\delta^{2}H$ and ^{17}O-excess using Picarro's patented Cavity Ring-Down Spectroscopy (CRDS).

The L2130-*i* isotopic water analyzer measures concentrations of $\delta^{18}O$ and $\delta^{2}H$.

The analyzer can be deployed for monitoring applications in a lab or in the field, allowing in-situ analysis of trace and ambient amounts of isotopic water.

NOTE

In this manual, $\delta^{2}H$ denotes the $^{2}H/^{1}H$ stable isotope ratio. The equivalent notation δD may appear in the software or result files.

2.2 System Overview

This section provides an overview of the L2130-*i* and L2140-*i* isotopic water analyzer systems and their primary components. It describes the analyzer hardware, the external vacuum pump, and the basic system configuration required for operation.

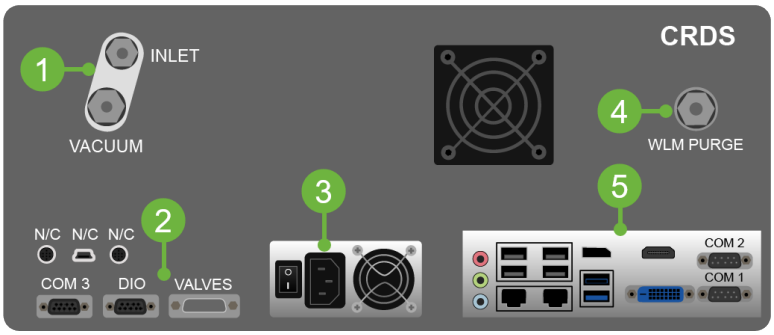
2.2.1 Analyzer

This section provides views of the analyzer front and back panels. More detailed information on panel features, functions, and connections are in section 5 Hardware Installation and Setup.

1 Soft Power Button

2 USB Port

Figure 1 - Front Panel



1 Sample Inlet and Vacuum Ports

2 Com/Valve Optional Ports

3 Main Power

4 WLM Purge Port (optional)

5 PC and Communication Ports

Figure 2 - Back Panel

2.2.2 A2000 Vacuum Pump

The A2000 vacuum pump is used to maintain cavity pressure inside the analyzer. The pump should be connected and running whenever the analyzer is in use.

Figure 3 - A2000 Vacuum Pump - Side Views

2.3 Analyzer Specifications

The following table provides the specifications for the L2130-*i* and L2140-*i* analyzers.

Table 2 - L2140-i, L2130-i L2140-iL2130-i Specifications

Parameter	Specification
Measurement Technique	Cavity Ring-Down Spectroscopy (CRDS)
Weight: Analyzer Weight: Pump	20.4 kg (45 lbs.) Should be lifted by two people. A2000: 6.5 kg (14.4 lbs)
L2140-*i* / L2130-*i* Analyzer Dimensions	Depth: 44.5 cm (17.5”) Width: 43.2 cm (17.0”) Height: 19.1 cm (7.5”) Height without Feet: 17.8 cm (7.0”)
Dimensions – A2000 Pump	Length: 34.5 cm (13.6”) Width: 15.5 cm (6.1”) Height: 22 cm (8.7”)
Ambient Humidity Range	< 85% RH non-condensing

Parameter	Specification
Ambient Temperature Range	Vapor Sample: -10 °C to 45 °C (14 °F to 113 °F) Liquid Sample & System Operation: 10 °C to 35 °C (50 °F to 95 °F) Storage: -10 °C to 50 °C (14 °F to 122 °F)
Maximum Altitude (During operation)	3,048 m (10,000 ft)
Front/Rear Clearance	Front: 15.3 cm (6”); Rear: 15.3 cm (6”)
Sample Pressure	300 to 1000 torr (40 to 133 kPa)
Sample Flowrate	~40 sccm at 760 torr (101 kPa)
Required Accessories	Included: Pump (external), keyboard, mouse Supplied by Customer: LCD monitor
Operating System Data Outputs	Windows 11 RS–232, Ethernet, USB, Analog (optional) 0-10 V
L2130-*i*/L2140-*i* Power Requirements Startup Power Steady-state Power	100 – 240 VAC; 50/60 Hz (auto-sensing) <375 W at start-up, (analyzer and pump) 120 W (analyzer) 150 W (A2000 Pump)
Minimum Rated Circuit Current (Amperes)	10A @ 115 VAC 5A @ 230 VAC
Liquid Ingress Protection	None

2.4 Acronyms

This manual includes various acronyms. For definitions, see below:

Table 3 - Acronyms, Formulas, Units, and Symbols

Acronym	Definition
“ (as in 1/4”)	Inches
°C	degrees Celsius
%	Percentage
±	Plus–minus sign
<	Less than
>	Greater than
≤	Less than or equal to
≥	Greater than or equal to
‰	per mil
µg	Microgram
µL	Microliter
µm	Micrometer
µmol	Micromole
A	Ampere
AC	Alternating Current
AMC	Airborne Molecular Contamination
ASCII	American Standard Code for Information Interchange
atm.	Atmosphere; unit of pressure, approximately equal to atmospheric pressure at sea level. 1 atm. = 14.69595 psi (101.325 kPa)
AUX	Auxiliary Port
bar	Metric unit of pressure. 1 bar = 100,000 pascals (Pa)
cc	current calibration
CDA	Clean Dry Air
CEMS	Continuous Emissions Monitoring System

Acronym	Definition
CH_4	Methane
cm	centimeters
CO_2	Carbon Dioxide
COM	Communication Port
CRDS	Cavity Ring-Down Spectroscopy
CSV	Comma Separated Values
CPU	Central Processing Unit
DAS	Data Acquisition System (the Analyzer)
DC	Direct Current
DCU	Data Collection Unit
DIO	Digital Input/Output
DI, DIW	DI, DIW Deionized Water
DLY	Delay
DVI	Digital Visual Interface
EMC	Electromagnetic Compatibility
EMO	Emergency Off
ESD	Electrostatic Discharge
EtO	Ethylene Oxide
°F	Degrees Fahrenheit
ft.	Length in feet;1 ft. = 12” or 12 inches (30.48 cm)
GUI	Graphical User Interface
H_2CO	Formaldehyde
H_2O	Water, Water Vapor
HB	Hotbox

Acronym	Definition
HBr	Hydrogen Bromide
HDF	Hierarchical Data Format
HDMI	High-Definition Multimedia Interface
HMI	Human Machine Interface
Hz	Hertz
ID	Inside Diameter (i.e., .5” ID) or Identification (i.e., Slave ID)
Inj	Injection
I/O	Input/output
kg	kilograms
kPa	Kilopascal; unit of pressure; 1 kPa = 0.145 PSI
lbs	pounds
LAN	Local Area Network
LPM	Liters per minute of flow
m	Meters or month
mA	Milliampere
max	Maximum
min	Minimum
mL	Milliliter
mK	Millikelvin
mm	millimeters / millimetre
MPM	Multi-Point Manifold
N/C	No Connection
NC	Normally Closed
NH_3	Ammonia

Acronym	Definition
NMP	N-Methylpyrrolidone or 1-methyl-2-pyrrolidone
NO	Normally Open
NTP	Network Time Protocol
OD	Outside Diameter
P	Pressure
PAIAC	Phosphoric Acid Impregnated Activated Charcoal
PCBA	Printed Circuit Board Assembly
PC	Personal Computer
PDF	Portable Document Format
PFA	Perfluoroalkoxy – A chemically resistant polymer, suitable for use with sticky and aggressive gases
PLC	Programmable Logic Controller
PN	Part Number
ppb	parts per billion
ppm	parts per million
PS/2	IBM Personal System/2 (6-pin mini-DIN connector)
PSI (psi)	Pounds per Square Inch
PSIG	Pounds per Square Gauge
PTFE	Polytetrafluoroethylene
Pws	Water vapor pressure
QC	Quality Control
RAM	Random Access Memory
RH	Relative Humidity
RJ-45	Registered Jack (physical network interface)
RO	Relay Outputs

Acronym	Definition
RS232	Recommended Standard 232 (serial communication protocol)
SCCM	Standard cubic centimeters per minute
SLPM	Standard Liters Per Minute
SNTP	Simple Network Time Protocol
sec	Seconds
SSL	Secure Sockets Layer
SSR	Solid State Relay
SS/SST	Stainless Steel
SVGA	Super Video Graphics Array
TEC	Thermoelectric Cooler
TCP/IP	Transmission Control Protocol/Internet Protocol
Torr	Torricelli (unit of pressure equal to 1/760 atmosphere)
UM	User Manual
USB	Universal Serial Bus
UPS	Uninterruptible Power Supply
VA	Volt-Ampere
VAC	Volts Alternating Current
VAP	Vaporizer
VDC	Volts Direct Current
VOC	Volatile Organic Compound
XML	Extensible Markup Language
W	Watts
WB	Warmbox
WLM	Wavelength Monitor
WMS	Workplace Monitoring System

2.5 Text Conventions

The following conventions are used in the manual.

- *Italic* text identifies screen names and to emphasize important text or certain features.
- ***Bold Italic*** text identifies section reference links.
- **Bold** text is for actions to take (such as clicking on a UI button), caution and warning statements, and text you should type or select in screens.

3 Safety

This chapter describes the safety information, hazard classifications, and handling requirements for the analyzer. It defines the warning symbols used throughout this manual and outlines general safety precautions, regulatory certifications, and system-specific hazards, including laser safety.

Read and follow all safety instructions before installing, operating, or servicing the analyzer. Failure to comply with these guidelines may result in personal injury, equipment damage, or unsafe operating conditions.

3.1 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.

DANGER

DANGER indicates an imminently hazardous situation that, if not avoided, will result in death or severe injury.

WARNING

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

WARNING

HAZARDOUS VOLTAGE alerts user to areas that may expose a user to electrical energy that is high enough to cause injury or death.

WARNING

LASER WARNING alerts user of a laser danger.

CAUTION

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

HOT SURFACE

HOT SURFACE alerts user to potential injury from hot surfaces.

NOTE

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

REMINDER

REMINDER is a helpful hint for procedures listed in the text.

3.2 General Safety

This section describes the CDRH and CE certifications for class 1 lasers and regulatory conformity for the European Union.

CDRH Certification

This Picarro analyzer complies with 21 CFR Chapter 1, sub-chapter J, and is classified as a Class 1 laser system when all panels and covers are on.

CE Certification

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

WARNING

Using this analyzer in a manner not specified by Picarro may result in damage to the analyzer and render it unsafe to operate

WARNING

This analyzer is for indoor use only and has an ingress protection rating of IPx-0. Analyzer is not protected against exposure to water including dripping, spraying, splashing or immersion

⚠ WARNING

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

⚠ CAUTION

The analyzer contains no user serviceable components except the particulate filter, CPU fan, fan kit (hotbox and ventilation fans), and A2000 vacuum pump diaphragms and valves. To order user-replaceable parts and access video replacement instructions, see section .

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

⚠ CAUTION

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

⚠ WARNING

If mounting in a 19” rack, this analyzer cannot support itself using a front rack mount kit alone. It must be supported by a shelf, or by user-provided “L” type support brackets.

⚠ CAUTION

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 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.

CAUTION

Equipment Damage: Do not disconnect the AC power to the analyzer, vacuum line, or the AC power to the external vacuum pump while analyzer is operating. Damage may be caused by current surges if power is applied while attaching or removing cables.

WARNING

This analyzer weighs 45 lbs. (20.4 kg). Use the technique described below when lifting the analyzer.

1. Before lifting, inspect the unit for slippery substances or sharp edges.
2. Lift with two people, one on each side of the analyzer.
3. Crouch down and stay close to the unit. Always keep your back as straight as possible.
4. Position your feet for sturdy balance. Lift with your legs, not your back.
5. Do not twist the back while carrying the unit. Rotate direction with hip joints.
6. Lower the unit by bending at the knees.

3.3 Laser Safety

This section describes the laser safety classification, labeling, and handling requirements for the analyzer. While the system is designated as a Class 1 laser product during normal operation, it contains an embedded higher-power laser that may present a hazard if the enclosure is opened.

Follow all safety instructions, observe all warning labels, and restrict service access to qualified personnel operating in approved laser-safe environments.

⚠ WARNING

This equipment is classified as a Class 1 laser product with an embedded 3B laser in accordance with EN 60825-1:2014. Do not to open the enclosure where this label is placed; there are no user serviceable parts inside.

The following laser safety Label is affixed to the outer cover of the analyzer.

Figure 4 - Laser Safety Label – Affixed to Outside Cover of Analyzer

⚠ WARNING

The laser is a Class3B when exposed.
Only operate or service this device in accordance with the instructions in this guide, and only open the device in an approved laser safe service area using appropriate laser-safety glasses.

The following laser safety label is affixed to the inside of the analyzer:

Figure 5 - Laser Safety Label – Affixed to Inside of Analyzer

⚠ WARNING

Use of controls or adjustments or performance of procedures other than those specified herein may result in hazardous radiation exposure.

⚠ WARNING

Any light emitted from the front panel status indicator, regardless of color or state, indicates one or more lasers are on.

4 Unpacking

This section provides instructions for inspecting and unpacking the analyzer and its associated components. Picarro products are inspected and tested prior to shipment, and the packaging is designed to protect the equipment from damage during normal transit.

Upon receipt, carefully inspect all shipping containers and contents before installation. Promptly report any damage or missing items to Picarro. Retain all original packaging materials for future transport, relocation, or service return of the analyzer.

4.1 Inspect the Shipping Boxes

Inspect the condition of all boxes upon arrival. The larger box includes the analyzer and most of the accessories. 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.

NOTE

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

4.2 Unpack Components

While unpacking each shipping box:

- Inspect each item to ensure it is not damaged.
- If items are missing, contact Picarro.
- Keep the shipping materials to reuse when transporting the analyzer.
- Contact Picarro for options on transporting systems to remote labs.

⚠ WARNING

This analyzer weighs 45 lbs. (20.4 kg). Use the technique described below when lifting the analyzer.

1. **Before lifting, inspect the unit for slippery substances or sharp edges.**
2. **Lift with two people, one on each side of the analyzer.**
3. **Crouch down and stay close to the unit. Always keep your back as straight as possible.**
4. **Position your feet for sturdy balance. Lift with your legs, not your back.**
5. **Do not twist the back while carrying the unit. Rotate direction with hip joints.**
6. **Lower the unit by bending at the knees.**

4.3 Contents

This section lists the components shipped with the analyzer. Items may be packaged in one or more shipping containers depending on the system configuration and ordered accessories.

Verify that all expected components are present and undamaged before proceeding with installation. If any items are missing or damaged, contact Picarro or your local distributor.

Table 4 - Shipping Contents

Part (qty)	Description
 **Analyzer (1)**	Includes all the data acquisition, control, and communications hardware and firmware to perform all gas handling, spectral collection, and analysis.
 **AC Power Cables (1)**	A power cable with connectors appropriate to your country is provided. **Note:** The analyzer automatically adjusts to local voltage.

Part (qty)	Description
 Nut (1) and Ferrules (2)	For connecting input line to analyzer gas input.
 Vacuum Hose (1)	Hose to connect the pump to the analyzer.
 Keyboard and Mouse (1)	Monitor is not included.
 Document Packet (1)	Includes this user manual and certificate of compliance (not shown).
 A2000 Vacuum Pump (1)	Provides vacuum required for sample gas sequencing into and out of the analyzer.

Part (qty)	Description
 AC Power Cable (1)	A power cable with connectors appropriate to your country is provided. **Note:** The vacuum pump voltage must be selected. See in section .
 Pump Manual (1)	Detailed instructions for pump.

5 Hardware Installation and Setup

This chapter describes the requirements and procedures for installing and configuring the L2130-*i* and L2140-*i* Isotopic Water Analyzers and associated peripherals. It identifies the items and tools required for installation, outlines applicable safety considerations, and describes environmental and ventilation requirements necessary for proper system operation.

This chapter also provides instructions for setting the external vacuum pump voltage and for performing the basic analyzer setup. Configuration procedures are included for **Dual Mode**, **Manual Mode**, and operation with the **Picarro Autosampler and High Precision Vaporizer (A0211)**. Dual Mode setup supports alternating measurements of ambient vapor and liquid calibration standards using a user-defined sequence and requires additional hardware and software components.

NOTE

Installation and setup procedures in this chapter are intended for trained personnel. Detailed operational procedures and system configuration options are described in subsequent chapters.

5.1 Items/Tools Required

- Analyzer and accessories included in shipment
- Pump and accessories included in shipment
- Peripherals and accessories included in the shipment according to your order
- 5/8” open end wrench
- 11/16’’ open end wrench
- Power cords for analyzer, pump, and peripherals

5.2 Installation Safety

Read this safety section in its entirety before proceeding.

WARNING

Two-person lift required: The analyzer weighs 20.4 kg (45 lbs). When lifting the analyzer, use the technique described in General Safety **(or follow your local regulations).**

⚠ WARNING

When the analyzer is being integrated to an external system, the safety of that system is the responsibility of the assembler of that system.

⚠ WARNING

Equipment Damage: Do not attach electrical power to or start the analyzer until after attaching and turning on the External Vacuum Pump. Do not disconnect the vacuum line while the analyzer is running. Failure to do so could result in damage to the optics.

⚠ WARNING

Picarro sells certain USB enabled devices, such as GPS, which are approved for use. Do not connect USB hubs or unauthorized USB devices (except flash drives, mice, and keyboards) to the USB ports. Unauthorized USB devices may interfere with the normal functioning of the analyzer.

⚠ WARNING

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

⚠ CAUTION

Lines connected to the 1/4" Swagelok sample inlet connector must not exceed 5 PSIG of pressure. Picarro recommends 2 to 3 PSIG of pressure.

⚠ CAUTION

During installation, do not position the analyzer so that it is difficult to operate the electrical disconnecting device (such as an emergency off (EMO) switch or breaker).

⚠ CAUTION

When working with hazardous gases, remove the pump exhaust muffler, adapt a tube to the vacuum pump exhaust port and direct the exhaust to a safe place for venting the mixture of sample gases. For instructions, see 17 Troubleshooting.

⚠ CAUTION

Use the AC power cables supplied with the analyzer or a similarly rated cable. Check with Picarro technical support if you have questions about power cable replacement. An inadequately rated power cable can result in equipment damage.

⚠ CAUTION

Cords shall be rated for the maximum current for the equipment and the cable used shall meet the requirements of IEC 60227 or IEC 60245. Cords certified or approved by a recognized testing authority are regarded as meeting this requirement. The connector type used should be: IEC320 C13.

⚠ CAUTION

Equipment Damage: It is imperative that the analyzer have adequate ventilation and/or cooling to maintain the ambient temperature below 35 °C when operating. Do not place the pump or the instrument in any enclosure without providing adequate forced air flow.

⚠ CAUTION

Do not plug or block any perforations in the chassis of the instrument. Do not put anything near the instrument that will impede the air flow. Failure to provide adequate airflow, especially clearance at the front and rear panels, to ensure proper airflow and/or cooling to the analyzer will result in overheating of the analyzer causing a shutdown and potential damage. There should be 6” (15 cm) of clearance in the front and back of the analyzer.

⚠ CAUTION

To determine if the ventilation is adequate in an enclosure, monitor the temperature of the air near the instrument and adjust ventilation so that the ambient temperature is within specification. As a guide, the ambient temperature of the air around the instrument cannot exceed the specifications listed below.

Thermal Specifications	Min	Max	Description
Ambient Operating Temperature	10 °C	35 °C	Worst-case environmental limits (unless otherwise specified)

⚠ CAUTION

If the analyzer has been stored at less than 10 °C (50 °F), allow the components to equalize to room temperature before starting the installation process.

5.3 Ventilation Considerations

The instrument and pump require adequate ventilation in order to function properly. Do not plug or block any perforations in the chassis of the instrument. Don't place anything near the instrument that will impede the air flow.

5.4 Pump Voltage Setting

Set the A2000 vacuum pump input voltage to the correct level for your area by rotating the voltage selector switch located on the side of the pump next to the fuse holder.

1. Fuse
2. Input Voltage Selector

Figure 6 - Vacuum Pump Voltage Selection

5.5 Basic Water Analyzer Setup

This section describes how to set up and start the analyzer for standalone operation to measure ambient water vapor. The analyzer can operate and report isotope values without liquid standards or peripheral accessories; however, calibration against liquid standards is required to obtain accurate quantitative results.

Refer to Figure 7- Electrical Connections below.

1. Remove the analyzer and the external vacuum pump from their respective shipping containers.
2. Place the analyzer on a cart or table.
3. Place the external vacuum pump near the analyzer on a cart, table, or on the floor.

   NOTE

   The A2000 vacuum pump is shipped with the Swagelok inlet adapter (PN 20639859) uninstalled. Before connecting the pump, install the adapter using the provided customer installation instructions.

4. Unpack the analyzer accessories (vacuum line, manual, and certificate of compliance).

   Store the certificate of compliance in a safe place. It may be required if you contact Picarro for service or questions.

5. Remove the caps from the analyzer SAMPLE inlet and VACUUM connection ports. Save the caps so they can be reinstalled when the analyzer is stored, moved or shipped.
6. Remove the caps from the pump vacuum inlet. Save the caps for reuse in case the analyzer and pump is stored, moved, or shipped.
7. Connect the provided vacuum line between the analyzer port labeled VACUUM and the pump vacuum inlet (Refer to Figure 7).

   Hand tighten the nut, then make an additional 1/4 turn with an 11/16” wrench.

8. The exhaust port of the external vacuum pump has a muffler attached for noise reduction. If desired, attach a tube to the pump exhaust port and direct it to a safe place for venting the mixture of sample gases for air/N2 and H20. For instructions, see Hardware Installation and Setup.
9. Connect a monitor to one of the DVI monitor ports at the analyzer back panel. Once powered up, the analyzer will detect the connection and adjust the resolution to match the monitor.
10. Connect a mouse and keyboard to a pair of USB ports.
11. Check that the A2000 pump voltage input switch is set correctly.

12. . Ensure the power switch on both the analyzer pump are set to OFF.
13. Attach the power cable to the analyzer and pump.

    This completes the basic analyzer installation.

NOTE

The analyzer has a universal power supply that automatically adjusts to power sources ranging from 100-240 VAC, 47 to 63 Hz, 10 A max.

NOTE

The A2000 pump does not automatically adjust to power sources. If using the A2000 vacuum pump, ensure its input voltage is set to the correct level for your area by rotating the voltage selector switch located on the side of the pump next to the fuse holder (see Pump Voltage Setting.

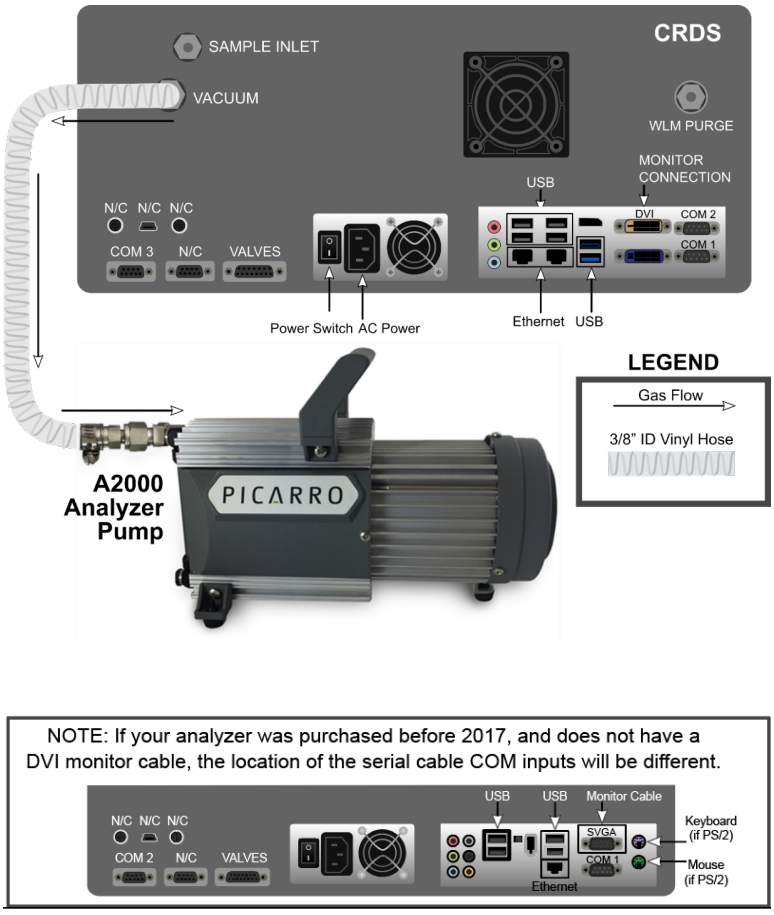


Figure 7 - Basic Water Analyzer Setup with A2000 Pump

5.5.1 Sample Gas Inlet Connection (SST Tubing)

If your analyzer is supplied with connectors for stainless steel tubing, follow these steps.

1. Slide the nut onto the 1/4" OD **stainless steel (SST)** tubing, with the threaded end facing the tube end.
2. Slide the back ferrule onto the tubing, followed by the front ferrule, as shown in the following figure.

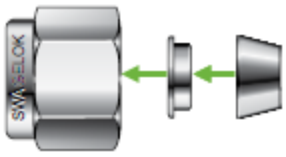


Figure 8 - Orientation of Inlet Nut and Ferrules

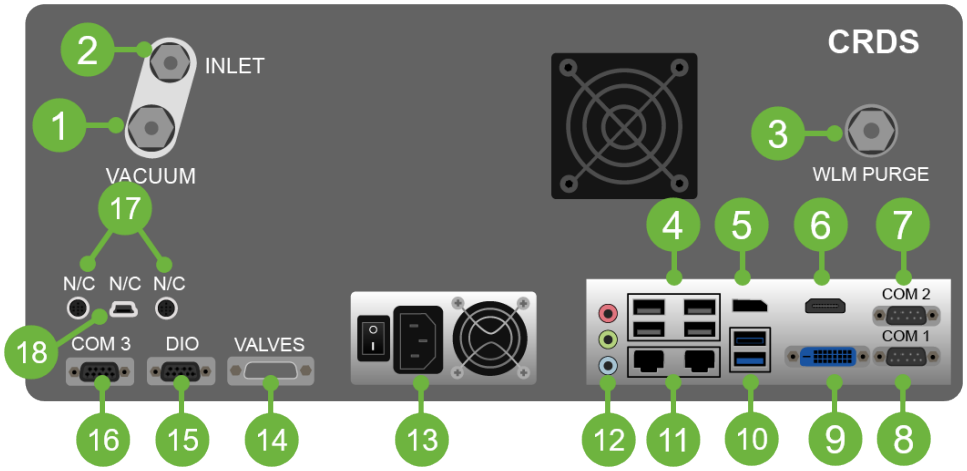
3. **Insert** the tubing into the **INLET fitting** on the back panel of the analyzer, pushing it in as far as possible.
4. Slide the nut forward and **hand-tighten it onto the fitting**.
5. Using a 9/16" wrench **(not included), further tighten the nut by 1-1/4 turns**.

When reconnecting SST tubing:

1. Inspect the ferrules. If you see any damage, replace the ferrules and follow the directions above for making a new connection.
2. If there is no damage, hand tighten the connector to the analyzer sample inlet.
3. Using a 9/16" wrench, tighten the nut 1/6 of a turn (60°).

5.5.2 Electrical Connections

Refer to the following figure and its callout list for electrical connection points.



1. External Vacuum Pump Port
2. Gas Sample Inlet
3. WLM Purge Port (optional)
4. USB Ports (4 ea)
5. Display Port
6. COM 2 Port
7. COM 1 Port
8. DVI-D Video Monitor Port (typical)
9. DVI-I Video Monitor Port
10. USB Ports (2 ea)
11. Ethernet Ports – RJ-45 (2 ea)
12. Audio In/Out Ports
13. AC Power Input and Power ON Switch
14. Valve Control Port (Solenoid valves)
15. DIO (Only for PAL autosampler connection)
16. COM 3 Port (Connected but typically not used.)
17. Analog EIC Output (Optional upgrade)
18. USB for Logic Board (Not connected)

Figure 9 - Annotated Back Panel Diagram

5.6 Dual Mode Setup

Refer to the following images in this topic.

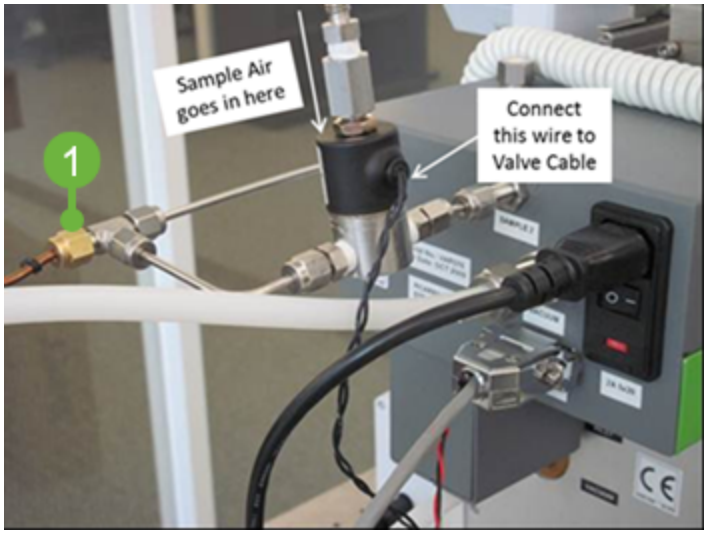
Dual mode is used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. The measurement mode alternates between analyzing ambient vapor and liquid standards based on a user defined sequence.

Dual Mode setup requires an **A0211 High Precision Vaporizer**, an **A0340 (or A0325) Autosampler**, and **A0912 Dual Mode Configuration hardware and software for vapor calibration**. Dual mode uses a high-precision method for liquid calibration. Each injection cycle takes 9 minutes.

1. Carefully unpack the peripheral boxes and prepare the facility.
2. Review the section, 5.2 Installation Safety before proceeding .
3. Install the analyzer and its external vacuum pump per the instructions in sections 5.1 Items/Tools Required through).
4. Install the Autosampler and Vaporizer.

   Refer to the Installation chapter in the A0340 Autosampler User Manual (PN 40-0094) or A0325 Autosampler User Manual (PN 40025) for detailed installation instructions.
5. Attach the vaporizer switching valve assembly to the vaporizer inlet ports labelled **Purge** and **Sample 2** (Figure 10 - Vaporizer Switching Valve Assembly Connected to Vaporizer and Figure 11 - Connections to Back of Vaporizer).
6. Attach the switching valve wire pair to the connector with the red/white wire pair that is attached to the Vap Valves cable connector.

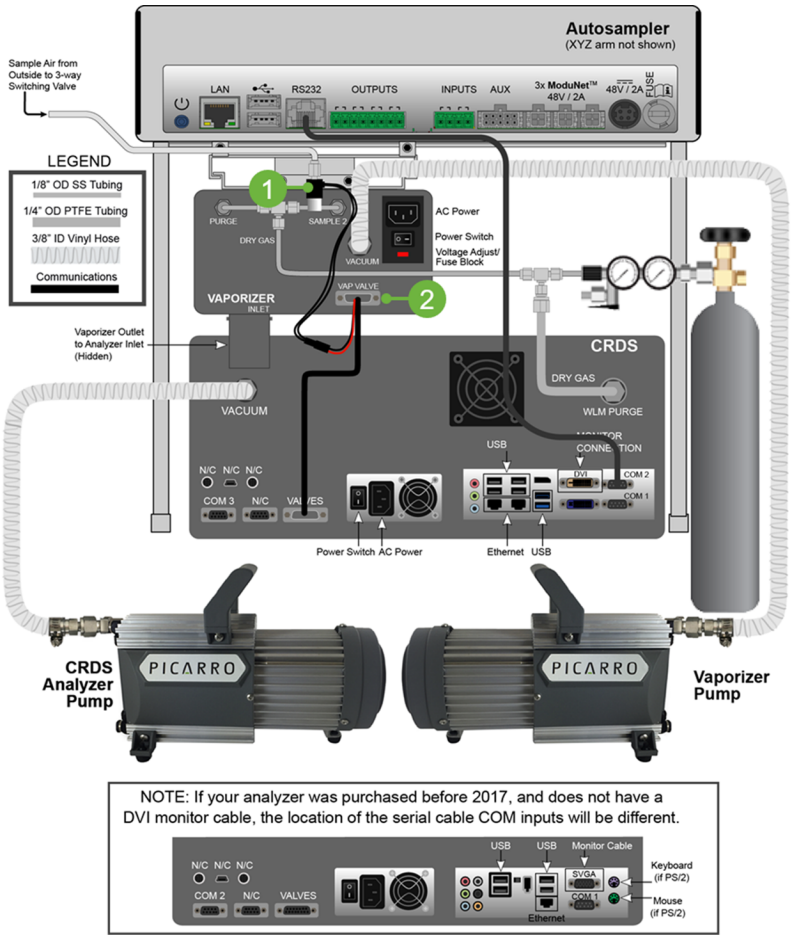
7. Attach the Zero Air gas line (shown as copper line in Figure 10 - Vaporizer Switching Valve Assembly Connected to Vaporizer) to the tee fitting on the vaporizer switching valve assembly.
8. Sampling tubing for measuring ambient water vapor should be connected to the top of the solenoid valve with the intake line routed outdoors.



1 From Zero Air dry gas source, (Zero Air is used for Dual Mode for ambient measurements).

Figure 10 - Vaporizer Switching Valve Assembly Connected to Vaporizer

Figure 11 - Connections to Back of Vaporizer



1. Vaporizer 3-way Switching Valve
2. Cable Assembly for Vaporizer Valve and Switching Valve

Figure 12 - Dual Mode Setup and Connections (Vaporizer Switching Valve Included)

5.7 Manual Mode Setup

Refer to Figure 13 - Manual Mode Setup and Connections below.

This mode is used for semi-automated measurement of liquid water samples with maximum precision.

The setup requires an **A0211 High Precision Vaporizer**. The user manually injects samples after prompt. The control of the vaporizer and the analysis of liquid samples are automated. Each injection cycle takes 9 minutes.

1. Inspect the boxes of Picarro products before opening. Carefully unpack the boxes and prepare the facility.

2. Please review the important safety notes before continuing on with the installation. See the section, 5.2 Installation Safety.
3. Install the analyzer and its external vacuum pump per the instructions in sections 5.1 Items/Tools Required through).
4. Place the vaporizer on top of the analyzer using feet of 0.5" (13 mm) thickness to set it to the appropriate height. Align the Inlet port (analyzer) with the delivery port of the vaporizer.
5. Attach a (N_2 or Dry Air) Gas line to the vaporizer and the analyzer (see section 6 Water Analyzer Dry Gas Supply Setup).
6. Attach the hose at the vaporizer's vacuum port and connect it to the second External Vacuum Pump. Attach the power cable to the External Vacuum Pump, but keep the power switch off.
7. Connect the vaporizer and the analyzer using a Valve Cable and the gas delivery port from the vaporizer (see VAPORIZER TO ANALYZER CONNECTIONS).
8. Check the Power Connections to the Machines: Make sure all power cables are attached to the power outlets on the analyzer, Vaporizer, and two External Vacuum pumps. However, keep the power switch off.
9. Carefully slide the complete system into position: Small movement of the components relative to one another is OK. However, do not overly force the system. Check for obstacles if the unit does not slide easily.
10. Plug all the power cables (including the one for the monitor) into a power supply. Switch ON the components in the following order

    a. External Vacuum Pumps (for both the analyzer and the vaporizer).

    b. Everything else.

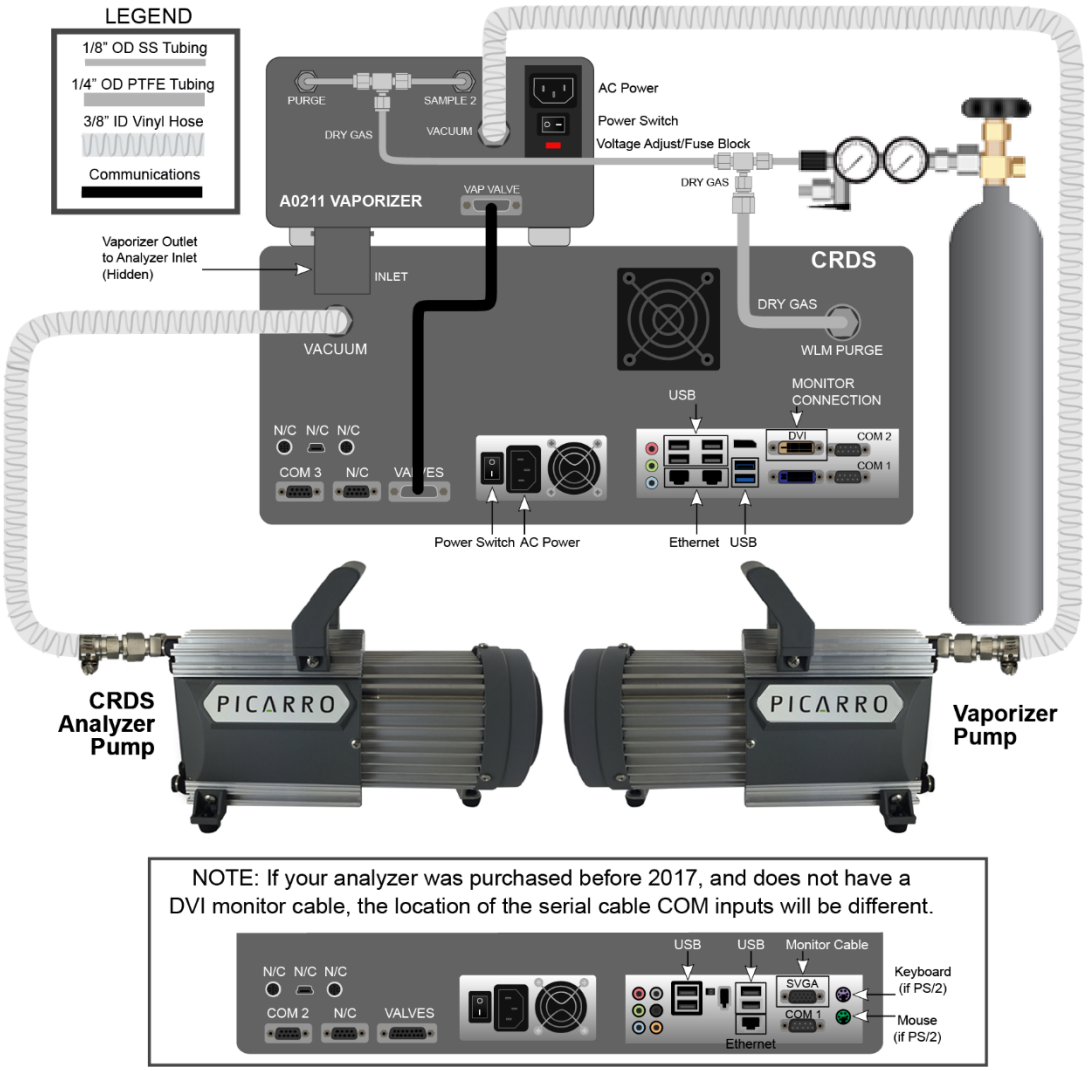


Figure 13 - Manual Mode Setup and Connections

5.8 Autosampler and Vaporizer (A0211) Setup

This setup is used for automated injection of liquid waters. It consists of two modes that utilize the same hardware: High Precision Mode (same as Standard Mode) and High Throughput Mode.

Refer to Figure 14 - Picarro Autosampler-High Precision Vaporizer Setup and Connections diagram below.

1. Inspect the boxes of Picarro products before opening. Carefully unpack the boxes and prepare the facility.
2. Please review the important safety notes before continuing on with the installation. See SAFETY.

3. Install the analyzer and its External Vacuum Pump (see analyzer and Vacuum Setup).
4. Install the Picarro Autosampler (see Installation | Picarro Autosampler chapter in the A0340 Autosampler User Manual (PN 40-0094) or A0325 Autosampler User Manual (PN 40025).
5. Supply dry gas to the analyzer (see Chapter 6, Water Analyzer Dry Gas Supply Setup).
6. Carefully slide the complete system into position: Small movement of the components relative to one another is OK, as the units are well locked. However, do not overly force the system: check for obstacles if the unit does not slide easily.
7. Power up the system: Plug in all the power cables (including the one for the monitor) into the appropriate power supply. Switch ON the components in the following order:

   a. External Vacuum Pumps (for both the analyzer and the vaporizer).

   b. Everything else

NOTE

The software to operate the instrument will start automatically after the operating system has loaded. The user interface will appear a few seconds after the instrument software starts. See section 8.1 Startup.

NOTE

Allow approximately 30 minutes for the analyzer to warm up before isotope data is available. During this period, only pressure and temperature readings are displayed.

NOTE

Remember that for the SDM operation, the Vaporizer temperature should be set to 140°C. For all the other coordinator modes, the temperature should be set to 110°C.

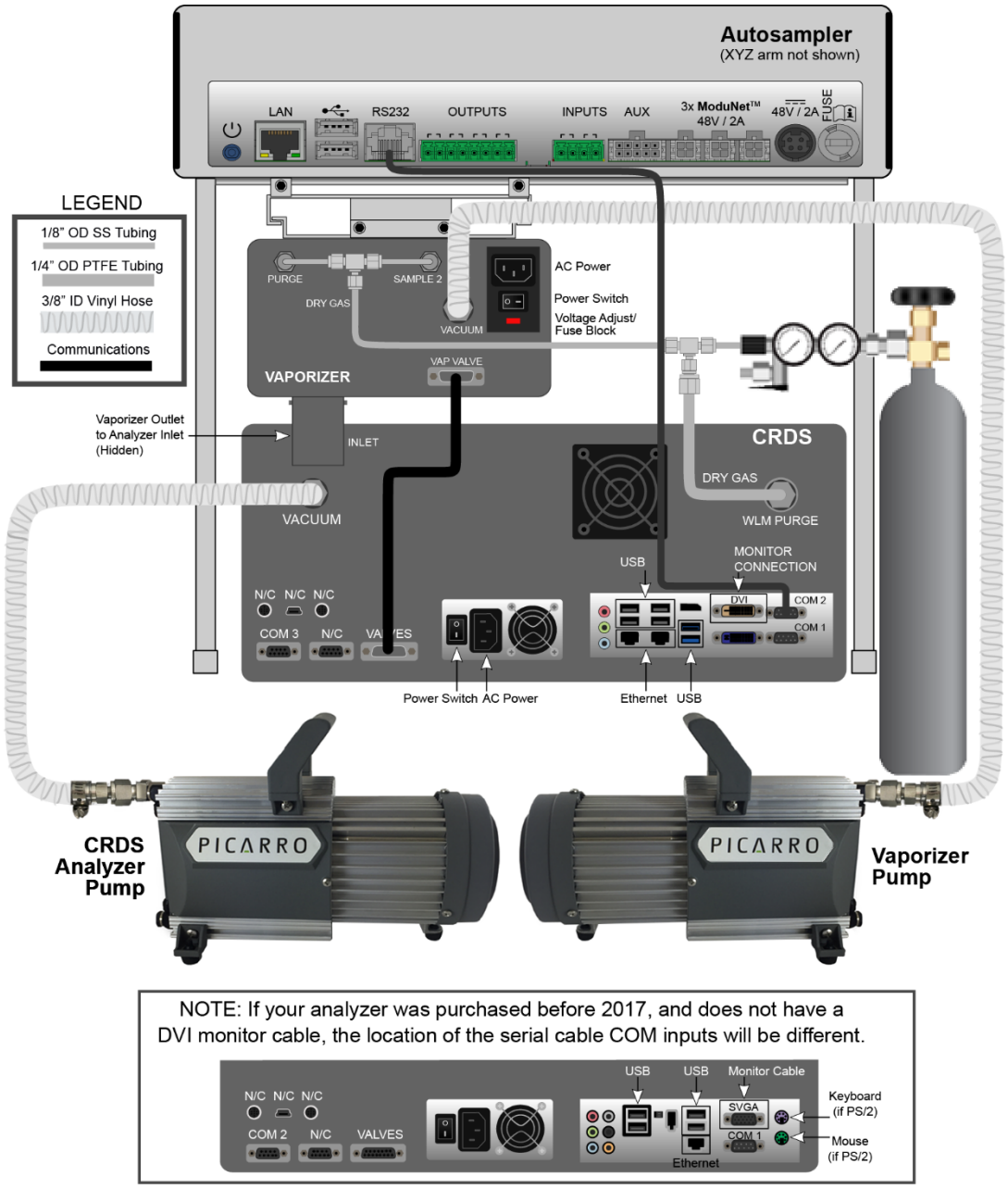


Figure 14 - Picarro Autosampler-High Precision Vaporizer Setup and Connections

6 Water Analyzer Dry Gas Supply Setup

The Picarro L2140-i and L2130-i analyzers each can work in many configurations, allowing a wide application of the analyzer. This section describes how to set up the dry gas supply for all these configurations. Find the section in this chapter that relates to your setup and then complete the dry gas supply installation steps.

- **Manual Mode Setup:** See 6.1 Dry Gas Configuration A.
- **Picarro Autosampler – High Precision Vaporizer (A0211) Setup:** See 6.1 Dry Gas Configuration A.
- **Picarro Autosampler – High Throughput Vaporizer (A0212) Setup:** See 6.2 Dry Gas Configuration B.
- **Basic Water Analyzer Setup:** No dry gas supply necessary
- **Dual Mode Setup:** See 6.3 Dry Gas Configuration C.
- **Induction Module Setup:** See A0213 Induction Module to CRDS Setup User Manual (PN 40039)
- **SDM Setup:** See A0101 Standards Delivery Module CRDS Setup User Manual (PN 40-0005)

NOTE

The Wavelength Monitor (WLM) purge is an optional feature and is not required for normal instrument operation. It is recommended when operating the instrument in humid environments. For additional information, see 6 Water Analyzer Dry Gas Supply Setup.

6.1 Dry Gas Configuration A

Refer to the following figure Figure 15 - Dry Gas Configuration A.

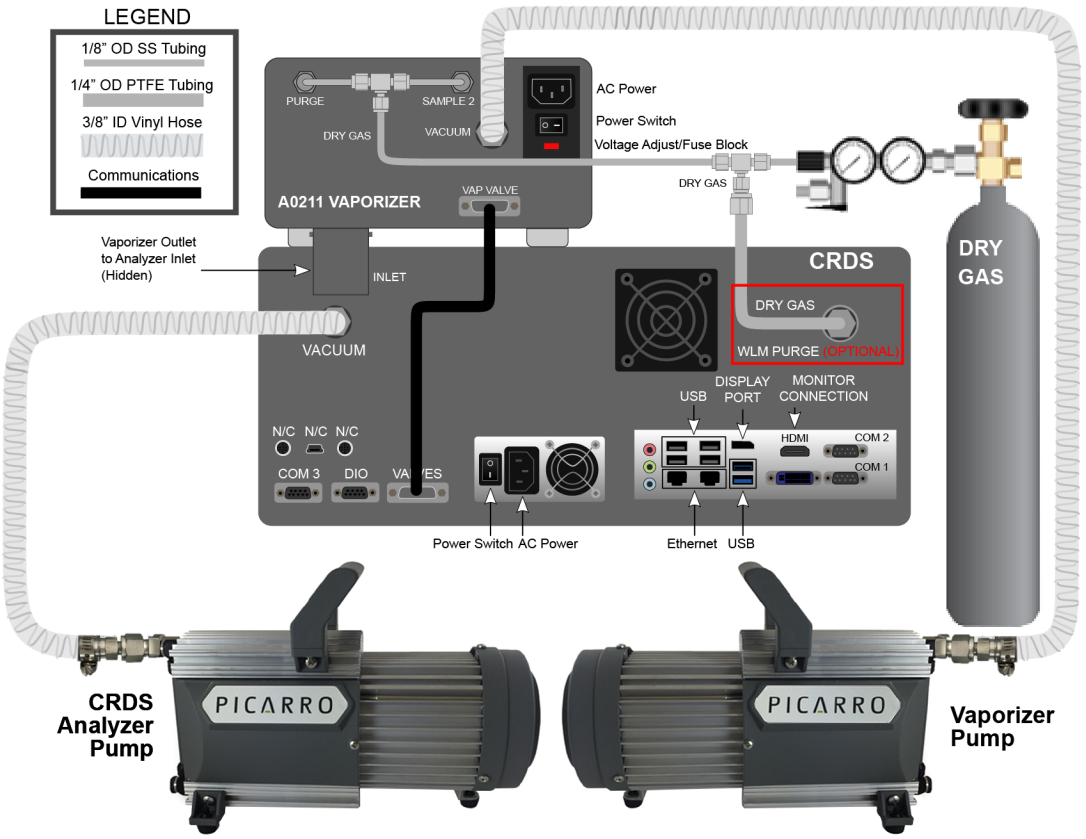
A dry gas supply is required for both the analyzer and the vaporizer. The gas must be regulated to 2.5 psi (0.17 bar) at the analyzer inlet. Pressure regulator kits are available from Picarro (PN A0921 or A0923).

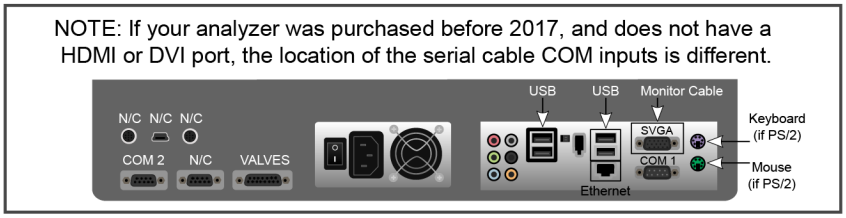
NOTE

The A0921 regulators come with CGA connectors, which may not be compatible with gas tanks used in your region.

Below, you will find a complete part list and diagram on how to connect dry gas to the water analyzer.

1. Attach the (N_2 or Dry Air) Gas Line to the analyzer: Attach a Gas line from the WLM Purge Port (optional) on the analyzer to the N_2 Regulator, which connects to a (nitrogen or dry air) gas cylinder.
2. To connect 1/4” dry gas tube to the Wavelength Monitor Purge (WLM Purge) Port on the analyzer, use the Push Connector that is attached to the port. The connector is in two pieces: The Outer Flap and the Inner Flap.
3. To connect the tube to the port, simply push the tube into the connector and then pull the tube back. If there is a space between the inner flap and the outer flap, this means that the tube is locked to the port. Do not twist and turn. To take the tube out of the port, push the Outer Flap in against the Inner Flap, and while doing this, pull out the tube. This will cause the gripping mechanism to release from the tube.





1. Q1-14B-580 Air Liquide Scott Regulator
2. SS-OGM2-S2-A Swagelok Toggle Valve
3. SS-T2-S-028-20 Swagelok 1/8" OD stainless steel tubing
4. SS-200-3 Swagelok 1/8" stainless steel Tee union
5. SS-400-R-2 Swagelok 1/8" (adapter fitting) to 1/4" (tube fitting) Reducing Union
6. 5033K31 McMaster-Carr 1/4" OD PTFE tubing

Figure 15 - Dry Gas Configuration A

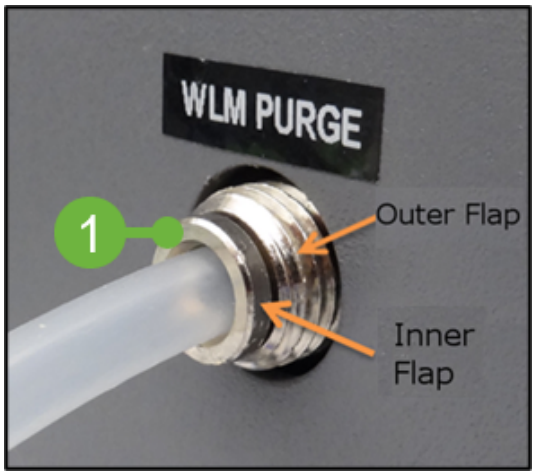
NOTE

Additional tools and parts are required, some others recommended. For the complete list, please click on the link below which, if you haven't already joined, will require you to have signed up for a Picarro community account.
https://picarro.box.net/shared/static/r19c3z8etk.pdf

4. Attach the Gas (N_2 or Dry Air) Line to the Vaporizer: Using either output from a (nitrogen or dry air) gas cylinder (should be at a pressure of 2.5 ± 0.5 psig (0.17 ± 0.03 bar)) or from the gas supply/regulator, attach the gas line to the open third leg of the gas line that connects the vaporizer purge and the sample ports (that is shipped connected to the vaporizer).

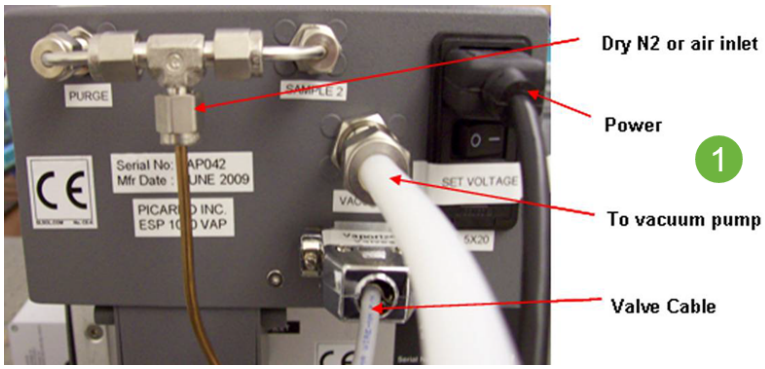
Figure 16 - Gas Regulator

Above is an N_2 Regulator: The semi-transparent tube on the left is routed to the 'WLM Purge" Port on the analyzer. The copper-colored tube on the top left comes from the 'Purge' and the 'Sample' ports on the Vaporizer. The copper-colored tube on the bottom right goes to the (N_2 or Dry Air) Gas Cylinder.



1 WLM purge port located at analyzer back panel

Figure 17 - WLM Purge Connections



1 Gas and electrical connections at rear of vaporizer

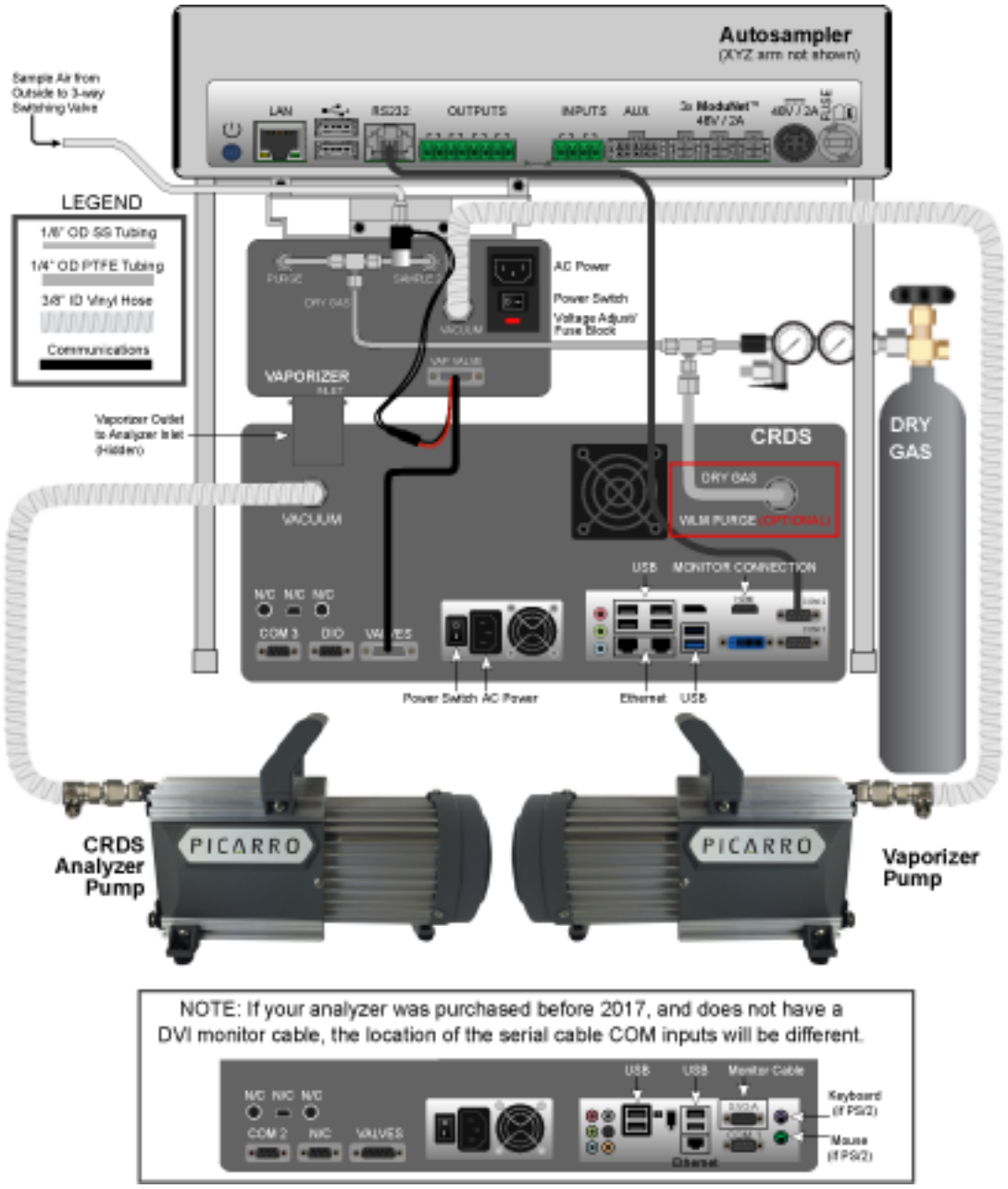
Figure 18 - Vaporizer and Analyzer Connections

NOTE

If the analyzer remains on dry gas without a sample signal for an extended period (for example, several hours or days), the frequency axis can drift, resulting in incomplete spectra. Symptoms may include increased measurement intervals or intermittent data dropouts when sampling resumes. If this occurs, disconnect and turn off the dry gas source and allow the analyzer to measure room air until normal operation is restored.

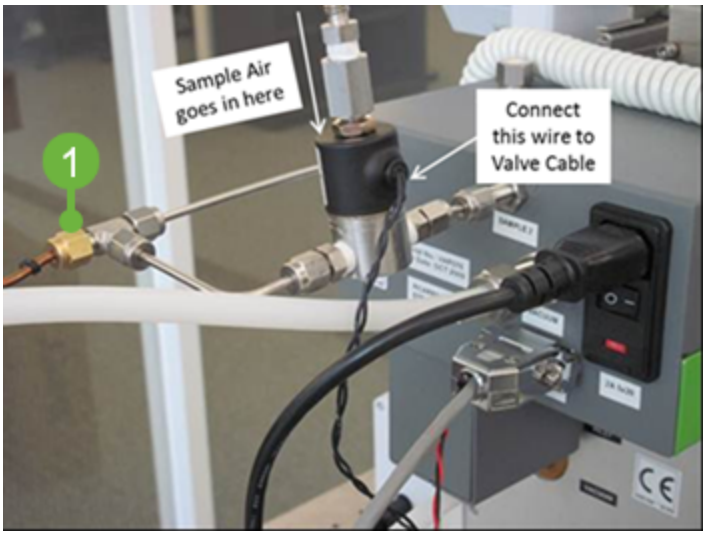
6.2 Dry Gas Configuration B

The gas connection for the **Dual Mode** setup is similar to the Dry Gas Configuration A except that it also has a Vaporizer Switching Valve. Follow the Dry Gas Configuration A, but also connect the Vaporizer Switching Valve to the back of the Vaporizer according to the schematic and images below.



1. Vaporizer 3-way Switching Valve
2. Cable Assembly for Vaporizer Valve and Switching Valve

Figure 19 - Dry Gas Configuration B



1 Vaporizer 3-way Switching Valve

Figure 20 - Vaporizer Switching Valve Connected to Vaporizer

NOTE

If the analyzer remains on dry gas without a sample signal for an extended period (for example, several hours or days), the frequency axis can drift, resulting in incomplete spectra. Symptoms may include increased measurement intervals or intermittent data dropouts when sampling resumes. If this occurs, disconnect and turn off the dry gas source and allow the analyzer to measure room air until normal operation is restored.

6.3 Dry Gas Configuration C

For the SDM setup, you only need to supply dry gas directly to the CRDS analyzer as show in the following diagram.

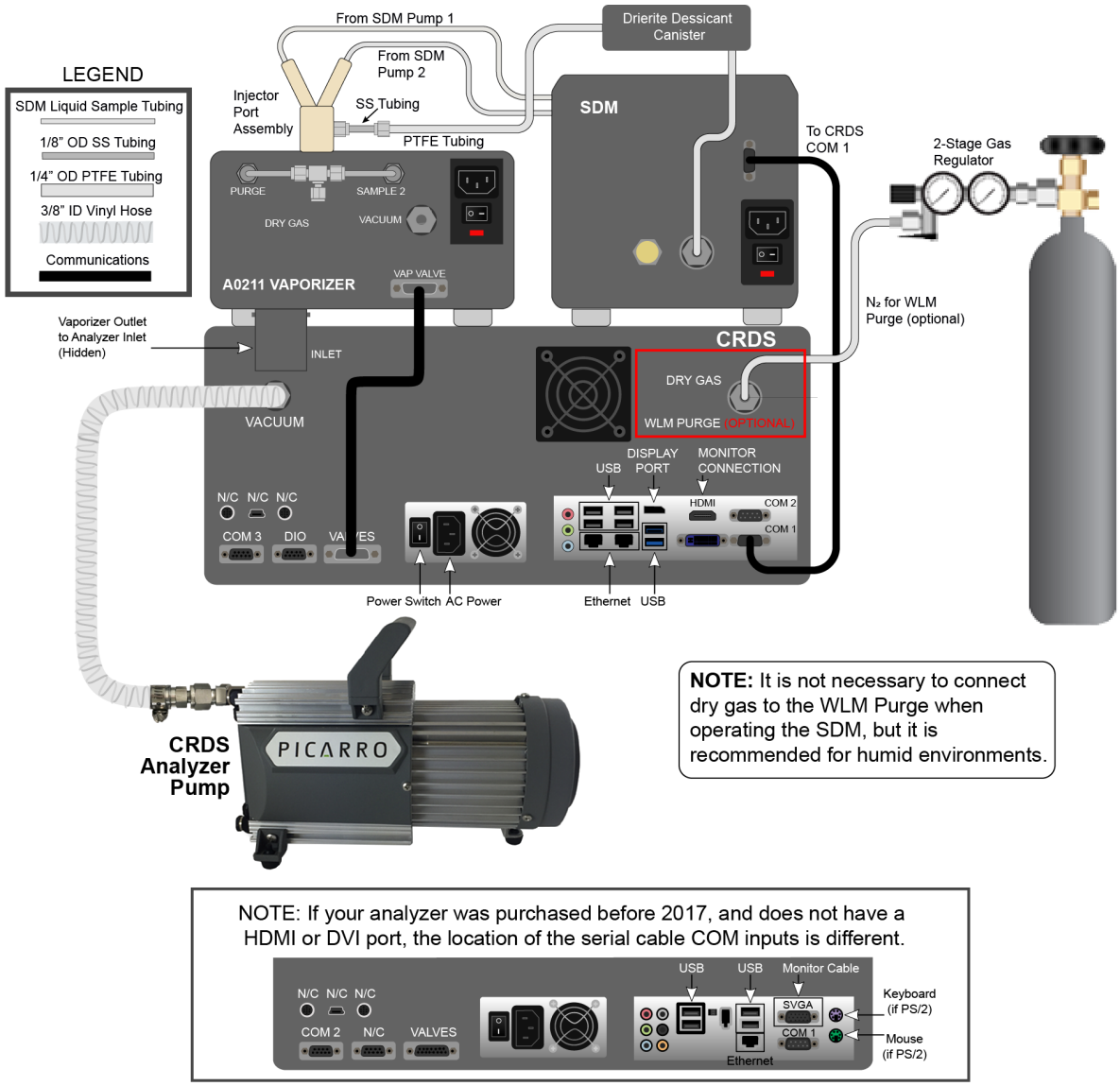


Figure 21 - Dry Gas Configuration C

To connect a 1/4" dry gas tube to the WLM Purge Port (optional) back of the analyzer, use the Push Connector attached to the port.

The connector is in two pieces: The Outer Flap and the Inner Flap. To connect the tube to the port, simply push the tube into the connector and then pull the tube back.

If there is a space between the inner flap and the outer flap, this means that the tube is locked to the port. Do not twist and turn. To take the tube out of the port, push the Outer Flap in against the Inner Flap, and while doing this, pull out the tube. This will cause the gripping mechanism to release from the tube.

Wavelength Monitor (WLM) Purge (optional)

The WLM purge port supplies dry gas to the analyzer warm box, where the wavelength monitor (WLM) controls laser targeting within the system's optical feedback loop. Inside the warm box, the laser travels along an open path of approximately 10 cm at 45 °C. Because the laser is tuned to a water absorption frequency, elevated ambient humidity within this path can cause light attenuation before it reaches the WLM, potentially resulting in measurement drift as environmental conditions change. Supplying dry gas minimizes this effect by reducing water vapor absorption along the optical path.

Is the WLM purge necessary?

In most laboratory conditions, the WLM purge is not required. Its benefit is minimal at typical indoor humidity levels, and it is generally recommended only when operating in humid environments, typically above 3% water content (30,000 ppm).

NOTE

The WLM purge consumes approximately 120–140 mL/min of dry gas continuously. If operating from a limited gas supply (such as a tank), leaving this port unconnected is typically more practical unless high humidity conditions are expected.

If you connect the WLM purge:

- If a dry gas supply is already in use for the vaporizer (for example, a High Precision or High Throughput Vaporizer), the simplest approach is to install a T-fitting and share the same gas source.
- Dry gas regulator kits with the required fittings are available from Picarro for N_2 (PN A0921) or zero air (PN A0923).
- The purge gas does not need to match the cavity matrix gas. Both N_2 and air are acceptable, regardless of the analyzer operating mode (Air or N_2).

NOTE

If the analyzer remains on dry gas without a sample signal for an extended period (for example, several hours or days), the frequency axis can drift, resulting in incomplete spectra. Symptoms may include increased measurement intervals or intermittent data dropouts when sampling resumes. If this occurs, disconnect and turn off the dry gas source and allow the analyzer to measure room air until normal operation is restored.

7 Vaporizer to Analyzer Connections

This chapter describes the procedures for connecting the vaporizer to the analyzer. It includes instructions for installing the valve controller cable and for connecting the gas delivery line between the vaporizer and the analyzer.

Procedures are provided for systems configured with or without an autosampler and include alignment requirements, handling of the vaporizer insulation box, and final positioning to ensure proper sample delivery and reliable operation.

7.1 Valve Controller Cable

Attach the 15 pin end of the grey valve cable to the port labelled Vap Valves on the vaporizer and connect to the port labelled VALVES on the analyzer (third connector from the left at the bottom row of the analyzer).

7.2 Gas Line Connection

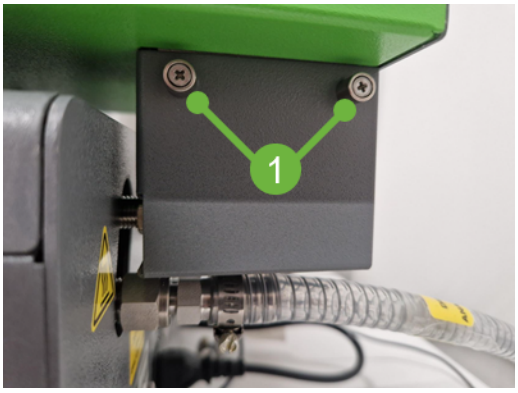
This section describes how to connect the gas delivery line between the vaporizer and the analyzer. Procedures are provided for systems configured with and without an autosampler, including alignment requirements and installation of the vaporizer insulation box to ensure proper fit and reliable sample delivery.

1. **(With Autosampler):** If an Autosampler is integrated with your system, carefully align the analyzer and the autosampler relative to each other such that the gas delivery line hanging from the vaporizer is aligned with the inlet port of analyzer. Do not bend the delivery port in the process.

   If the delivery port is not horizontally aligned with the analyzer inlet port, gently move the position of the vaporizer on the autosampler by loosening the mounting clamps and retightening them after alignment.

2. **(Without Autosampler):** If an Autosampler is not used with your system, attach the feet to the vaporizer underside or place an object under to level the vaporizer outlet connection to the analyzer inlet.
3. Follow the procedure below and connect the gas line from the vaporizer to the analyzer as follows.

a. Remove the insulation box by removing the Phillips screws securing it (two on each side), as shown in Figure 22. Removing the insulation box provides easier access to the analyzer inlet.



1 Phillips screws

Figure 22 - Vaporizer Insulation Box - Screws

b. Align the vaporizer sample line fitting with the analyzer inlet and hand-tighten the nut onto the analyzer inlet as shown in the Figure 23.

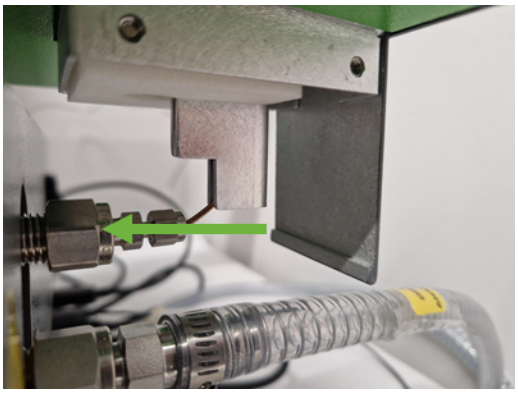
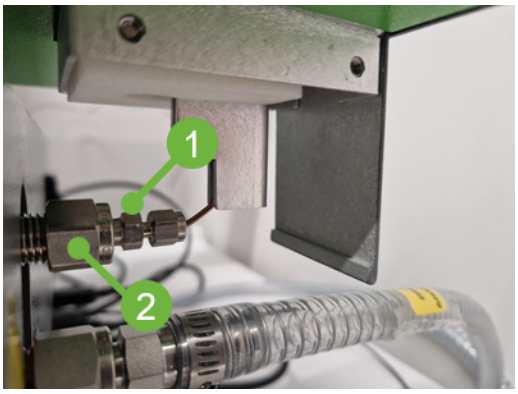


Figure 23 - Vaporizer Alignment to Analyzer Inlet

c. Using a 5/16-in. wrench, hold the union fitting stationary while tightening the nut with a 9/16-in. wrench, as shown in Figure 24.



1. Hold the union station using 5/16" wrench
2. Tighten nut using 9/16" wrench

Figure 24 - Vaporizer Connection to Analyzer Inlet

NOTE

Verify that the 9/16-in. sample line remains properly aligned with the aluminum guide and is not under stress or excessive bending.

d. Move the vaporizer forward, leaving enough space to reinstall the insulation box.
e. Reinstall the insulation box.
f. Carefully push the autosampler (if used) and/or vaporizer forward until there is no gap between the insulation around the vaporizer outlet and the analyzer. See Figure 25.

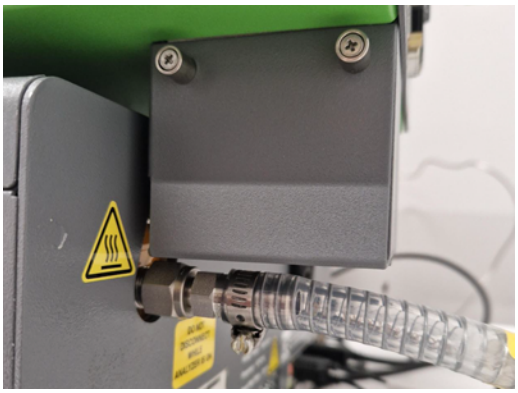


Figure 25 - Vaporizer to Analyzer Installation Complete

8 Basic Operation

This section explains how to operate the analyzer using the GUI. It describes system startup, shutdown, and recovery procedures, desktop features. GUI Functions are detailed in section CRDS Data Viewer Overview.

Before continuing, review the important safety notes in the Safety section.

⚠ CAUTION

If one accidentally over-saturates the instrument with water, it is very important to NOT turn the instrument off. Rather, let the instrument pull either room air or dry air/ N_2 through for a few days to dry out the cavity until the instrument can make normal measurements again. If the instrument is turned off right after the accident, water will condense and contaminate the cavity rendering it useless with a very costly cavity repair required for the instrument to operate correctly.

⚠ CAUTION

Always turn on the external pump before powering up the analyzer. This ensures a safe start-up sequence. Failure to do so could result in damage to the cavity optics.

8.1 Startup

This section describes the initial startup sequence for the analyzer, including required connections, power-up steps, and system initialization. It outlines how the analyzer software loads, how system readiness is indicated, and the conditions that must be met before measurement data becomes available.

1. Make sure the pump vacuum hoses are connected between the analyzer and its pump, and the Vaporizer and its pump.

   ⚠ CAUTION

   Always turn on the external pump that is attached to the analyzer before powering up the analyzer. This ensures a safe start-up sequence.

2. Verify the power cables to vacuum pumps are plugged in.
3. Switch power on at the pumps.
4. Verify the power cable to the analyzer is plugged in.
5. At the analyzer back panel, press the main power switch to the **ON** (“**I**”) position.

6. If needed, press the round **Soft Power** button on the front panel. The indicator LED will illuminate green.

   The software will start automatically, and the analyzer will display a CRDS Software Loading Status window (Figure 26), then the CRDS Data Viewer window (Figure 27) once loading is complete. Data Viewer features are detailed in section 10 CRDS Data Viewer Overview.

Figure 26 - Startup; Software Loading Sequence

The analyzer will not begin producing data until the cavity temperature and pressure have reached their operational set points. A message will be displayed in the Status Log window of the data viewer (see Figure 27, bottom panel) when each set point is reached. An explanation of the most common status log messages can be found in section 10.8 Analyzer Status Log.

In the case of the L2130-*i* or L2140-*i* analyzer, these are 80°C and 50 Torr. Warm up typically takes about one hour. By design, the cavity pressure will not start to decrease until the cavity temperature is close to its set point. Ideally, the analyzer is open to room air during the warm up, i.e., there is nothing attached to the “Gas Inlet” on the rear of the analyzer. This is desired because ambient water vapor will provide a good signal for the Picarro Wavelength Monitor (WLM) which provides the frequency control for the spectral measurement.

Data will be saved automatically once the analyzer starts to produce data. The data in the GUI is the continuous real time read out from the analyzer. User data is stored in:

C:\Userdata\DataLog_User \YYYY\MM\DD, where Y=year, M=month, D=day.

Further details can be found section 14 File Management.

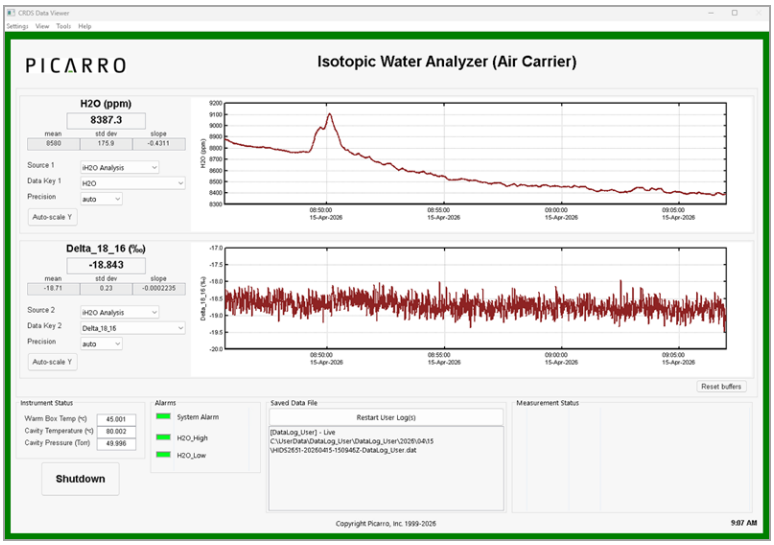


Figure 27 - GUI/Data Viewer Screen

8.2 Shutdown

This section describes the recommended procedure for safely shutting down the analyzer to prevent damage to critical internal components. Proper shutdown is essential to avoid trapping high-moisture gas within the cavity, which can condense as the instrument cools and cause damage to the optical surfaces.

It also outlines required precautions during shutdown, including maintaining gas flow and proper use of the software controls to ensure the analyzer and supporting hardware are powered down in a controlled manner.

⚠ CAUTION

A flow of clean, relatively dry gas should always be directed to the instrument for several minutes prior to shutting down. Trapping a high-moisture content gas sample in the cavity can cause condensation damage to the mirrors as the instrument cools from its operating temperature.

⚠ CAUTION

Do not turn off the pump or disconnect the vacuum line while the instrument is operating.

⚠ CAUTION

If you have trouble turning off the analyzer software, do not use the Windows Task Manager to kill the processes. Instead, double-click on the "Stop Instrument" icon in the Diagnostics folder on your desktop and select the default option to stop the software with the drivers running. See Figure 28 below.

8.2.1 Flow Clean, Dry Gas

1. With the pump still running, switch to a source of clean, dry gas at the sample inlet and allow it to run until the water channel reading on the GUI falls below 0.2% (2000 ppm). This will prevent any damage from condensation to the cavity surfaces. This dry gas may be from a tank (target 2-3 PSIG pressure) or from a desiccant column like the Drierite column, C0360, sold on store.picarro.com).

8.2.2 Shutdown

1. Click on the **Shutdown** button located on the left side of the Data Viewer window.
2. A window will pop-up (Figure 28) prompting the user to confirm the shutdown. Once confirmed, the analyzer software and hardware will turn off. (Note: If three options are given on an older instrument, choose the "For **Shipment**" option.)
3. Manually turn off the pump(s) and dry gas (only if system requires it).

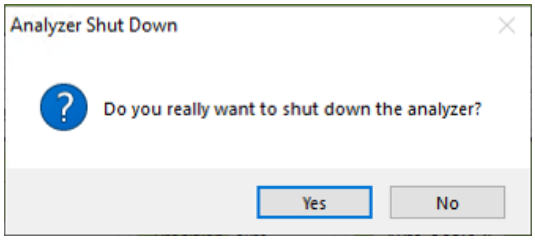


Figure 28 - Shutdown Confirmation Pop-Up Dialog

After clicking **Yes** to confirm, the analyzer software, then the computer OS will shut off after a few minutes. Leave any dry gas or desiccant attached to the inlet during this process.

4. Once the instrument fans audibly turn off and the **green power button light** on the front panel turns off, switch off the pump(s) using the **rocker switch** on the pump. As a good practice, also switch off the **main power** at the rear of the analyzer.

8.3 Analyzer Restart after Electrical Power Outage

If power to the analyzer is cut-off for any reason the analyzer will cease operation. However, when the power is reapplied, the analyzer will restart automatically, the Picarro software tools will properly close out previous files and open new files for data collection so that

previously collected data, instrument diagnostics and other parameters recorded up to the time of power outage are retained.

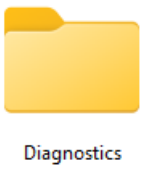
If short power outages are common in the user location, Picarro recommends using an uninterrupted power supply (UPS) to protect the data stream and the health of the cavity.

8.4 Desktop Icons and Folders

This section describes the desktop icons and folders installed on the analyzer system and their functions. These shortcuts provide access to software tools used to operate the analyzer, manage sample processing, view and analyze data, and perform diagnostic and configuration tasks.

Table 5 - Desktop Icons and Folders

Location	Icons
	
	 Example only: number varies by analyzer model.
	

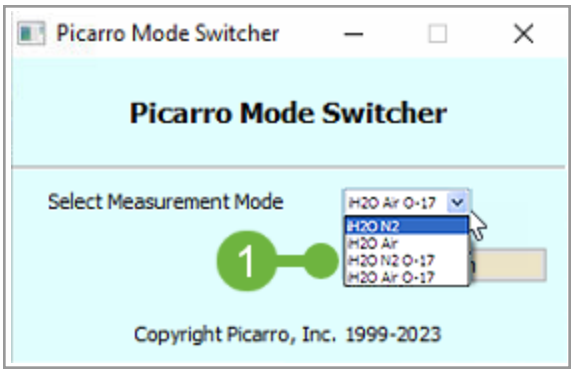
Location	Icons
	

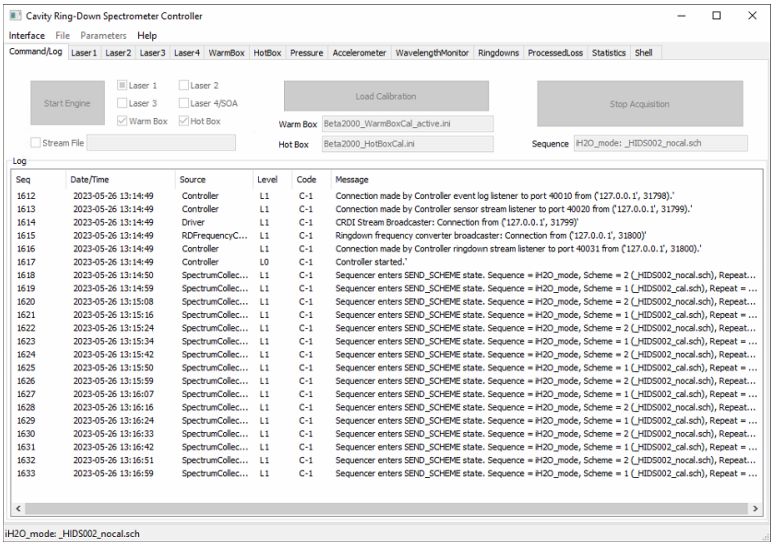
8.4.1 Desktop Icons

The Desktop Icons provide quick access to the primary software tools used to operate, monitor, and manage the analyzer. These shortcuts allow the user to start and control the instrument, manage sample processing, switch measurement modes (if available), view diagnostic information, and access data visualization utilities.

Table 6 - Desktop Icon Descriptions

Icons	Description
	**Autosampler:** Launches the Autosampler UI software for managing sample processing tasks.
	**Start Instrument:** If the instrument software is already running, this restarts the software. If the instrument software has been shut down, this starts the software.
	**Coordinator Launcher (not present on all configurations):** Clicking on this icon opens a window that allows you to choose the proper coordinator to operate peripheral modules on certain analyzers.

Icons	Description
	**Picarro Mode Switcher (not present on all configurations):** When clicked, a window opens that allows you to switch between various measurement modes. Most analyzer models are configured for one mode and may not include the Mode Switcher. If the analyzer has multiple modes, this allows the user to switch between them easily.
	 **Note**: Available L2130-*i* or L2140-*i* Measurement Modes Figure 29 - Picarro Mode Switcher

Icons	Description
	**Picarro Controller:** Opens a diagnostic interface intended for Picarro Support, providing real-time visibility into analyzer internal temperatures, pressure, and spectroscopy data. While the interface includes user-accessible functions, instrument parameter changes must only be performed under the direction of Picarro Support.
	 Figure 30 - Picarro CRDS Controller Window
	**Autosampler Configurator:** Opens the Autosampler Configurator, which is used to configure the autosampler and train module positions, create offline configurations, and train component locations required for autosampler operation.
	**ChemCorrect:** is a post-processing tool that identifies potential chemical contamination in isotope measurements and helps improve data accuracy through quality assessment and correction methods.

Icons	Description
	**Picarro Computer Icon:** The Windows Computer Icon is renamed to the analyzer serial number.
	**Data file Viewer**: When clicked, a window opens that allows you to convert between *.dat and H5 data files and to make various graphical representations of your data over time periods longer than what is available in the software buffer. The instructions on using the Data File Viewer software are described in B Data File Viewer.

8.4.2 Switching Between Measurement Modes

The Picarro Mode Switcher allows users to operate the analyzer in various modes. Switching between measurement modes is accomplished with a few easy steps:

1. Activate the mode switcher interface by double-clicking the Picarro Mode Switcher icon on the desktop (8.4.2 Switching Between Measurement Modes).
2. To switch modes, click the drop-down menu, select the desired measurement mode, and then click the launch button.
3. Confirm your selection when prompted by the confirmation dialog box.
4. The analyzer software will then re-start in the new measurement mode. There is no need to turn off the vacuum pump(s) or any other peripherals during this process

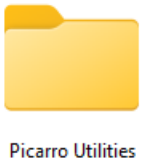
8.4.3 Post-Process ChemCorrect

ChemCorrect software is now included in all Picarro water isotope analyzers. The software allows post-acquisition analysis of discrete sample data generated by the coordinator. For more information, see section 13 ChemCorrect™ Software.

8.4.4 Picarro Utilities Folder

The Picarro Utilities folder provides access to tools used for data recalibration, analyzer configuration, and data file review.

Table 7 - Picarro Utilities Folder

Icon/Folder	Description
	**Data Recal:** When clicked, a window opens that allows you to recalibrate your data based on known, certified data.
	**Setup Tool:** When clicked, a window opens that allows you to edit various settings for your analyzer (See A Setup Tool and Communication for information.
	**Data file Viewer:** (see).

8.4.5 Diagnostic Folder

The Diagnostic folder provides tools for managing analyzer operation during abnormal or emergency conditions. The **Stop Instrument** function opens the Stop CRDS Software pop-up, which allows you to shut down the analyzer in an emergency. For standard shutdown procedures, see Section 8.2 Shutdown.

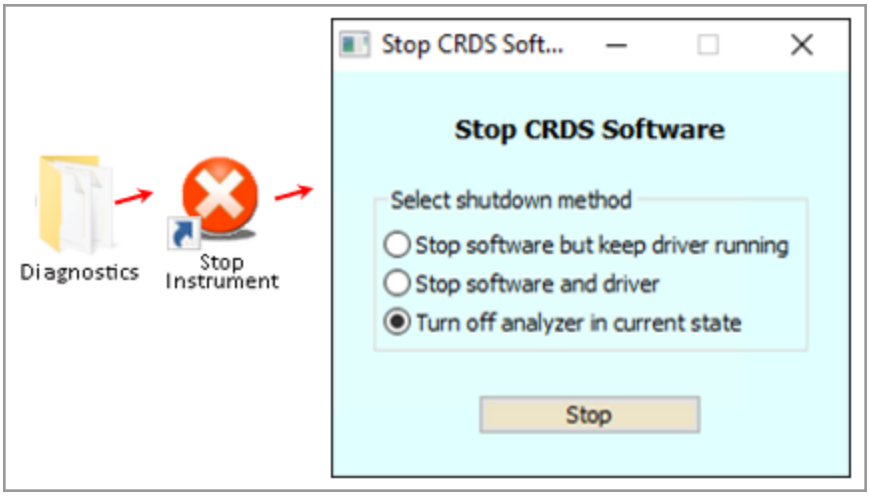


Figure 31 - Stop CRDS Software Pop-up

The Stop CRDS Software pop-up offers three shutdown methods:

- **Stop software but keep driver running:** Closes the analyzer software only. The driver continues to control cavity pressure/temperature and sample flow continues. Use this option when changing instrument settings, such as port or column configuration in the Setup Tool, or when modifying scripts.
- **Stop software and driver:** Also stops the driver, closing the valves and stopping flow; the cavity is left at low pressure. Use this option only when changing the system time by more than 30 seconds. (Routine time-server synchronization does not require this.)
- **Turn off analyzer in current state:** Immediately shuts down software and hardware, leaving the cavity at operating (low) pressure. Use only if the analyzer will be restarted soon, such as when moving it to a nearby bench or lab.

⚠ CAUTION

Unlike the standard shutdown procedure (Section 8.2), these emergency shutdown methods do not flush the cavity with dry gas before shutdown. Use these options only when necessary. Before the next normal shutdown or any extended power-off period, restore dry gas flow to ensure the cavity can be properly purged.

9 Measurement Setup Modes

The analyzer supports multiple measurement setup modes to accommodate different sampling workflows, including ambient vapor measurement, automated liquid injection, and manual sample analysis. Each mode combines specific hardware configurations and coordinator software settings to meet varying accuracy, throughput, and automation requirements.

The following sections describe the available setup modes, including Dual Mode, Manual Mode, and Autosampler-based configurations, along with their operational requirements and typical use cases.

9.1 Dual Mode Setup

Dual Mode measures ambient water vapor continuously and periodically interrupts that measurement to run automated injections of liquid calibration standards. This setup requires the A0211 High Precision Vaporizer, an Autosampler, and the A0912 Dual Mode Configuration. Each injection cycle takes just over 7 minutes, including cleaning and stabilization steps.

The A0912 Dual Mode Configuration adds a 3-way valve at the rear of the analyzer. In its normally-open (resting) position, the valve routes ambient sample air to the analyzer. During a calibration injection, the coordinator switches the valve to draw from a dry gas supply instead. Because the analyzer also measures ambient air in this mode, the dry gas supply must be Zero Air rather than N_2 — ambient air contains oxygen, and using Zero Air keeps the gas matrix during calibration consistent with the ambient matrix being measured.

9.1.1 Operation

This section describes the steps required to begin analyzer operation using the coordinator and autosampler system. It covers system readiness checks, software startup, and initial parameter configuration required before starting measurements.

1. Before continuing, review the important safety notes in the Safety section.
2. Make sure the hardware setup is complete and the system turned on in the correct sequence.
3. Once turned on, the main CRDS Data Viewer of the analyzer will open automatically on the desktop screen. To understand all the functions of the main CRDS Data Viewer, see section: CRDS Data Viewer Overview. A sequence of start-up messages will also appear in the Status Log Message window of the main CRDS Data Viewer. For definition, see section: 10.8.1 Common Status Log Messages.
4. Make sure the temperature of the High Precision Vaporizer stabilizes at 110°C by viewing the read out on the front of the vaporizer.

5. Make sure the Picarro Autosampler software is running, that the Autosampler has been trained, methods and jobs defined, and samples loaded. For detailed setup instructions, refer to the Picarro A0340 Autosampler User Manual (PN 40-0094) or the Picarro A0325 Autosampler User Manual (PN 40025).
6. Double click on the Coordinator Launcher icon on the analyzer's desktop. The coordinator software allows the analyzer to take measurements from multiple samples and is used to control the sample source and match the corresponding real time read out with the sample source. To learn more about the coordinator software (running the software, loading sample description, functions of the coordinator window), see section 11 Coordinator Software. Choose and launch an appropriate coordinator mode from the choices in the drop down menu of the coordinator launcher window. The Dual Mode Setup can operate in one coordinator mode.
7. Once launched, before the Coordinator window opens up, the User Editable Parameters window will pop up Figure 32.

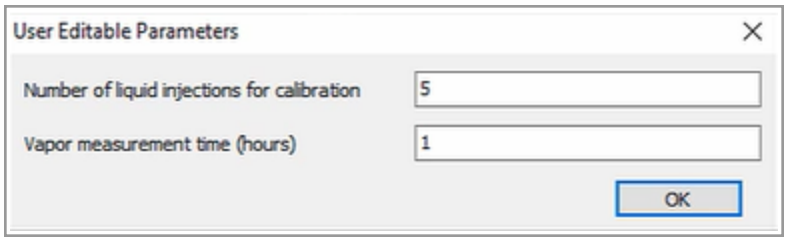


Figure 32 - User Editable Parameters Window

This allows measurement of liquid isotopic water standards at fixed time intervals during the measurement of the vapor phase to verify calibration. Measurement will always start with liquid injections.

- If no liquid samples are to be measured, enter '0' in the field for liquids. It will then measure the vapor continuously.
- If no vapor samples are to be measured, enter '0' in the field for vapors. It will then run only the liquid samples specified in the Autosampler job.
- If the analyzer is already running and these parameters need to be changed, it will require exiting and restarting the Picarro coordinator software.

NOTE

Analysis of liquid samples requires that both the coordinator software and autosampler job be started. Be sure to start the Autosampler Controller software before launching the Dual Mode Coordinator. Once the Autosampler Controller software is open, you may start the Dual Mode Coordinator. Once open, click "Run" on the Autosampler Controller software.

The coordinator alternates between two phases: a calibration block, where it requests a set number of liquid injections from the Autosampler, and a vapor block, where it measures ambient air for a fixed duration. Once the vapor block ends, the coordinator starts a new calibration block by asking the Autosampler for its next scheduled injections — it does not track vials or standards itself; that sequencing lives entirely in the Autosampler job.

Set "Number of liquid injections for calibration" in the Coordinator to match the total injections in one line of the Autosampler job. For example, an Autosampler line configured for ports A1–A2 at 10 injections each totals 20 injections; enter 20 in the Coordinator. If using two or more standards, this value can also be an integer multiple of one line's total.

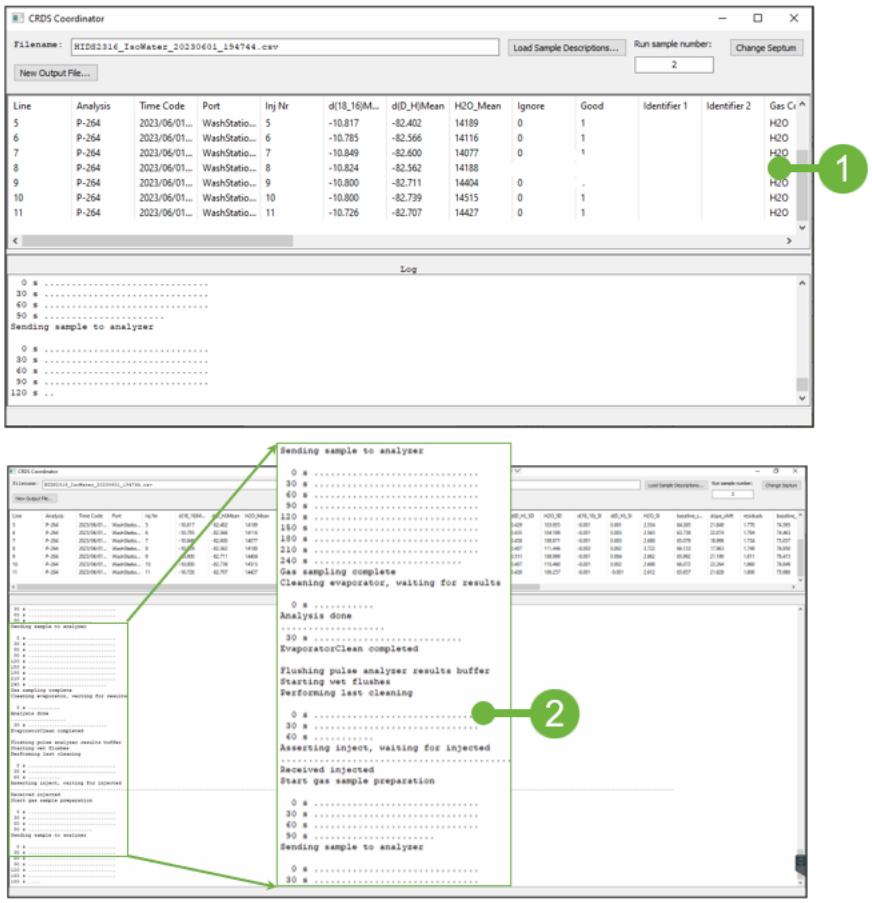
To run multiple unattended calibration/vapor cycles, configure that many corresponding lines in the Autosampler controller before starting — one line per cycle. If the coordinator finishes a vapor block and the Autosampler has no further lines queued, it will wait indefinitely for a new Autosampler job rather than repeating the previous one.

For drift checks using a single standard, rather than configuring multiple Autosampler lines, one line can be set to a higher injection count that's an integer multiple of the Coordinator's calibration block size. For example, a single line of 100 injections will support ten 10-injection calibration blocks before the Autosampler job needs to be renewed. The practical injection count from one vial is still limited by its volume, so size the line accordingly.

Once the injection number and vapor measurement duration parameters have been entered and the '**OK**' button is clicked, the coordinator window will pop up on your desktop. The different software elements will indicate whether liquid or vapor is being measured.

8. Once launched, the coordinator will automatically start collecting data. The data will also be available in the GUI as pulses. To customize pulse analysis or to adjust the peak of pulse data, see the section Best Practices and Operational Tips.

Figure 33 - Coordinator Launcher



1 Coordinator window

2 Coordinator Window – Expanded to illustrate typical steps and additional data

Figure 34 - Coordinator Window

9.1.2 Data

The coordinator writes calibration and vapor measurement results to a CSV file in C:\IsotopeData. Each row includes the injection or vapor reading along with its isotope values, timestamps, and sample/tray identifiers from the Autosampler.

For raw analyzer data (HDF5/h5 format), see 14 File Management and B Data File Viewer.

9.2 Manual Mode Setup

Manual Mode Setup is used for semi-automated measurement of liquid water samples, where the user manually injects samples while the analyzer controls vaporization and data acquisition. This mode is suitable for workflows that require flexibility in sample handling without the use of an autosampler.

The following section describes the operational requirements, supported coordinator modes, and procedures for performing measurements using Manual Mode.

9.2.1 Operation

1. Before continuing, review the important safety notes in Safety.
2. Make sure the hardware setup is complete and the system turned on in the correct sequence.
3. Once powered on, the main **CRDS Data Viewer** opens automatically on the desktop. For information about the functions of the CRDS Data Viewer, see CRDS Data Viewer Overview.

   NOTE

   A sequence of startup messages also appears in the Status Log Message window of the CRDS Data Viewer. For definitions of these messages, see Common Status Log Messages.

4. Verify that the **High Precision Vaporizer** temperature has stabilized at **110 °C**.

   NOTE

   Before starting measurements, ensure that the analyzer is operating in the correct measurement mode. Select the measurement mode that matches the dry gas supplied to the vaporizer (N_2 or zero air). For instructions, see 8.4.2 Switching Between Measurement Modes.

5. Double click on the **Coordinator Launcher** icon on the desktop.

   The coordinator software allows the analyzer to take measurements from multiple samples and is used to control the sample source and match the corresponding real time read out with the sample source. To learn more about the coordinator software (running the software, loading sample description, functions of the coordinator window), see section 11 Coordinator Software.

   From the drop-down menu, select and launch the appropriate Coordinator mode. The Coordinator window opens.

   Manual Inject is a semi-automated coordinator mode: it prompts you to inject each sample, then automates vaporizer control and analysis. Each injection cycle takes 9 minutes.

- The **L2130-*i*** supports one **Manual Inject** Coordinator mode for measuring:
  - $\delta^{18}O$
  - $\delta^{2}H$
- The **L2140-*i*** supports two Manual Inject Coordinator modes:
  - **Manual Inject** — Measures $\delta^{18}O$ and $\delta^{2}H$.
  - **O17 Manual Inject** — Measures $\delta^{18}O$, $\delta^{2}H$, and $\delta^{17}O$, and calculates 17O-excess.

For descriptions of all Coordinator modes supported by Picarro water isotope analyzers, see 11.4 Coordinator Modes for Picarro Water Isotope Analyzer .

6. Once launched, the coordinator will direct the user on when to manually inject samples and it will automatically start collecting data. The data will also be available in the GUI as pulses. To customize pulse analysis or to adjust the peak of one's data pulses, see the section Best Practices and Operational Tips.
7. The status bars at the bottom of the Coordinator window will allow one to know if the analyzer is ready for a manual injection or not. If ready, the sample description (if preloaded) will appear. If not loaded, a description can be added. Manually inject the sample and then press the Injected button in the lower right corner of the Coordinator window. The coordinator software will prepare the sample in the vaporizer in high precision mode (same as Standard Mode). It will take approximately 9 minutes until it is ready for the next injection.

9.2.2 Data

The coordinator writes measurement results to a CSV file in C:\IsotopeData. Each row includes the injection reading along with its isotope values, timestamp, and the sample description entered at the time of injection.

For raw analyzer data (HDF5/h5 format), see 14 File Management and B Data File Viewer.

9.3 Picarro Autosampler and High Precision Vaporizer Setup

This setup is used for automated injection and analysis of liquid water samples using the **Picarro Autosampler** and **High Precision Vaporizer**. It ships with two coordinator modes: **High Precision**, for maximum accuracy, and **High Throughput**, for faster cycling.

A Coordinator software upgrade adds **Standard** (a renamed High Precision), **Express**, and **Survey** modes, which trade some precision for speed.

For **L2140-*i*** systems, **High Precision 17O** mode is also available for $\delta^{17}O$ and 17O-excess measurements.

See section Coordinator Modes for Picarro Water Isotope Analyzer for the full list of modes available for your analyzer and software version, and section Parameters Recommended for Standard, Express, and Survey Modes for recommended injection counts, volumes, and discard settings for each mode.

9.3.1 Operation

1. Before continuing, review the important safety notes in chapter Safety.
2. Make sure the hardware setup is complete and the system is turned on in the correct sequence.
3. Once turned on, the main CRDS Data Viewer of the analyzer will open automatically on the desktop screen. To understand all the functions of the main CRDS Data Viewer, see CRDS Data Viewer Overview. A sequence of start-up messages will also appear in the Status Log Message window of the main CRDS Data Viewer. For definition, see Analyzer Status Log.
4. Make sure the temperature of the High Precision Vaporizer has stabilized at 110°C by viewing the read out on the front of the vaporizer.

   NOTE

   Before starting measurements, ensure you are in the correct measurement mode. Select the measurement mode that matches the dry gas supplied to your Vaporizer (either N2 or zero air). See the section Basic Operation for instructions.

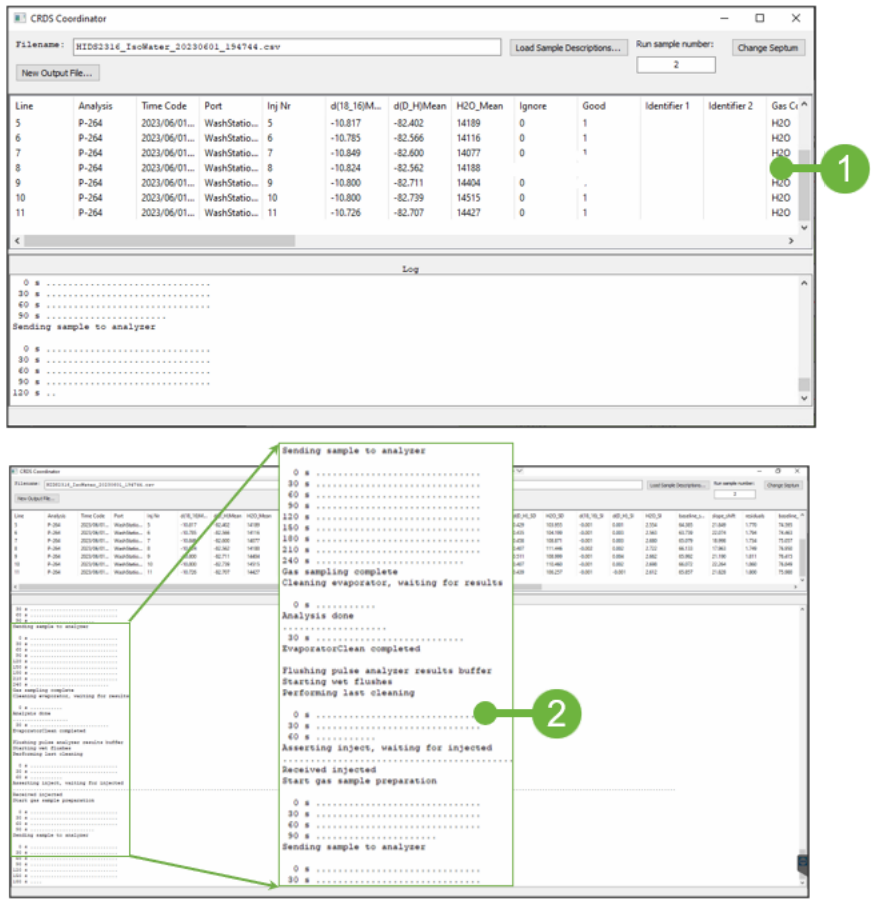
5. Make sure the Picarro Autosampler software is running, that the Autosampler has been trained, methods and jobs defined, and samples loaded. For detailed setup instructions, refer to the Picarro A0340 Autosampler User Manual (PN 40-0094) or the Picarro A0325 Autosampler User Manual (PN 40025).
6. Double click on the Coordinator Launcher icon on the analyzer's desktop. The coordinator software allows the analyzer to take measurements from multiple samples and is used to control the sample source and match the corresponding real time read out with the sample source. To learn more about the coordinator software (running the software, loading sample description, functions of the coordinator window), see section 11 Coordinator Software. Choose and launch an appropriate coordinator mode from the choices in the drop down menu of the coordinator launcher window. The coordinator window will pop up.

   NOTE

   Analysis of liquid samples requires that both the coordinator software and autosampler job be started. Be sure to start the Autosampler Controller software before launching the Coordinator. Once the Autosampler Controller software is open, you may start the Coordinator. Once open, click "Run" on the Autosampler Controller software.

7. Once launched, the coordinator will automatically start collecting data, assuming the Autosampler job has been started. The data will also be available in the GUI as pulses. To customize pulse analysis or to adjust the peak of pulse data, see the section Best Practices and Operational Tips.

Figure 35 - Coordinator Launcher



1 Coordinator window

2 Coordinator Window – Expanded to illustrate typical steps and additional data

Figure 36 - Coordinator Window

9.3.2 Data

The coordinator writes measurement results to a CSV file in C:\IsotopeData. Each row includes the injection reading along with its isotope values, timestamps, and sample/tray identifiers from the Autosampler.

For raw analyzer data (HDF5/h5 format), see 14 File Management and B Data File Viewer.

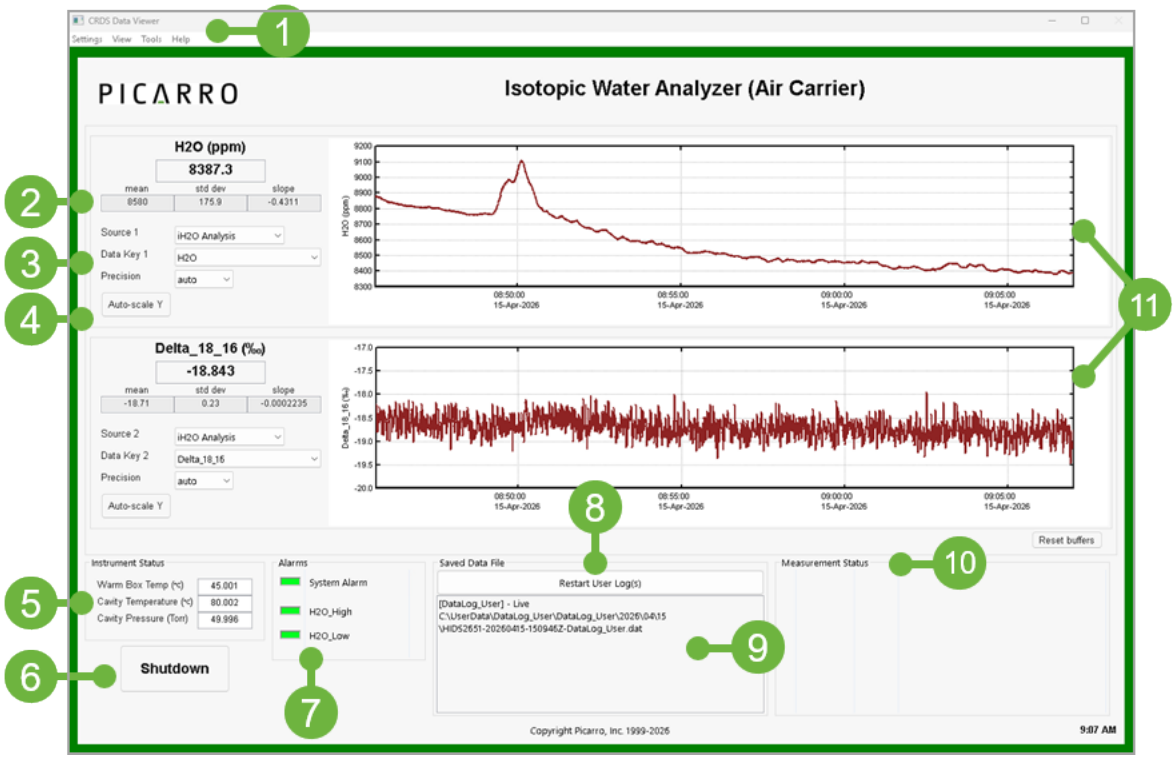
To screen results for chemical contamination and apply a linear-regression calibration based on the measured standards, see ChemCorrect™ Software.

9.4 Picarro Autosampler and High Throughput Vaporizer Setup

Picarro removed the High Throughput Vaporizer (part number A0212) from the price list in December 2013. Since that time, we have not shipped new High Throughput Vaporizers.

10 CRDS Data Viewer Overview

The features of the Data Viewer shown in Figure 37 are described in the following sections.



1. Settings, View, Tools, and Help menus
2. Digital Readouts and Statistics
3. Data Source, Data Key, Precision settings
4. Axis Auto Scaling
5. Instrument Status
6. Shutdown button
7. Alarm Panel
8. Restart Log Buttons
9. Data Log; Filename, and Path
10. Status Log Window
11. Data Windows

Figure 37 - Layout of Analyzer Data Viewer

10.1 Settings, View, Tools, and Help Menus

The menus in the application provide access to display controls, calibration tools, and diagnostic features. This section describes the available options in the Settings, View, Tools, and Help menus, including functions for changing GUI modes, adjusting display behavior, accessing calibration utilities, and viewing instrument version information.

10.1.1 Settings Menu

Left clicking on the **Settings** menu pulls down a menu that has one entry: **Change GUI Mode from Standard to Service (or Change GUI mode from Service to Standard if it is already in service mode)**.

This is the access point to a password protected service mode (default password is **picarro**) where additional operational and measurement parameters are available in the data keys. Selecting and clicking on this entry opens the Cavity Ring-Down Spectrometer Controller.

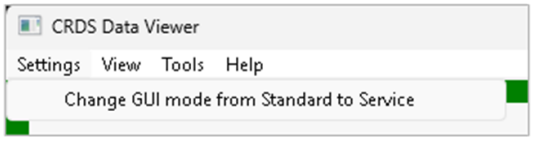


Figure 38 - CRDS Settings Menu options

10.1.2 View Menu

The View menu provides options for controlling the display of graphs and on-screen information:

- **Lock Time Axis When Zoomed / Unlock Time Axis**: When enabled, forces both graphs to use the same time scale during zoom operations.
- **Show/Hide Statistics**: Toggles the display of measurement statistics. See Section 10.3 Digital Readouts for more information.
- **Show/Hide Instrument Status**: Toggles the display of instrument status information. See 10.4 Instrument Status for more information.

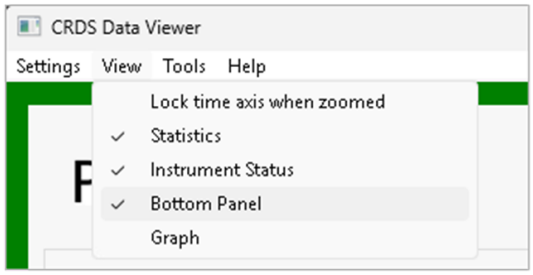


Figure 39 - CRDS View Menu Options

10.1.3 Tools Menu

This menu item has two entries:

1. **User Calibration:** Opens the password protected user calibration window (default password is **picarro**).

Calibration slope and intercept can be entered, and their effects are immediately seen in the data. See section Updating the Instrument Calibration for Accurate On-Screen Readings, for more information.

2. **Show/Hide Sequencer GUI:** Toggles the display of the external valve sequencer window (user may need to hit **alt-tab** to bring it to the front).

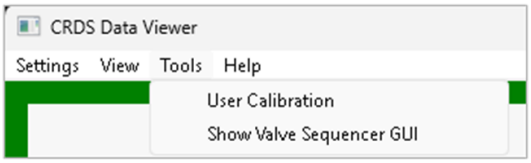


Figure 40 - CRDS Tools Menu Options

10.1.4 Help Menu

About: Displays the version number of the instrument.

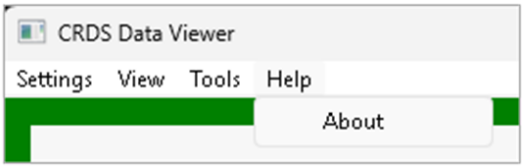


Figure 41 - CRDS Help Menu Options

10.2 Alarms Panel

This panel is used to monitor the status of the internal instrument alarms. These indicators are gas concentration alarms, such as “H2O Too High/Low” depending on instrument configuration. The gas concentration alarm icons are off (grayed) when the respective concentrations are below a certain value, and they are illuminated red when the respective concentrations are above/below a certain value.

⚠ CAUTION

High/low alarm settings are not intended as a safety measure as configured at the factory, either with respect to human health or the health of the analyzer. It is up to the customer to determine the meaning and level of a “high” or “low” value based on their application.

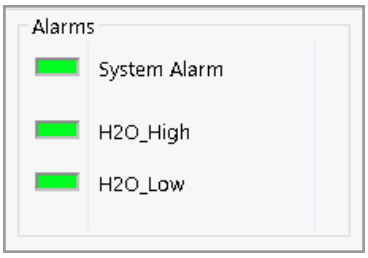


Figure 42 - Alarms Panel

To view the alarm set point, click on the **Alarm Icon** and a dialog box will appear indicating the alarm setting and allow the user to enable it or change the setpoint.

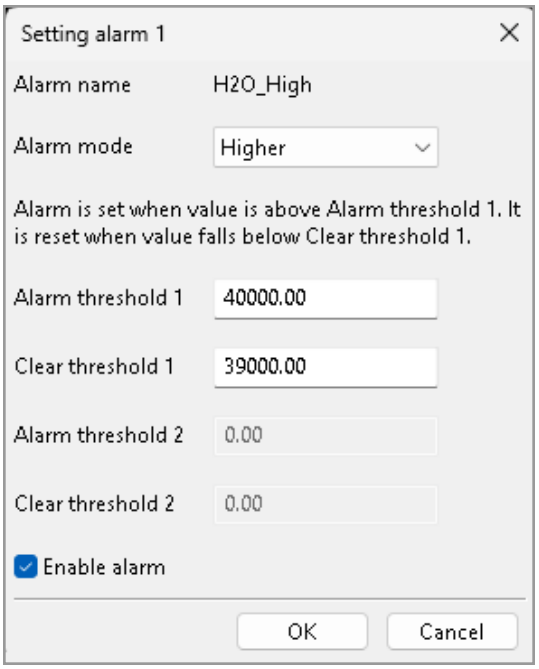


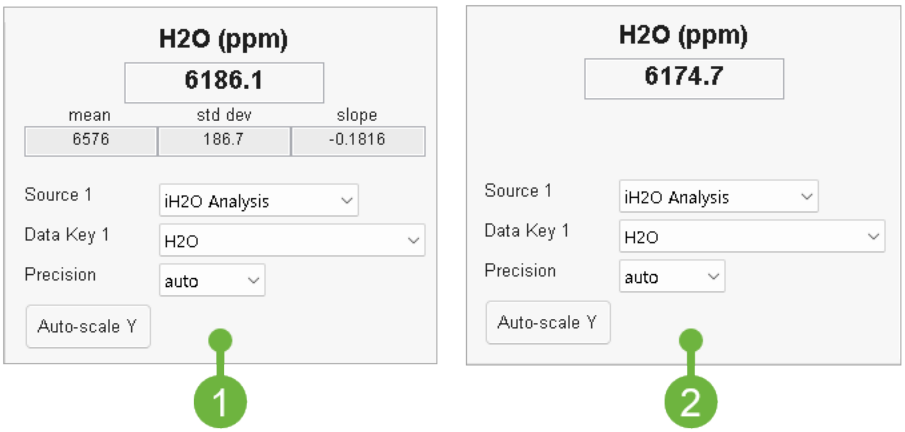
Figure 43 - Alarm Settings Dialog Box Example

Type the value you wish to set the alarm to and click the **OK** button or **Cancel** if you do not wish to change the alarm value. If you do nothing, the dialog box will disappear, and the alarm value will remain unchanged. The units are those that appear in the GUI graph.

10.3 Digital Readouts

Displays the latest value recorded for the selected Data Key for each Data Window. Changing the Data Key changes the Digital Readout as well as the Data Window view. If the **Show Statistics** entry is enabled in the **View** menu, the mean, standard deviation, and slope of the data in the graph is dynamically calculated and indicated below the digital concentration readout. These numbers change to reflect statistics of whatever data is in the

data window. **Zooming** into a section of existing data will show the statistics statically for that time period, while the digital readout above the statistics continues to update with the latest value.



1 Show Statistics Enabled

2 Show Statistics Disabled

Figure 44 - Digital Readouts Panel

10.4 Instrument Status

If these parameters are enabled through the **Show Instrument Status** entry in the **View** menu on the main toolbar, digital readouts for Warm Box temperature, Cavity Temperature and Cavity Pressure are displayed to the left of the main trend graphs.

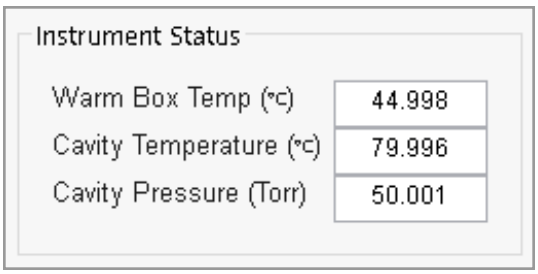


Figure 45 - Instrument Status Panel

10.5 Shutdown and Restart User Logs Buttons

This section describes the Shutdown and Restart User Log(s) buttons, which allow users to safely shut down the analyzer and manage instrument data logging during operation.

10.5.1 Shutdown Button:

Shuts down the analyzer. See section 8 Basic Operation for more information.

Figure 46 - Shutdown Button

10.5.2 Restart User Log(s) Button

The analyzer automatically records all data collected on the instrument as .dat files. These are described further in 14 File Management.

To start a new data file (time-coded to the current second), click the **Restart User Log(s)** button. The new file name should be visible beneath the button in a few seconds.

Figure 47 - Restart User Logs Button

10.5.3 Data Log Filename and Path

The filename and path of the active data log is displayed in this pane. The indicator is grayed-out when there is no active data log before gas measurement reporting begins. A new file is generated when the instrument starts reading gas concentrations, (e.g., “201301Z”) and subsequently at 1 hour increments (e.g., “211301Z”, “221301Z”). A new day folder (e.g., “2023\06\01”) will be generated at midnight, as will month and year folders at the appropriate times.

Figure 48 - Data Log File Name and Path

10.6 Data Window

The data window displays a graph of any stream of data vs. system time, with a format of hh:mm:ss. The user can select which data streams are displayed using combinations from the **Data Source** and **Data Key** pull down menus. The precision displayed can be adjusted using the **Precision** menu. Auto-Scaling of the **Y-axis** is also available. Clicking any Autoscale button autoscales its Y-axis if the plot hasn’t done this automatically.

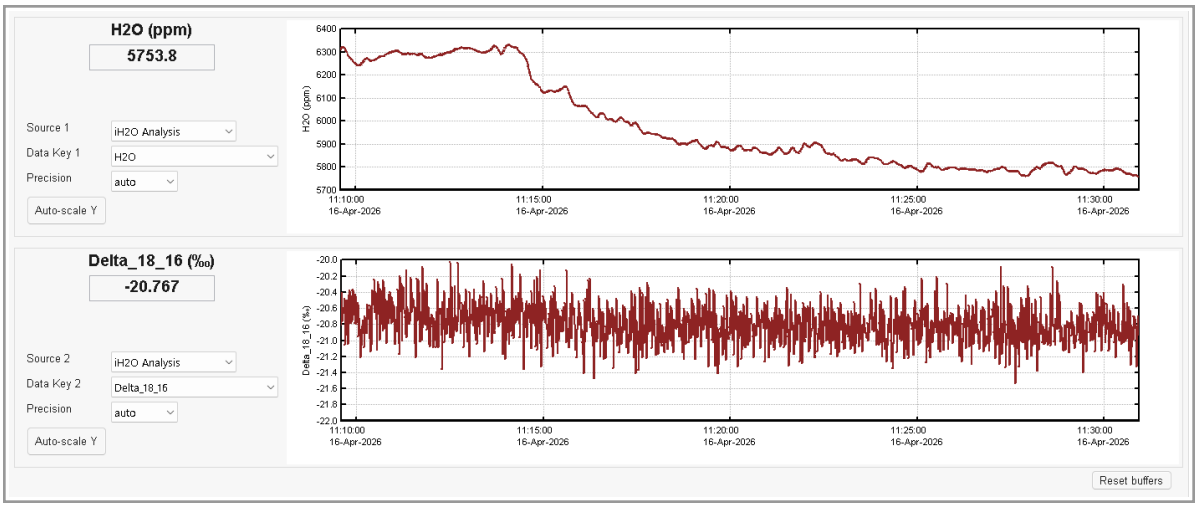


Figure 49 - Data Window Panel

10.7 Data Source, Data Key, and Precision Controls

The Data Source, Data Key, and Precision pull-down menus control how data is selected and displayed in the data window. Together, these controls determine which data stream is shown and how its values appear on the graph.

The **Data Source** and **Data Key** menus are used to select the type of data displayed. When Instrument Analysis (where Instrument represents the system installed) is selected, gas concentration data is shown. When Sensors is selected, the display shows system parameters such as optical cavity pressure, cavity temperature, electronics temperature ("DASTemp"), and wavelength monitor temperature ("WarmBoxTemp").

The **Precision** pull-down menu controls the number of digits displayed on the y-axis. The default setting is Auto, which automatically selects an appropriate display precision for most applications. Users can manually select between 0 and 4 digits of precision if required. This setting affects only how data is displayed in the data window and does not affect the precision of saved data in log or results files.

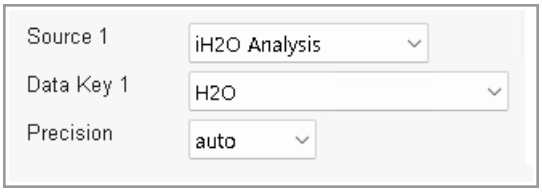


Figure 50 - Data Source, Data Key, Precision Controls

10.8 Analyzer Status Log

This window displays instrument status messages, in the following form: **YYYY,MM,DDhh:mm:ss,** then '**Generic message text.'**

10.8.1 Common Status Log Messages

Following are the most common messages that appear:

- **Pressure Stabilizing/Locked: Displayed when** the valve control system begins to allow flow through the analyzer and stabilizes the pressure inside the cavity.
- **Temperature Locked: WB (HB): When the temperatures of the warmbox (wavelength monitor) and hotbox (cavity) have stabilized.**
  This is typically the longest step in the startup sequence. **Startup:** Depending on ambient temperature, the analyzer and its hotbox temperature set point, this step may take as little as 20, or as much as 60 minutes. **Restart:** If the instrument is only stopped briefly, this may take a few seconds to a few minutes.
- **Preparing to Measure:** Spectral scanning has started. Concentration measurements will be available in approximately 30 seconds. The instrument will continue to scan and report concentration measurements until the instrument is shut down.
- **Measuring:** This is the normal mode of operation after startup has completed.

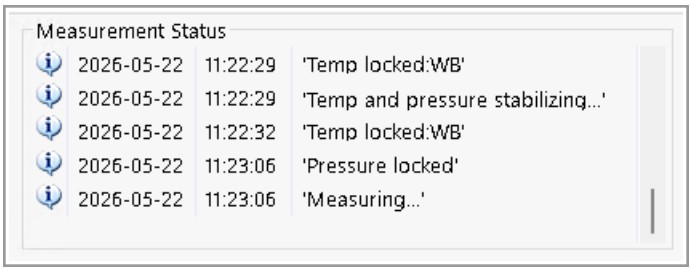


Figure 51 - Analyzer Status Log

10.9 Reset Buffers Button

Click this button to clear the internal data buffer of the GUI (this clears the current data traces from the graphs). This has the effect of clearing all data in the data window. Pressing this button has no effect on any of the data log files stored by the instrument.

Figure 52 - Reset Buffers Button

10.10 Graph Zooming and Panning

The data graph provides interactive zooming and panning controls that allow users to closely inspect specific regions of interest or return to a full-data view as needed. These controls support mouse-based actions and keyboard modifiers to adjust the graph scale, navigate along the axes, and automatically rescale the display for clearer data interpretation.

Zooming In/Out

To zoom in on a specific region of the graph, move the cursor to the area of interest, **click/hold** the left mouse button, **thendrag** as desired to create a box that covers the region of interest (see Figure 53 - Data Graph Zoom Function). When the box is drawn, release the left button and the boxed area will automatically scale to fill the data window.

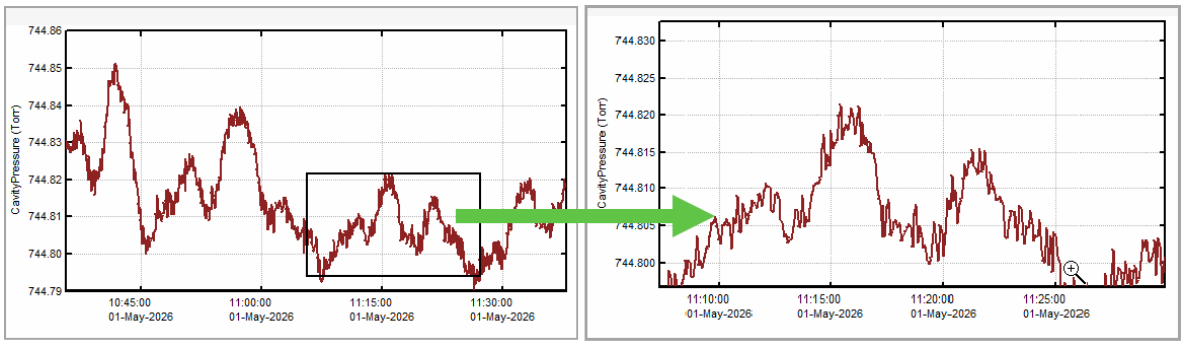


Figure 53 - Data Graph Zoom Function

To zoom back out to see all data in the buffer, **double-clickthe left button** within the graph display. **To zoom out indefinitely**, right click. Right clicking multiple times zooms out further. **To auto scale** the y-axis of either graph, use the auto-scale buttons below the graph.

To Zoom the X and Y axes: hold down the control button and move the cursor up/down or left/right using the right mouse button.

Lock/Unlock Time Axis

Zoom and pan features are often useful when time axes are locked, and the user wishes to align the Y axis in multiple plots. To lock or unlock the time axis of each graph during zooming, from the **View** menu, select **Lock time axis when zoomed** or **Unlock time axis**.

Panning

To pan the data in the X or Y axis: hold down the control button and drag the cursor using the left mouse button.

11 Coordinator Software

To measure discrete samples or to control external peripherals and accessories a separate software tool (Coordinator) is used to control the sample source and match the corresponding real time read out with the sample source. The Coordinator programs that are accessible to a user are dependent on the system configuration.

NOTE

Although this section will provide an overview to the concept of Coordinators, it does not necessarily provide the detail on all Coordinators available on a Picarro water isotope system. Instead, refer to the separate User Manual provided with each of your Picarro accessories:

- **A0101 SDM (Standards Delivery Module) User Manual (PN 40-0005)**
- **A0213 IM (Induction Module) User Manual (PN 40039)**
- **A0214 MCM (Micro Combustion Module) User Manual (PN 40022)**
- **A0217 CWS (Continuous Water Sampler) User Manual (PN 40003)**

11.1 How to Run Coordinator Software

The Coordinator software is used to control sample analysis by linking the analyzer measurement process with the sample source (for example, manual injection or autosampler operation). It manages measurement sequencing, associates results with sample identifiers, and displays real-time output during analysis.

The following procedure describes how to launch the Coordinator software, select the appropriate coordinator mode, and begin sample analysis.

1. First, make the required hardware connections for your system of interest. Afterwards, turn on the analyzer and wait for the CRDS Data Viewer of the analyzer's software to open up automatically on your desktop screen.

2. Next, launch the coordinator software by double clicking on the **Coordinator Launcher** icon on your desktop.
3. After double clicking on the Coordinator Launcher icon, a window will appear. Choose the appropriate coordinator from the drop down menu, and then click the **Launch** button. Make sure that the chosen coordinator is supported by your hardware connections and that samples are ready to be analyzed.

Figure 54 - Coordinator Launcher Window

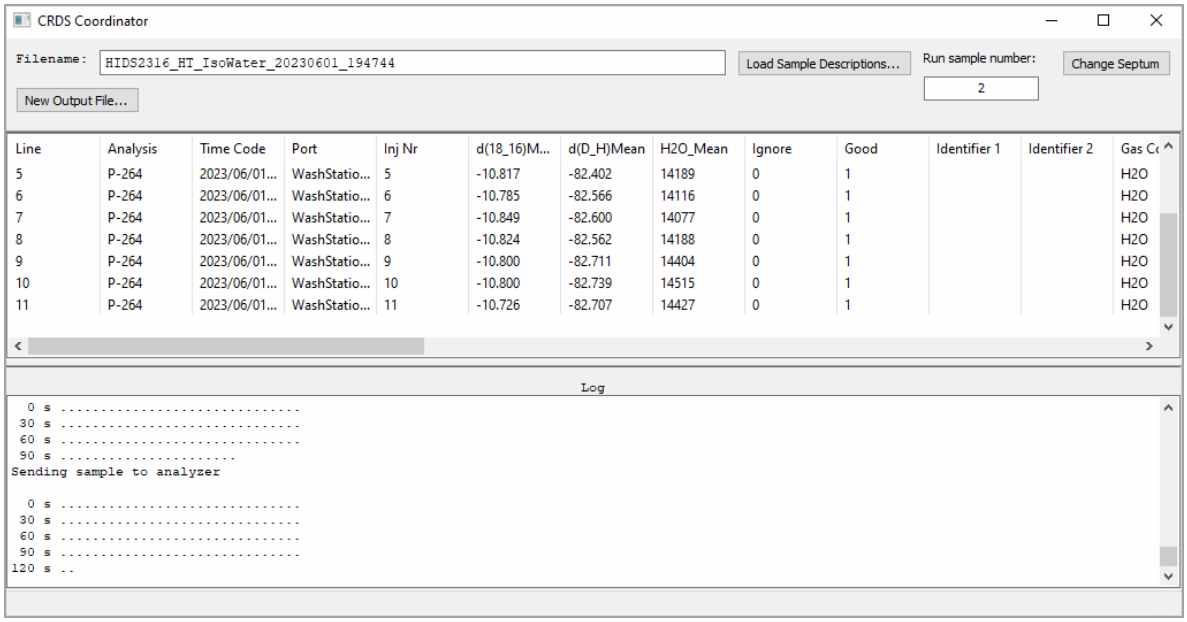


Figure 55 - CRDS Coordinator Window

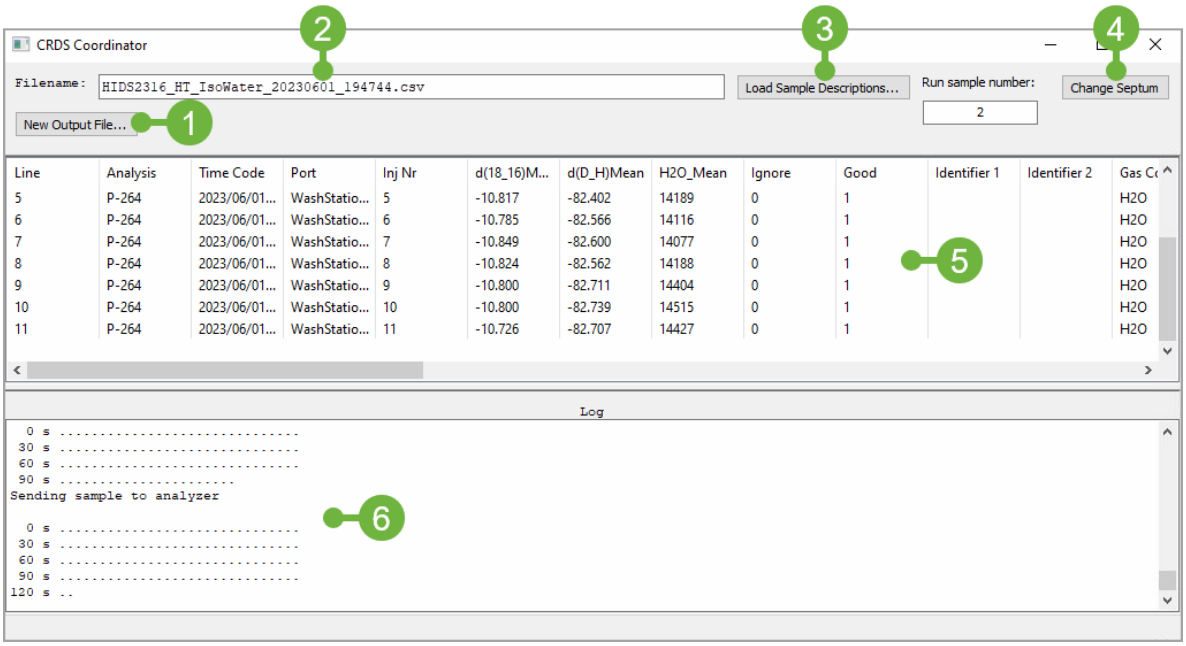
NOTE

The look of the window may vary depending on the configuration of your analyzer.

4. After clicking on the **Launch** button, the coordinator window (Figure 55 - CRDS Coordinator Window) will pop up. (Depending on the coordinator mode chosen, you may or may not be asked to set parameters for your analysis). From the Coordinator window, you will be able see results from sample analysis,

11.1.1 Coordinator Window Descriptions

This section describes the elements of the Coordinator window and their functions during operation. It explains how output data is generated and managed, how sample information is incorporated, and how system actions and analysis results are displayed to the user.



1. New Output File Button
2. Coordinator Output Filename
3. Load Sample Descriptions Button
4. Change Septum Button
5. Upper Portion of Window
6. Lower Portion of Window

Figure 56 - Coordinator Window Descriptions

1. **Coordinator Output Filename:** Can be seen in the upper left of the Coordinator window. It follows an automated convention of:

   model, serial number, mode, year, month, date, and time. For example:

   HIDS2316_HT_IsoWater_20230601_194744.csv

   This means the coordinator file output was taken using analyzer HIDS2316 in high throughput isotopic water analysis starting on 1 June 2023 at 7:47:44 pm.

2. **New Output File Button:** Clicking on this button will save the data that you see on the coordinator window into a file, and then clear the data from the Coordinator Window.

3. **Load Sample Descriptions Button**: Located around the upper right corner of the Coordinator Window. The button allows the user to include a description for each vial in the data file output on the coordinator window.
4. **Change Septum Button:** Used to pause the Autosampler and the vaporizer in the middle of an analysis to physically change the septum on the vaporizer.

   In order to load the sample description file, press the button labeled **Load Sample Descriptions**. A dialog box will appear. Select the sample description file, and then click **Open**. If a certain tray (front or rear) is not being used, use the 'Cancel' button to dismiss the dialog.
5. **Upper Portion of The Window:** Each row represents the analysis results from a single injection. The types of columns are pre-selected by Picarro to include the most useful values for isotopic water analysis and for diagnostic indications.

   The values for the columns, unless otherwise noted, are the average value for time period of the injection, which was marked in red on the CRDS Data Viewer. Values of the form *_SD are standard deviations for that same time period. The time period is selected by trigger thresholds based on the water vapor concentration. The analyzer is characterized and specified based on the factory default trigger thresholds—changing these values is not recommended, please contact Picarro if you feel this is necessary.
6. **Lower Portion Of The Window (labeled "Log"):** This window displays the action that is currently taking place. For those actions that take some time to complete, a period is displayed each second and a new line is started every thirty seconds to show progress.

11.2 How to Make the Sample Description File

NOTE

The A0340 Autosampler software labels vial positions by row (A, B, C...) and vial number within each row (1–10). The sample description file uses the original sequential vial numbering across the full tray instead — for example, vials C1–C5 in the Autosampler software correspond to vial numbers 21–25 in the description file.

The sample description file should be in CSV (comma separated value) format. Use the supplied NotePad++ software. Write the sample descriptions in the format as shown below.

Tray,Vial,Identifier 1,Identifier 2

1,1,Picarro 00,standard

1,2,Picarro 11, standard

1,3,Picarro 22, standard

1,4,WA 1,first sample from Washington

1,5,WA 2,second sample from Washington

1,6,CA 1, first sample from California

1,7,CA 2, second sample from California

1,8,Picarro 00, standard

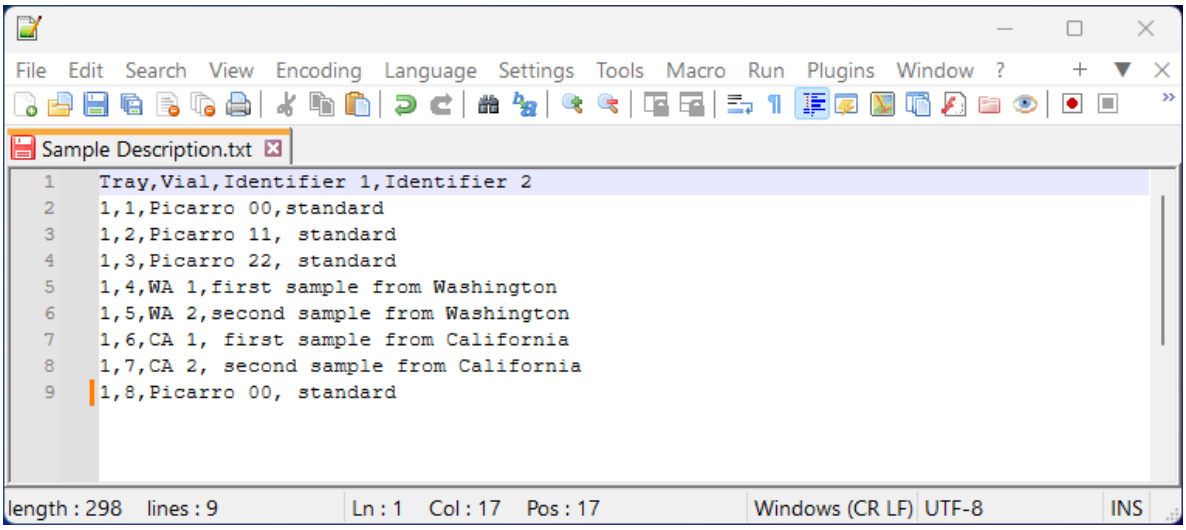


Figure 57 - Sample Description Example

After the first line (which should contain the column heading), each line should represent a sample description for the analysis results from a single injection. The lines in the file may be arranged in any order. The capitalization and spacing of the first line must exactly match the provided example. MS Excel can be used if the file is saved in CSV format. It is recommended to generate the file using Windows operating systems (as on the analyzer) as there are differences in CSV format between different operating systems. It is permissible to load the sample description files at any time during the data collection. The output file is rewritten to use the new sample descriptions, so that the most recently loaded descriptions are always used.

11.3 Parameters Recommended for Standard, Express, and Survey Modes

The original protocol for water isotope analysis was 6 injections per sample, averaging the last 3 data points to obtain the isotopic values of the sample. This still meets the analyzer's factory specification. Based on further characterization of memory effects in the vaporizer, Picarro now recommends at least 8 injections per sample for improved accuracy, with 10 injections as the standard recommendation, still averaging only the last 3 data points.

Using the Express mode, Picarro recommends running 10 injections per sample: the first 6 are overlapping "wet flush" injections used to purge memory faster, followed by 4 standard-length injections. As with Standard Mode, only the last 3 data points are averaged.

Before launching the Express coordinator, please set number of injections to 10, and volume of sample to 1.8 µl, in the Autosampler user interface.

Using the **Survey** mode requires only one injection.

Before launching the Survey coordinator, please set number of injections to 1, and volume of sample to 2.5 µl, in the Autosampler user interface.

The following table summarizes Picarro's recommendations for processing samples.

Table 8 - Picarro Recommendations for Processing Samples.

Coordinator	Number of Injections*	Sample Volume* (µl)	Number of Injections to Discard**
Standard	10	1.8	7
Express	10	1.8	7
Survey	1	2.5	0

*Edits are done to the autosampler software method tab.

**Edits are done to the ChemCorrect post processing parameters.

NOTE

Six injections (discarding the first 3) still meets factory specification but is no longer the recommended default. For applications requiring the highest achievable accuracy — such as establishing an in-house working standard — see the Picarro Calibration Guide for guidance on using a significantly higher injection count with an extended discard count.

NOTE

When using samples with large isotopic range, more injections can be added to help reduce the memory effect.

11.4 Coordinator Modes for Picarro Water Isotope Analyzer

The CRDS analyzer needs to be equipped with the appropriate hardware to support a coordinator mode.

Table 9 - Available Coordinator Modes

Hardware	Associated Coordinators
High Precision Vaporizer (A0211) CRDS Analyzer (L2130-*i* or L2140-*i*)	Manual Injection
High Precision Vaporizer (A0211) Autosampler (A0340 or A0325) CRDS Analyzer (L2130-*i* or L2140-*i*)	**L2130-*i*:** • High Precision* (same as Standard Mode) • High Throughput* • Standard** (same as High Precision Mode) • Express** • Survey** **L2140-*i*** • High Precision* • High Throughput* • High Precision ^{17}O* • Express** • Survey** *Only available without Coordinator software upgrade ** only available with coordinator upgrade
High Precision Vaporizer (A0211) Autosampler (A0340 or A0325) CRDS Analyzer (L2130-*i* or L2140-*i*) Vaporizer Switching Valve (A0912)	Dual Mode Dual Mode ^{17}O (if L2140-*i*)
High Precision Vaporizer (A0211) Micro Combustion Module (A0214) CRDS Analyzer (L2130-*i* or L2140-*i*)	MCM Manual Mode

Hardware	Associated Coordinators
High Precision Vaporizer (A0211) Standards Delivery Module (A0101) CRDS Analyzer (L2130-*i* or L2140-*i*)	Standards Delivery Module (SDM)
High Precision Vaporizer (A0211) Micro Combustion Module (A0214) Autosampler (A0340 or A0325) CRDS Analyzer (L2130-*i* or L2140-*i*)	MCM High Precision MCM High Throughput
Induction Module (A0213) CRDS Analyzer (L2130-*i* or L2140-*i*)	Induction Module
Continuous Water Sampler CRDS Analyzer (L2130-i or L2140-i)	Continuous Water Sampler

11.4.1 Description of Different Coordinator Modes

Picarro Coordinator modes define how the analyzer acquires and processes measurements for different sample types, workflows, and performance requirements. Each mode is optimized for a specific application, such as high-precision laboratory analysis, high-throughput screening, continuous monitoring, or specialized configurations involving additional hardware modules.

Selecting the appropriate Coordinator mode is an important step in configuring the analyzer, as it determines the sequence of operations, measurement timing, and required system components. Some modes operate automatically with autosamplers, while others require user interaction or additional hardware.

The following sections describe the available Coordinator modes, their intended use cases, and key operational characteristics.

1. **High Precision (also called Standard after a Coordinator software upgrade):** Used to measure liquid water samples with maximum precision. Automatically injects and measures liquid samples. Each injection cycle takes 9 minutes.

2. **High Throughput:** Used for faster measurement of liquid water samples with good precision. Automatically injects and measures liquid samples. Each injection cycle takes 4 minutes. High Precision and High Throughput operate in the exact same fashion, except that the steps of sample preparation and analysis are faster in High Throughput.
3. **Express*:** Used for faster measurement of liquid water samples while retaining high precision. Uses 10 injections per sample — 6 overlapping "wet flush" injections (~1.5 minutes each) followed by 4 standard-length injections (~5 minutes each) — discarding the first 7 to achieve optimal memory reduction.
4. **Survey***: Used for super-fast measurements of large sample batches at moderate precision, enabling efficient sample sorting. By manually rearranging samples according to survey results, the memory effect between adjacent samples can be reduced. Each injection cycle takes 95 seconds; we recommend 1 injection per sample.

   NOTE

   ***Express and Survey are only available with a Coordinator software upgrade.**

5. **Manual Inject:** Used for semi-automated measurement of liquid water samples with maximum precision. Requires A0211 High Precision Vaporizer. User manually injects samples after prompt; vaporizer control and analysis are automated. Each injection cycle takes 9 minutes.
6. **Dual Mode (labeled "Dual Liquid/Vapor" in the Coordinator Launcher dropdown):** Used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. Requires A0211 High Precision Vaporizer, A0912 Dual Mode Configuration hardware, and an Autosampler. Alternates between analyzing ambient vapor and liquid standards based on a user-defined sequence. Each injection cycle takes just over 7 minutes, including cleaning and stabilization steps.
7. **Standards Delivery Module (SDM):** Used for measurement of ambient vapor coupled with automated injection of liquid calibration standards. Requires A0211 High Precision Vaporizer and A0101 Standards Delivery Module. Alternates between analyzing ambient vapor from multiple points and a continuous stream of vaporized standard, based on a user-defined sequence. A calibration measurement takes approximately 20 minutes per concentration/standard. Before operating in SDM mode, set the vaporizer temperature to 140°C.
8. **IM CRDS (Induction Module):** Requires the Induction Module. Used for isotopic analysis of water extracted from samples such as soil, plants, or tissues.
9. **Micro Combustion Module (MCM):** Used to measure liquid water samples while destructively removing potential contaminants, with maximum precision. Requires A0211 High Precision Vaporizer, A0214 Micro Combustion Module, and an Autosampler. Each

injection cycle takes 9 minutes. In addition to controlling the valve sequence for liquid sample injection, the MCM coordinators also control MCM heating to ensure removal of interfering organics.

10. **Continuous Water Sampler (CWS):** Used for continuous, real-time measurement of water. Requires A0217 Continuous Water Sampler. No discrete sampling is required; automatically switches between calibration standards and samples using four inlet ports.

NOTE

The L2140-*i* can operate in four instrument modes (iH2O N_2, iH2O Air, iH2O N_2 O-17, and iH2O Air O-17). 17O-excess measurements rely on longer injections and averaging for precision rather than fast cycling, so Express and Survey modes are not offered for the O-17 instrument modes — only the O-17 variants of High Precision, Dual Mode, and Manual Inject (High Precision 17O, Dual Mode 17O, and O17 Manual Inject) are available.

11.4.2 Description of Column Headers Used in Coordinators

The following table provides information regarding the column headers presented in the Coordinator output files available on a Picarro water isotope analyzer. The table below lists the possible fields in the coordinator results file header:

Coordinators vary by analyzer product number, therefore not all columns will be visible on an individual analyzer.

Table 10 - Column Headers Used in Coordinators

Item	Description
Line	Line counter. Each line represents a single injection or data point (for vapor measurements in the dual mode).
Analysis	Sequential number of the sample run over the history of the analyzer.
Time Code	Time the line was recorded in “Year/Month/Day Hours:Minutes:Seconds.” This time stamp is linked to the local time of your computer’s clock.
Port	Reports the vial position on the tray where the autosampler is sampling from.
Inj Nr	Sequential injection number from the port (vial).

Item	Description
d(17_16)Mean	The average $\delta^{17}O$ value, in per mil (‰), measured at that interval (Line). The typical raw data acquisition rate on a L2140-i is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration. Only available on a L2140-i.
d(18_16)Mean	The average $\delta^{18}O$ value, in per mil (‰), measured for that injection (Line). The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration.
d(D_H)Mean	The average $\delta^{2}H$ value, in per mil (‰), measured for that injection (Line). The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration.
E17_Mean	The average ^{17}O-excess value, in per mil (‰), measured for that injection (Line). ^{17}O-excess is the deviation the expected relationship between $^{17}O/^{16}O$ and $^{18}O/^{16}O$ ratios and is defined by: E17_Mean = ln[d(17_16)Mean + 1] – 0.528ln[d(18_16)Mean + 1] The typical raw data acquisition rate on a L2140-i is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated. Post-processing is required for calibration. Only available on an L2140-i.
H2O_Mean	The average water concentration, in ppm, is measured for that injection (Line). The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore this represents the average of 1 Hz data points across the water pulse. The averaging window is shown in red on the CRDS Data Viewer. The reported delta values are not calibrated.

Item	Description
Ignore	-1 or 0: -1 indicates the measurement should be ignored and is based on the first three injections from each sample vial being ignored due to sample-to-sample isotopic memory.
Good	0 or 1: 1 indicates that the mean H_2O concentration is within the required range. 0 indicates that the mean H_2O concentration is outside the required range.
Vapor d(17_16)	Only reported when operating in Dual Mode. Populated when the Dual Mode is measuring ambient vapor. Raw $\delta^{17}O$ output from the analyzer with no averaging. The typical raw data acquisition rate on a L2140-i is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second. Only available on a L2140-i.
Vapor d(18_16)	Only reported when operating in Dual Mode. Populated when the Dual Mode is measuring ambient vapor. Raw $\delta^{18}O$ output from the analyzer with no averaging. The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second.
Vapor d(D_H)	Only reported when operating in Dual Mode. Populated when the Dual Mode is measuring ambient vapor. Raw $\delta^{2}H$ output from the analyzer with no average. The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second.
Vapor E17	Only reported when operating in Dual Mode. Populated when the Dual Mode is measurement ambient vapor. Raw ^{17}O -excess output from the analyzer with no averaging. The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second. Only available on a L2140-i.
Vapor H2O	Only reported when operating in Dual Mode. Populated when the Dual Mode is measurement ambient vapor. Raw H_2O concentration output from the analyzer with no averaging. The typical raw data acquisition rate on a L2130-*i* or L2140-*i* is ~ 1 Hz, therefore during the vapor measurement phase a line will be created every ~ 1 second.
Identifier 1	First identifier of the sample. Only populated if a sample description file is loaded when the coordinator is open.

Item	Description
Identifier 2	Second identifier of the sample. Only populated if a sample description file is loaded when the coordinator is open.
Gas Configuration	Indicates the type of gas being measured. Water isotope analyzers measure water vapor sample.
Timestamp Mean	Unix timestamp.
d(17_16)_SD	Standard deviation of the measured $\delta^{17}O$ across an injection's averaging window. The averaging window is shown in red on the CRDS Data Viewer. Only available on a L2140-i.
d(18_16)_SD	Standard deviation of the measured $\delta^{18}O$ across an injection's averaging window. The averaging window is shown in red on the CRDS Data Viewer.
d(D_H)_SD	Standard deviation of the measured $\delta^{2}H$ across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
H2O_SD	Standard deviation of the measured H_2O concentration across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
E17_SD	Standard deviation of the measured ^{17}O-excess across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer. Only available on a L2140-i.
d(18_16)_SI	The slope of the measured $\delta^{18}O$ across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
d(D_H)_SI	The slope of the measured $\delta^{2}H$ across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
H2O_SI	Slope of the measured H_2O concentration across an injection's averaging window. The averaging window is show in red on the CRDS Data Viewer.
baseline_shift	The average value for baseline shift, in ppb/cm, measured for that injection (Line). Baseline_shift is a spectral term that is measured on the L2130-*i* and L2140-*i*. It is the change in the constant term of the fitted baseline, relative to an empty cavity baseline which is measured at the Picarro factory. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.

Item	Description
slope_shift	The average value for slope shift, in ppb/cm, measured for that injection (Line). Slope_shift is a spectral term that is measured on the L2130-*i* and L2140-*i*. It is the change in the linear term of the fitted baseline, relative to an empty cavity baseline which is measured at the Picarro factory. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.
residuals	The average value for residuals, in ppb/cm, measured for that injection (Line). Residuals is a spectral term that is measured on the L2130-*i* and L2140-*i*. This term represents the root mean squared residual of the least-squares fit of the measured spectra versus the expected spectra. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.
baseline_ curvature	The average value for baseline curvature, in ppm*cm, measured for that injection (Line). Baseline_curvature is a spectral term that is measured on the L2130-*i* and L2140-*i*. This term represents the quadratic term in the fitted baseline. This column can be used to track potential spectral interference and data integrity. See ChemCorrect section.
interval	Average of the elapsed time between each fitted spectrum for an injection's averaging window.
ch4_ppm	The average methane concentration, in ppm, is measured for that injection (Line). This column can be used to track potential spectral interference and data integrity. Methane concentration is not calibrated and should not be used directly to determine the methane concentration in the water source.
h16od_adjust	This term represents an adjustment applied to WLMh16od_offset, a filtered and scaled frequency error derived from least-squares fit. h16od_ adjust is only reported on the L2130-*i* and L2140-*i*. This column may be used to the Picarro Technical Support team in diagnosing wavelength locking.
h16od_shift	This term represents an adjustment applied to WLMh16od_offset, a frequency error derived from least-squares fit. h16od_shift is only reported on the L2130-*i* and L2140-*i*. This column may be used to the Picarro Technical Support team in diagnosing wavelength locking.

Item	Description
n2_flag	Flag for reported the measurement mode at the time of measurement. n2_flag will equal 1 for operation in the N2 mode, and equal to 0 for operation in the Zero Air mode.
DAS Temp	Temperature measured at the DAS board in the Picarro analyzer.
Tray	.Tray name (a number for the older versions of the Autosampler)
Sample	Vial sample number.
Job	Line in the autosampler job queue.
Method	Autosampler method that is associated with the autosampler sequence.
Error Code	Error code associated with Autosampler operation.

12 Calibration

This chapter describes the procedures and best practices for calibrating the Picarro isotopic water analyzer to ensure accurate isotope measurements. It explains the use of primary, secondary, and working standards; outlines recommended calibration methodologies for different sampling configurations; and provides guidance for updating and verifying analyzer calibration.

Calibrating your Picarro water isotope analyzer involves three steps:

- Measuring the isotopic composition of known standards
- Determining the relationship between the measured value and the known value
- Adjusting the settings on the analyzer to account for any difference between the measured and known values, so that the on-screen readings are accurate.

Picarro recommends calibrating your Picarro L2130-i or L2140-i analyzer using liquid water samples. All water isotope standards should have accepted values for δ18O and δ2H. If applicable, the standards should also be calibrated for 17O-excess. Picarro recommends

NOTE

Upon manufacturing, Picarro guarantees the performance of your analyzer with respect to precision. The system is also calibrated using isotope standards, however Picarro does not certify the analyzer for accuracy. It is the responsibility of the instrument user to verify the factory-calibration and to calibrate the instrument for accuracy.

12.1 Primary and Secondary Standards

The isotopic composition of a water sample is typically determined relative to the known value in a standard using the delta notation and expressed as per mil (‰):

$$\delta^2H = \left(\frac{\left({}^2H/{}_1H \right)_{sample}}{\left({}^2H/{}_1H \right)_{standard}} - 1 \right) \times 1000$$

$$\delta^{18}O = \left(\frac{\left({}^{18}O/{}_{16}O \right)_{sample}}{\left({}^{18}O/{}_{16}O \right)_{standard}} - 1 \right) \times 1000$$

$$\delta^{17}O = \left(\frac{\left({}^{17}O/_{16}O\right)_{sample}}{\left({}^{17}O/_{16}O\right)_{standard}} - 1 \right) \times 1000$$

These delta values can be used to construct secondary parameters:

Deuterium-excess (expressed as per mil (‰)):

$$d - excess = \delta^{2}H - 8 \times \delta^{18}O$$

^{17}O-excess (expressed as per mil (‰)):

$$^{17}O - excess = 1000 \times ln\left(\frac{\delta^{17}O}{1000} + 1\right) - 0.528 \times 1000 \times ln\left(\frac{\delta^{18}O}{1000} + 1\right)$$

There are three international “primary” standards:

- **VSMOW2 –** Vienna Standard Mean Ocean Water 2
- **SLAP2 –** Standard Light Antarctic Precipitation 2
- **GISP –** Greenland Ice Sheet Precipitation

The GRESP standard is replacing the GISP standard that was available until 2012. The table below shows the isotopic compositions of each standard:

Table 11 - Isotopic Compositions of VSMOW2, SLAP2 and GRESP Standards

	$\delta^{18}O$ (‰)	$\delta^{2}H$ (‰)	^{17}O-excess (‰)	$\delta^{17}O$ (‰)
VSMOW2	0 ± 0.02 [1]	0 ± 0.3 [1]	0 [2]	0 [2]
SLAP2	-55.50 ± 0.02 [1]	-427.5 ± 0.3 [1]	0 [2] –0.015±0.005 [3]	-29.6968 [2] –29.741±0.100 [3]
GRESP	-33.40 ± 0.04 [1] -33.45 ± 0.034 [4] -33.426 ± 0.028 [5]	-258.0 ± 0.4 [1] -257.87 ± 0.52 [4] -258.20 ± 0.08 [5]	0.025 ± 0.005 [4] 0.038 ± 0.008 [5]	-17.7784 ± 0.02 [4]

[1] IAEA, [2] Schoenemann et al. (2013), [3] Wostbrock et al. (2020), [4] Vallet-Coulomb et al. (2021), [5] Keinan and Goldsmith (2023)

The $\delta^{18}O$ and $\delta^{2}H$ values are defined based on publications by the International Atomic Energy Agency (IAEA):

VSMOW2 and SLAP2:

https://nucleus.iaea.org/sites/AnalyticalReferenceMaterials/Shared%20Documents/ReferenceMaterials/StableIsotopes/VSMOW2/VSMOW2_SLAP2.pdf

GRESP:

https://nucleus.iaea.org/sites/AnalyticalReferenceMaterials/Shared%20Documents/ReferenceMaterials/StableIsotopes/Gresp/RS_GRESP-2021.pdf

There is no consensus on the $\delta^{17}O$ reference values for SMOW2, SLAP2 and GRESP. The table above provides an overview of the commonly assigned values as suggested by Schoenemann et al. (2013), Wostbrock et al. (2020), Vallet-Coulomb et al. (2021), and Keinan and Goldsmith (2023).

Picarro provides a Secondary Water Isotopes Standard Kit (part number C0356) that is based on standards provided by the United States Geological Survey [USGS]:

Table 12 - USGS Standards

Standard	$\delta^{18}O$ (‰)	$\delta^{2}H$ (‰)
USGS46	–29.80 ± 0.03	–235.8 ± 0.7
USGS47	–19.80 ± 0.02	–150.2 ± 0.5
USGS48	–2.224 ± 0.012	–2.0 ± 0.4

Since the IAEA and USGS primary and secondary standards are expensive and sample limited, each laboratory should develop their own working standards. Example sources of working standards include:

- **Local precipitation (variable isotopic composition)**
- **Local tap water (variable, related to local precipitation)**
- **Kona Deep, Destiny Deep Sea Water (~ 0 ‰)**
- **Snow or ice from your favorite alpine region (depleted)**
- **Tap water from your colleagues across the globe (variable)**

The isotopic composition of a secondary standard should first be measured against a primary standard. Once calibrated with respect to the VSMOW-SLAP isotope scale, it can be used for routine, daily calibration. About 1.2 L of secondary standard would be enough for a year's supply. This assumes each standard is measured 2x per day using a standard 2 mL autosampler vial, and that the analyzer is operated 300 days per year (2 mL / vial x 2 standard vials / day x 300 days = 1.2 L).

References

- Schoenemann, S. W., Schauer, A. J., & Steig, E. J. (2013). Measurement of SLAP2 and GISP $\delta^{17}O$ and proposed VSMOW-SLAP normalization for $\delta^{17}O$ and ^{17}Oexcess. Rapid Communications in Mass Spectrometry, 27(5), 582–590.
- Wostbrock, J. A. G., Cano, E. J., & Sharp, Z. D. (2020). An internally consistent triple oxygen isotope calibration of standards for silicates, carbonates, and air relative to VSMOW2 and SLAP2. Chemical Geology, 533, 119432.
- Vallet-Coulomb, C., Couapel, M., & Sonzogni, C. (2021). Improving memory effect correction to achieve high-precision analysis of $\delta^{17}O$, $\delta^{18}O$, $\delta^{2}H$, ^{17}O-excess and d-excess in water using cavity ring-down laser spectroscopy. Rapid Communications in Mass Spectrometry, 35(14), e9108.
- Keinan, J., & Goldsmith, Y. (2023). A simple method for rapid removal of the memory effect in cavity ring-down spectroscopy water isotope measurements. Rapid Communications in Mass Spectrometry, 37(19), e9600

12.2 Tools, Equipment and Samples Required

1. Waters with known isotope signatures, i.e., a verified $\delta^{18}O$, $\delta^{2}H$ and ^{17}O-excess (if applicable) value.
   - **Picarro recommends all labs purchase one supply of primary isotope standards from IAEA or USGS. These primary standards should not be used on a daily basis. Instead, they can be used to calibrate secondary or in-house standards.**
   - **Secondary or in-house standards that bracket the isotope space of your sample set. A set of three working water isotope standards is also available from Picarro (part number C0350). These standards have been calibrated for δ18O and δ2H against the VSMOW-SLAP scale.**
2. 2 mL sample vials with caps. Picarro sells water isotope kits for 500 or 1,000 samples (part number C0328 and C0329, respectively). These kits include 10 µL syringes, 2 mL glass vials with caps and injection port septa. Quantities vary based on the kit selected; visit the Picarro Store for more information: https://picarroinc.force.com/picarrosupport
3. Pipette for transferring water from primary storage (e.g., pressurized stainless steel barrels) to secondary storage (e.g., sealed amber vials) and eventually into sample vials (2 mL sample vials with caps and septa).
4. Permanent marker or label maker for labeling sample vials.
5. Refrigerator (or freezer) for storing water standards. If storing waters in the freezer, ensure the water is either stored in an expandable container or that the container has ample room for water expansion upon freezing. Also ensure the water is completely defrosted before conducting any analysis or sub-sampling from the water. For additional information on storing water isotope standards, please see section .

12.3 Calibration Methodology

You should calibrate your samples using water standards that are introduced to the analyzer using an identical (or as close to identical) methodology as the samples.

- **For clean liquid water samples, analyze your standards using the same method, i.e., with the High Precision Vaporizer and Autosampler.**
- **When using the Micro Combustion Module (MCM) to analyze plant waters and other contaminated waters, also analyze your standards using the MCM.**
- **For ambient atmospheric monitoring, calibrate your system using liquid water standards of known isotopic composition using a Standards Delivery Module or dual mode kit. You can also design your own lab-built nebulizer or bubbler. For ambient atmospheric studies, calibrate for both accuracy in delta space and the dependence of delta value on water vapor concentration.**
- **For matrix bound water analyzed using the Induction Module (IM), measure your liquid water standards using the sample introduction methodology and heating recipe.**
- **For the Continuous Water Sampler, produce large volumes of tertiary water standards that can be analyzed on the CWS. Calibrate these standards using the High Precision Vaporizer and Autosampler.**

NOTE

Picarro isotopic water analyzers are not calibrated for water vapor concentration. If high accuracy water vapor concentration is desired, calibrate your system with a dew point generator that can introduce vapor streams of known concentration.

12.4 Performing Calibration Measurements

Since the Picarro analyzer is extremely linear, it is only necessary to use three calibration standards to calibrate each isotopic species (two points define the calibration line and a third intermediate point is used for verification). The exact value of each calibration standard is not of particular importance, as long as they span a representative range of values over which the analyzer will typically be operated. Although it is not necessary to use more than three standards, additional standards can be used to further constrain the linear calibration coefficients.

Each calibration standard should be introduced into the analyzer for an interval long enough for the analyzer to yield a stable measurement of that sample. In the case of water isotopes, it is important to ensure sample-to-sample isotopic memory is overcome prior to using injection pulses for calibration. For example, if there is a significant difference in the isotopic composition of two adjacent standards, it is important to increase the number of injections per vial for the purpose of calibration. For example, if the system is calibrated directly with VSMOW and SLAP, which represent the largest natural variability in oxygen and hydrogen

isotopes, Picarro recommends at least 10 injections are made per vial prior to averaging 3-5 injections for the purpose of calibration. Such a high number of injections is not required for samples that are more closely spaced in isotopic composition.

For routine daily calibration, secondary standards can be interspersed with samples during a given run. The order in which you run the standards can provide information about parameters, such as drift and sample-to-sample isotopic memory, which are helpful in assessing data quality. Picarro recommends the following daily calibration procedure:

- **Measure three standards that bracket the expected composition of samples at the beginning of the autosampler run.**
- **Measure one of those standards again in the middle of the autosampler run.**
- **Measure the three same standards again at the end of the autosampler run.**

At the completion of the autosampler sequence, the standards can be used to construct a bracketed calibration. Plot the measured values of the standards on the x-axis, and the known values (versus VSMOW-SLAP) of those standards on the y-axis. A linear regression can then be used to correct your sample data to the VSMOW-SLAP scale. If necessary, the standard that was run at the beginning, middle and end of the autosampler sequence can be used to correct drift. Finally, remember that standard operating procedure is to discard the first three injections for any sample vial and then average the remaining injections to get the value of that water. The total number of injections made, and the number discarded can be optimized based on performance requirements and the sample-to-sample jumps in isotope space. It is possible to correct sample data to the VSMOW-SLAP scale by post-processing the Coordinator output data. Alternatively, Coordinator data can be analyzed using ChemCorrect™. Finally, if there is a desire to update the on-screen readings, the Picarro software can be updated by following the instructions given in the next section.

12.5 Updating the Instrument Calibration for Accurate On-Screen Readings

Once you have measured your standards, you can use either of the two methods described below to calibrate the analyzer. **Method 1** requires you to make a graph (known standards versus measured standards) to calibrate the analyzer. **Method 2** does not require you to make a graph; however, the effect of this calibration is harder to reverse than Method 1.

Method 1: Using the CRDS Data Viewer to Update the On-Screen Readings

For isotope standard measurements, plot the analyzer's reported isotope value on the horizontal (x) axis and the standards' known isotopic composition on the vertical (y) axis. This graph will help you to determine the linear relationship between the known calibration values and the analyzer's reported values.

Calculate a linear best-fit equation from the data. The slope and intercept of the best-fit line through these points are the two values that are used to calibrate the analyzer. Determining the linear relationship between the known values and the analyzer's reported values enables the calculation of a calibration offset (slope and intercept). This adds a correction term to the analyzer's factory or previous calibration.

The analyzer's calibration is intended to be altered infrequently. Instead of recalibrating frequently to increase the accuracy of the data, users often verify the calibration by measuring three or more water standards and using the same regression procedure described here to calculate an offset by which to correct their data offline (see previous section). In the calibration example data below, fitting the three standards yields the linear equation y = 0.9866x + 5.2658 with the slope m = 0.9866 and the intercept b = 5.2658. This equation would be used with x = raw data measured by the analyzer (labelled "CRDS Reported") to give y = corrected data (labelled "Certified" value).

Table 13 - Calibration Example Data

	CRDS Reported Value	Certified Value
Calibration Point #1	200.1	202.7
Calibration Point #2	600.3	597.6
Calibration Point #3	400.0	400.0

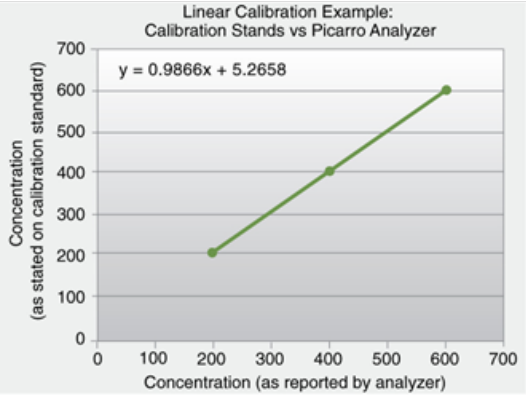


Figure 58 - Linear Calibration Example

Enter these calibration values into the software by selecting **User Calibration** from the **Tools** menu on the CRDS Data Viewer. Enter the slope and intercept for each species. This is a password-protected function, with the default password "picarro."

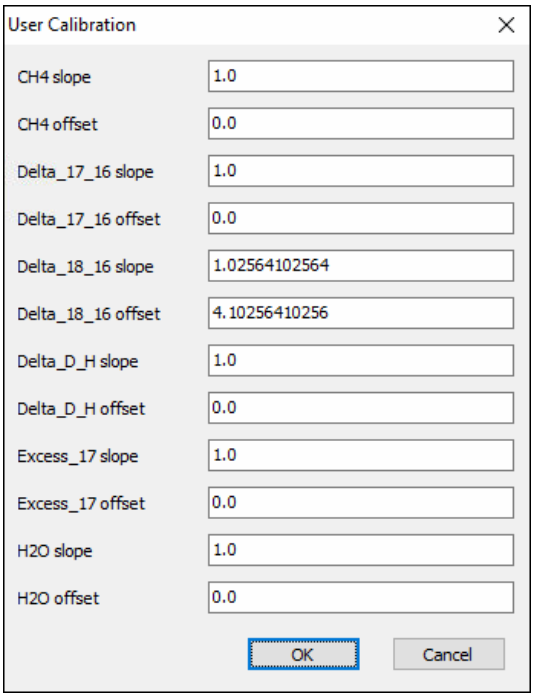


Figure 59 - User Calibration Dialog

After the calibration is entered, it will take effect immediately after clicking **OK**.

To return to the factory calibration, simply set the slope to "1" and the intercept to "0" for each species.

This calibration approach and functionality is available across all Picarro analyzers. In the example data given above the species measured were CO_2, CH_4 and H_2O concentration. The same method applies for isotope data, including $\delta^{18}O$, $\delta^{17}O$, $\delta^{2}H$.

Method 2: Using the "Picarro Data Recalibration Tool" to Calibrate the Analyzer

This tool can be used after you have performed the calibration measurements of standards with your Picarro analyzer.

The **Picarro Data Recalibration** ("Data Recal" icon) software can be found in the **Picarro Utilities** folder in the desktop, and it can be used to recalibrate the data analyzed by Picarro analyzers.

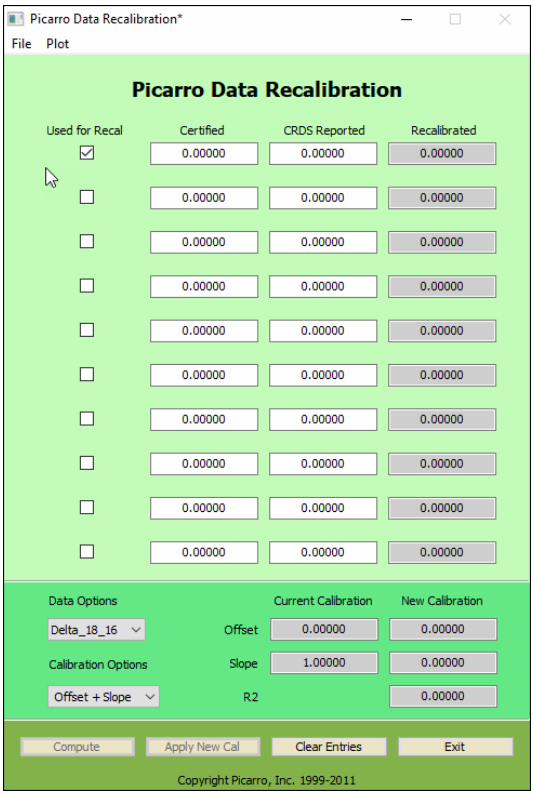


Figure 60 - Data Recalibration Tool

1. Double-click the **Data Recal** icon to pull up the window to the left.
2. Click on **Clear Entries** to reset the values in the "Picarro Data Recalibration" window.
3. Enter data values into the **Certified** (expected delta values) column.
4. Enter data values into the **CRDS Reported** (delta reported by Picarro analyzer) column.
5. Check the boxes in the **Used for Recal** column that you want the software to base the calibration on.
6. Click the **Compute** button located at the bottom of the window.

   The recalibrated values will appear in the rightmost column called **Recalibrated**.
7. Click **Apply New Cal** if you want to apply the calibration to your future measurements.
8. The default User Calibration Password is "picarro." Click OK to continue. NOTE: This action cannot be undone from the "Picarro Data Recalibration Window," but it CAN be undone in Method 1 in the "User Calibration" window.

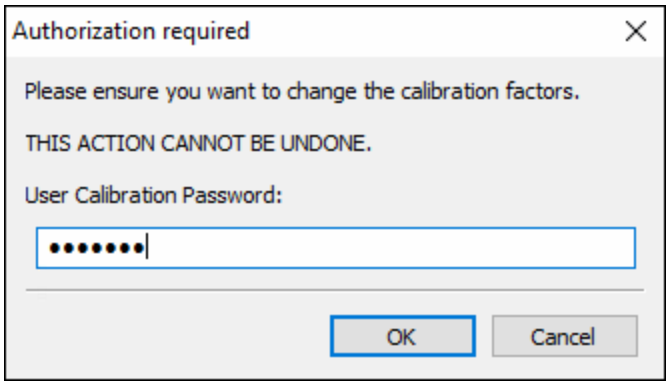
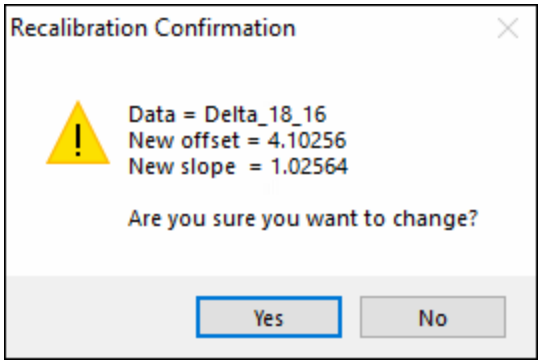


Figure 61 - Password Window

9. Review the values in the window (Figure 62 - Confirmation Windows), and click **YES** to confirm, then **OK** to continue.



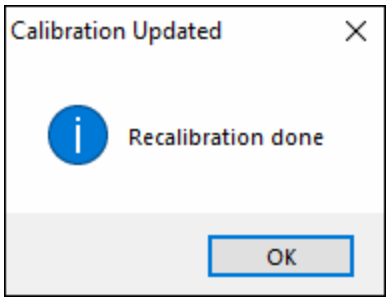


Figure 62 - Confirmation Windows

10. A Save Calibration Dialog window appears giving the option to save your calibration settings. Click **Cancel** if you don't want to save your new calibration setting.

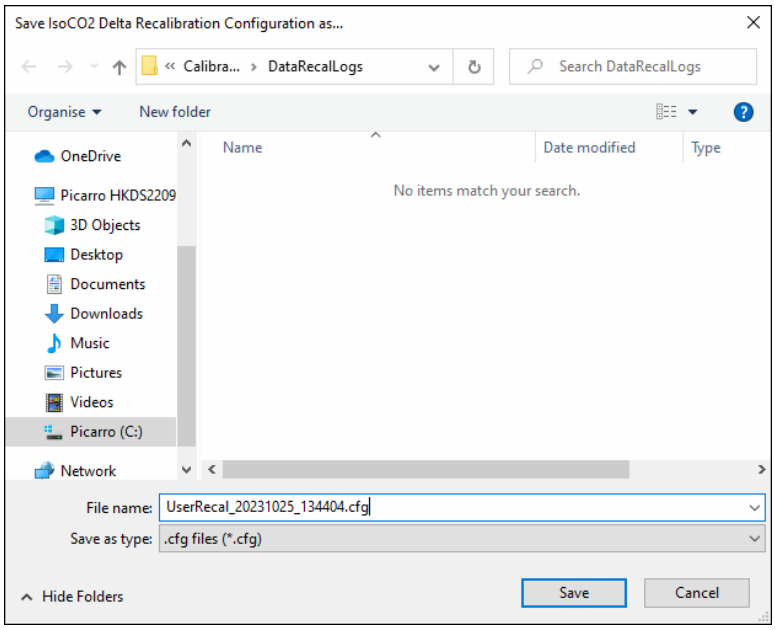


Figure 63 - Save Calibration Dialog

11. You have now calibrated your analyzer. The next time you do any sample measurements, the on-screen measurement readings will be based on the new calibration setting.

12.6 Literature and Other Useful Resources

There are many useful resources regarding calibrating systems for accurate water isotope measurements. A non-exhaustive list is below:

- Gröning, M. (2018). TEL Technical Note No. 03. Stable isotope internal laboratory water standards: Preparation, calibration, and storage. https://nucleus.iaea.org/sites/AnalyticalReferenceMaterials/SharedDocuments/Publications/TechnicalNotes/TELTechNote03_WaterInternalLaboratoryStandards.pdf
- Hachgenei, N., Vaury, V., Nord, G., Spadini, L., & Duwig, C. (2022). Faster and more precise isotopic water analysis of discrete samples by predicting the repetitions' asymptote instead of averaging last values. MethodsX, 9, 101656.
- Keinan, J., & Goldsmith, Y. (2023). A simple method for rapid removal of the memory effect in cavity ring-down spectroscopy water isotope measurements. Rapid Communications in Mass Spectrometry, 37(19), e9600.
- Terzer-Wassmuth, S., Wassenaar, L. I., Araguás-Araguás, L. J., Stumpp, C., & Terzer, S. (2023). Balancing precision and throughput of $\delta^{17}O$ and $\Delta'^{17}O$ analysis of natural waters by Cavity Ringdown Spectroscopy. L.I. Wassenaar, L.J. Araguás-Araguás et Al. MethodsX, 10, 102150.

- Vallet-Coulomb, C., Couapel, M., & Sonzogni, C. (2021). Improving memory effect correction to achieve high-precision analysis of $\delta^{17}O$, $\delta^{18}O$, $\delta^{2}H$, ^{17}O-excess and d-excess in water using cavity ring-down laser spectroscopy. Rapid Communications in Mass Spectrometry, 35(14), e9108.

13 ChemCorrect™ Software

ChemCorrect™ Software is a post-processing tool designed to improve the reliability of isotope measurements obtained from Picarro water isotope analyzers. In many real-world applications, water samples may contain trace chemical contaminants that can distort the measured optical spectrum and introduce bias or increased uncertainty in isotope results. Because removing these contaminants without altering the isotopic composition is often impractical, data-level correction is required to preserve sample integrity.

ChemCorrect addresses this need by evaluating spectral features associated with each measurement and comparing them to those of known, clean reference standards. Using statistical analysis, the software identifies deviations that may indicate contamination and flags affected samples for further review. Where applicable, ChemCorrect applies calibration and correction methods to align measured values with accepted isotope reference scales.

This section describes the underlying principles used by ChemCorrect to detect spectral interference, assess data quality, and support correction of contaminated samples.

13.1 Principle of Operation

Picarro CRDS has become a de facto standard for many water sample research areas, such as ice core, watershed, and aquifer studies. For various reasons, samples can contain a variety of chemical contaminants, which in some cases can lead to spectral interference that can degrade the accuracy of results. It is difficult to eliminate these contaminants from water samples without fractionating the isotope ratios and diminishing sample fidelity.

Proprietary software, called ChemCorrect, comes pre-loaded on your Picarro water isotope analyzer. This program solves the problem of data degradation and fidelity resulting from water samples contaminated with trace hydrocarbons. The software makes the a priori assumption that your standards are clean waters that do not contain any contamination. Then the program compares a number of features in the spectra from the samples and the standards, applies a statistical test to see if the samples are different from the standards, and assigns flags based on the statistical differences. These flags alert you to artifacts, potentially from contamination, which may affect the accuracy of your results. Finally, the software uses a linear regression to correct your samples to an isotope reference scale by comparing the measured values of your standards to their accepted values. For more information on organic interferences, see the Picarro application note: Plant Water: Accurate Water Stable Isotope Analysis of Organic Contaminated Water.

13.1.1 How Contaminants Impact The Optical Spectrum

Contaminants fall into one of the following three categories, based on the nature of the distortion to the optical spectrum:

1. Compounds that do not affect the spectrum (at concentrations up to 10-20% of the water sample). Most compounds fall into this category. In the presence of these contaminants, Picarro analyzers will report accurate and precise isotope values without bias or increase in noise.
2. Large compounds (with more than about 6-8 atoms) contribute a broad, spectrally unresolved absorption baseline beneath the target molecules. To first order, this baseline will cause no systematic bias to the reported values. Because optical absorption is a linear, additive process, the water vapor spectrum will 'float' on top of the contaminant baseline. The linearity and wide dynamic range of CRDS makes the technique particularly insensitive to these baseline offsets.
3. In some cases, however, this baseline offset is accompanied by a tilt of the spectrum with wavelength. This larger offset, if uncorrected, can cause bias in the measurements and degrade the precision of the instrument.
4. Small compounds (with fewer than 6-8 atoms) have spectrally resolved absorption lines that can interfere with the lines from the observed water vapor. This can lead to systematic errors in the reported isotope ratios. One example of such a molecule is methanol, which has a particularly complex absorption spectrum in this spectral region.

   ChemCorrect software uses known spectral interferences or general spectral patterns to identify trends due to contamination.

13.1.2 ChemCorrect on the L2130-*i* and L2140-*i*

The L2130-*i* and L2140-*i*, when operating in 'normal' measurement mode ($\delta^{18}O$ and $\delta^{2}H$), also measure spectral indicators that can be used to determine the integrity of the spectra and resulting data.

Using the spectral indicators listed below, the ChemCorrect software performs statistical tests to determine how those spectral features differ between the samples and the standards.

- **Residual:** The root mean squared residual of the least-squares fit to a spectra, in units of ppb/cm, is used to screen for potential small molecule contaminants, e.g., methanol.
- **Baseline Shift:** The spectral baseline is a good early indicator of a potential issue with a sample. The baseline shift term is a change in the constant term of a fitted baseline, in units of ppb/cm.
- **Baseline Curvature**: The spectral baseline is a good early indicator of a potential issue with a sample. The baseline curvature team is a change in the quadratic term of a fitted baseline, in units of ppb*cm.
- **Slope Shift:** The slope of the spectral baseline or change in the linear term of the fitted baseline, in units of ppb/cm, although not unique is also a useful indicator for moderately-sized molecules, e.g., ethanol that can interfere with nearby spectral features.

The software flags these indicators if they deviate from the thresholds set in ChemCorrect.

For example, a red flag can be triggered by any of the following:

- **The sample residual being 1.5 σ away from the mean of the standards residual**
- **The sample baseline shift being 18 σ away from the mean of the standards baseline shift**
- **The sample baseline curvature being 3 σ away from the mean of the standards baseline curvature**

Sometimes the software generates false positives by flagging features that do not arise from contamination. To reduce the number of false positives, the notification thresholds can be changed to be less stringent. This can be done by editing the ChemCorrect Instruction Set. If a user edits the Instruction Sets, we recommend changing the name of the Instruction Set so that it is possible to revert to the original set supplied by Picarro.

If a flag is raised, a number of things can be done. First, try some offline sample treatment methods, such as the use of activated charcoal. Second, if you suspect alcohols may be present in your samples, you can utilize Picarro's Micro Combustion Module (MCM) to remove those artifacts. Third, and as a last resort, you can analyze your samples using an alternative technique, such as Isotope Ratio Mass Spectrometry (IRMS). IRMS is not susceptible to spectral interference from alcohols; it can, however, introduce other analytical artifacts and have other interferences, such as mass interference, which can affect accuracy.

and replace it with your own content.

13.2 Analysis of Coordinator Output Files

The following Coordinator output files can be post-processed using ChemCorrect:

- High Precision
- High Throughput
- Manual Injection
- Standard
- Express
- Micro Combustion Module

ChemCorrect cannot be applied to data $\delta^{17}O$ and ^{17}O-excess data. Nor can it be applied to Coordinators generated during SDM, IM, Dual Mode, or Continuous Water Sampler Setups.

13.3 Preparing the Run Sequence

1. Each run needs at least 2 standards (3 is recommended but more is better) with known $\delta^{18}O$ and $\delta^{2}H$ values. These values create a linear fit, which is used in calibration of the samples.
2. The standards must be run one after another at the beginning of each sequence to be analyzed. The post processing software works sequentially and therefore requires the linearity of the known standards before it can correct the unknown values of the samples. It is recommended to include standards in the middle and end of the sample set as controls. An example is shown (Figure 64 - Run Sequence with Standards), vials with the CYAN stars indicate the standards:

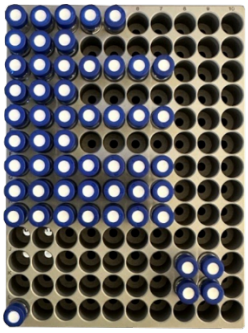


Figure 64 - Run Sequence with Standards

3. Due to memory, the first two to three injections of each vial should be ignored. Because of this, a minimum of six injections should be run per vial. The number of injections is set using the Autosampler Controller software (A0340 or A0325).

13.4 Files Required to Run ChemCorrect

ChemCorrect requires a standards file, an instruction set, and a source file (data output from the coordinator software that is in *C:\IsotopeData*). Each of these files are provided in .csv formats. To ensure the standards file format is preserved, Picarro recommends editing the file using Notepad++ which is provided with the analyzer.

A sample data file along with the standards and instruction files can all be found in the ChemCorrect main folder *C:\Picarro\ChemCorrectExe*.

13.4.1 Standards File

The standards.csv file must contain the name and known $\delta^{18}O$ and $\delta^{2}H$ values of each standard (relative to an isotope reference scale, typically VSMOW-SLAP for water isotopes). The names in the standards.csv file must match (case-sensitive) the names in the source file under “Identifier 1”. If they do not match, standards will be treated as samples.

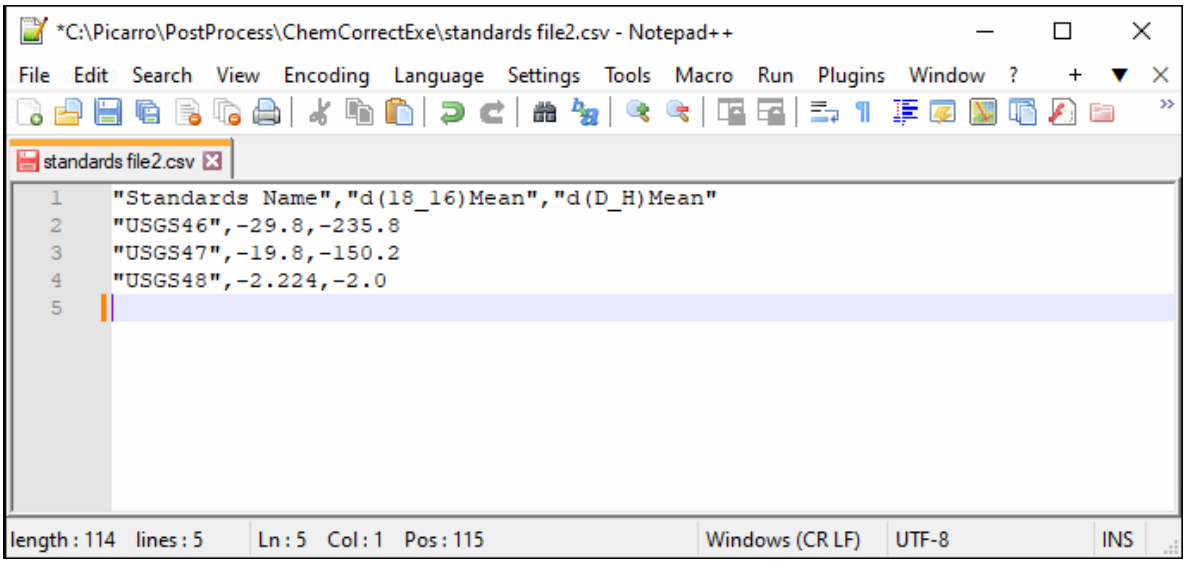


Figure 65 - Standards CSV File Example

13.4.2 Instruction Set

The instruction set is provided by Picarro.

- **L2130-i / L2140-i Instruction Set:** chemcorrect_inst avg_orgeval_10.csv

13.4.3 Source File

This is the output file from the Coordinator (stored in C:\IsotopeData). Before closing the Coordinator at the end of an Autosampler Sequence, it is advised to load the sample description file. Below is an example of a sample description file. Ensure that the “Identifier 1” for standards is identical to the “Standards Name” list in the standards file.

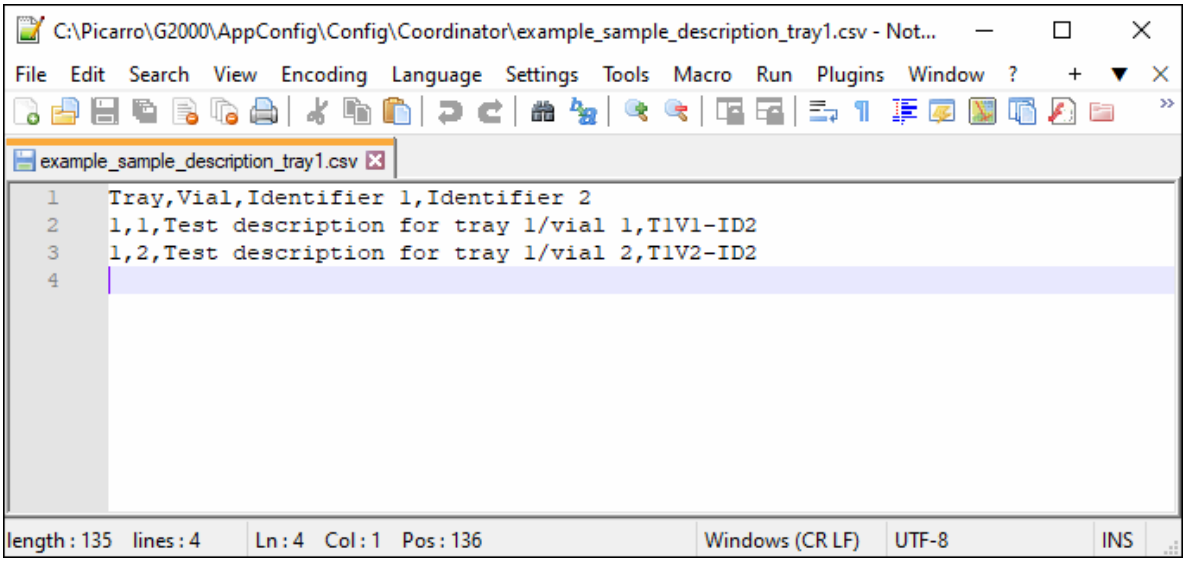


Figure 66 - Sample Description File

13.5 Running ChemCorrect

This section describes how to launch and configure ChemCorrect™ Software for post-processing isotope data. The software interface allows you to select the required input files, define processing parameters, and initiate analysis of Coordinator output data. Before running ChemCorrect, ensure that the appropriate source file, instruction set, and standards file are available and correspond to the analyzer and measurement type being used.

The following procedure outlines how to open ChemCorrect, configure the required fields, and start the analysis.

1. Double-click the ChemCorrect icon on the analyzer desktop. The ChemCorrect program will now open.
2. The top four boxes are the required fields: the most recent **Source** file name (sometimes empty), **Instruction Set** name, **Standards File** and the number of **Injections to Ignore**. You also have an option to plot additional graphs for other parameters.
3. To choose a different source file to be analyzed, click the **Source** button located on the bottom of the window. Then use the finder window to locate the desired raw data file and click **Open**.
4. To select a different instruction file than the one displayed, click the **Instruction Set** button located on the bottom of the window. Then use the finder window to locate the desired instruction file and click **Open**.
5. To change the number of injections to be ignored, highlight the existing number and type in the preferred one (required 2 but 3 is recommended). **Do not leave this field blank**.
6. When the correct source and instruction files are shown, click the **OK** button at the bottom of the window to start the ChemCorrect analysis.

Different Instruction Sets and Standards files are used for different analyzers.

Make sure there is a number here. Do not leave blank.

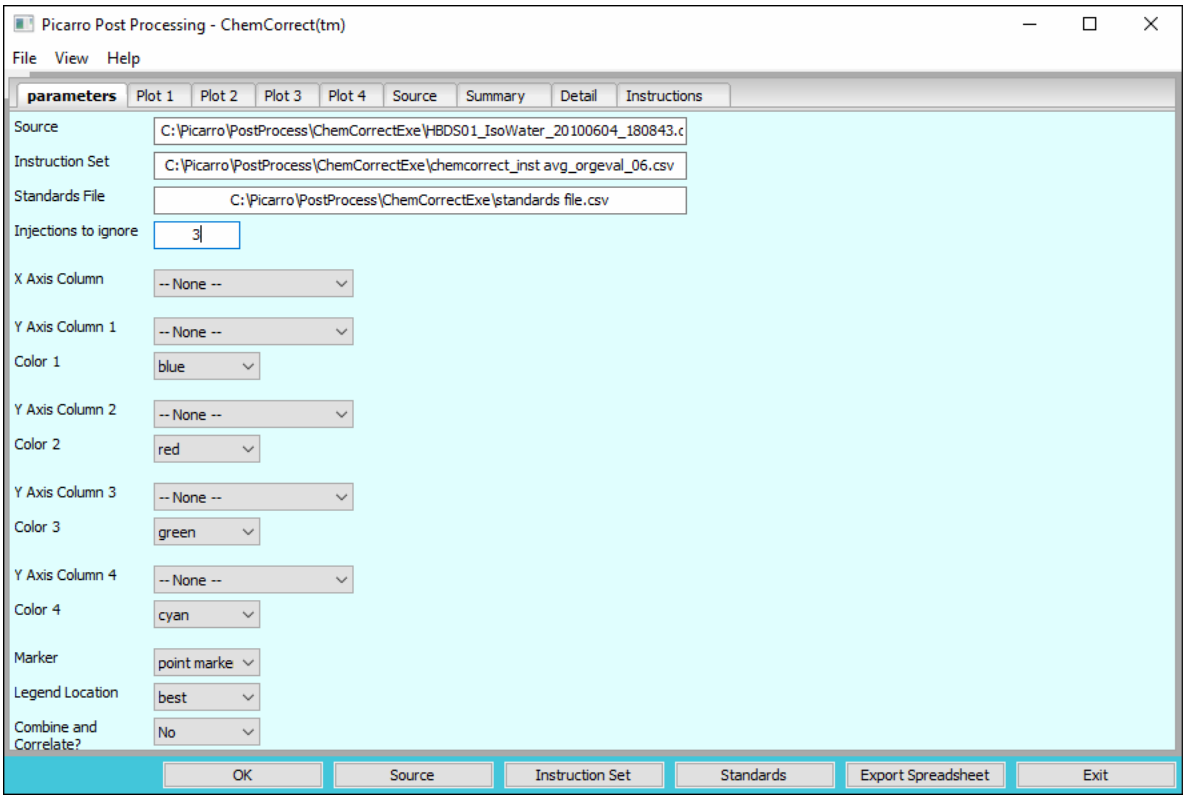


Figure 67 - ChemCorrect Window

13.6 Example Analysis

See the Figure 68 - ChemCorrect Analysis below.

1. Select **HBDS01_IsoWater_20100604_180843.csv** (which Picarro has provided in C:\Picarro\PostProcess\ChemCorrectExe\) as the source, and chemcorrect_inst avg_orgeval_10.csv as the instruction file. Then click **OK**.
2. The first display is called the **Summary**. Contained here are: the calibrated isotope values and visual indicators as to the severity of contamination by sample.
3. The CYAN rows are standards.
4. The GREEN rows are samples that have been determined to have little to no contamination.
5. The YELLOW rows are samples that contain trace values of contamination that may slightly shift the isotope values.
6. The RED rows are samples with severe contamination leading to inaccurate δ^2H and $\delta^{18}O$ readings.
7. A star next to a sample indicates a problem, e.g. missing rows in the source file resulting in an inaccurate calculation.

8. Red/yellow rows display relative contamination due to methane, methanol, or “other” hydrocarbons in the respective columns on the right.

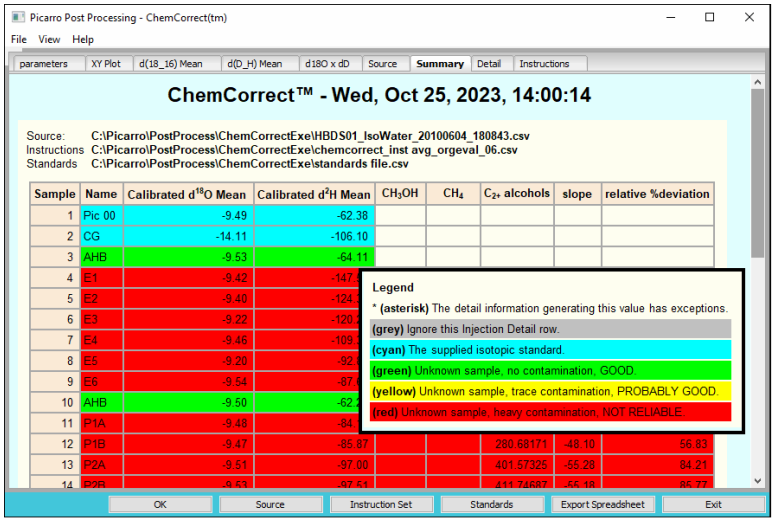


Figure 68 - ChemCorrect Analysis

9. There are other tabs that can be accessed by clicking on them in the top left corner of the window:
10. **Detail:** Summons a list of summarized charts by injection and sample chronologically. The un-calibrated and calibrated values, as well as the measurements taken to calibrate the values are included per injection. Below each chart is a summary.
11. **Source:** Displays the original raw data file without any changes or calibration.
12. **Instructions:** Displays the raw instruction file used by ChemCorrect as well as comments on the far right of each instruction.
13. **Additional plots** for visualizing your data.
14. At the bottom of the ChemCorrect window are additional buttons **OK**, **Export Spreadsheet**, and **Exit** buttons.
15. **OK:** Each time you reload the source and instruction sets, you can click OK again to process more data without closing and re-opening ChemCorrect. Once you make your edits, export the result to save your processed data.
16. **Export Spreadsheet:** Creates an excel spreadsheet complete with all the information contained in the four tabs in the ChemCorrect main window as well as all the data sets and formulas used to calibrate the isotope values.
17. **Exit:** Quits ChemCorrect.
18. The standards.csv file can be amended if needed, but the format must remain the same. To edit, simply open the file, make the desired changes, and click save. For the changes to be reflected in ChemCorrect, click the **OK** button at the bottom of the ChemCorrect.

19. For more advanced users, Instruction Sets can be edited to perform your required calculations.

NOTE

If editing the Instruction Set, we recommend changing the name of the Instruction Set so that it is possible to revert to the original set supplied by Picarro.

NOTE

Picarro recommends running the post processing within 7 days of initially acquiring the data. If a sample is flagged as contaminated, the post processing software will automatically set aside the associated spectral files. These files can be sent to Picarro for further analysis and spectral library development. Once set aside, these files will not be affected by the automatic file management software which is running on the analyzer.

NOTE

Due to the large amount of data generated by the analyzer a buffer of approximately 10 GB of spectral files are kept, after which point, they are erased. This corresponds to approximately 2 weeks of operation. Running the post processing ensures that any spectra associated with contamination are not erased.

14 File Management

The Picarro analyzer generates ASCII-format text output files that are updated after each batch of concentration measurements is complete. The data files are stored primarily in UserData folders and are also mirrored in folders which retain more situational data. Some analyzers also produce discrete measurements stored in separate isotope data folders. All user data is archived, compressed, and retained, either shortly after the measurements or at a later point, to optimize space on the hard drive.

This section describes how data generated by the Picarro analyzer is organized, stored, and maintained on the system. The analyzer produces multiple types of output files during operation, including real-time measurement data, event logs, and diagnostic data. These files are written in standardized formats and stored in defined directory structures to support data access, review, and troubleshooting.

In addition to active data storage, the system includes automated archiving and compression processes to manage disk usage while preserving historical records. Understanding the file structure, naming conventions, and storage locations is essential for retrieving measurement data, supporting post-processing workflows (such as ChemCorrect), and providing information for diagnostics or support.

The following sections describe the primary data directories, file types, naming conventions, and archiving behavior used by the analyzer.

14.1 User Data Folder

The User Data folder is located at:

C:\UserData\DataLog_User - with files arranged by year\month\day\hour.

The User Data files are in a simple text format (white-space delimited) with a DAT file extension. By default, each file stores one hour of data.

Using the **Setup Tool**, the user can select and customize the data columns, file length, total storage size and folder structure for the user data logs. Setup Tool is described in more depth in A Setup Tool and Communication.

Certain instruments may contain additional sub-folders under C:\UserData\ relating to time synced file formats, soil flux, or GPS data, among others. If the user has any questions about this file structure, they can contact Picarro Support.

14.2 Data File Name

The file name is generated from the analyzer serial number, the date, and the time when the file was started. The specific time stamp will depend upon the time the instrument was started and began measuring sample gas, so files seldom begin exactly at the top of the hour. For example:

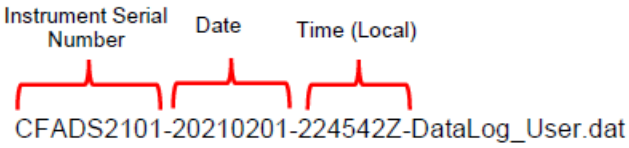


Figure 69 - Example Data File Name

- **CFADS2101** is the analyzer serial number
- **20210201** is the date, in format yyyymmdd (to allow chronological sorting of data files).
- **224542** is the time the file was started in the computer's Local Time as displayed in the lower right hand side of the Windows OS screen, 22:45:42, formatted as hhmmss using a 24-hour clock. Note that the time stamp of samples within the file is usually recorded in UTC (GMT) relative to the local time. For example, an analyzer in California will usually have a time stamp (UTC) within the file that is 8 hours ahead of the time stamp in the file name itself (UTC - 8).

14.3 Data Archive

The archive directory is:

C:\Picarro\G2000\Log\Archive

and has subdirectories:

DataLog_Private, ***DataLog_EventLogs***, *and* ***DataLog_Mailbox.***

DataLog_Private

These data files contain a comprehensive list of system parameters such as instrument temperatures and pressure, set points and spectroscopy. This additional information is not broadly relevant to the user for day-to-day operation but can be useful for diagnostic purposes. Files are stored by the convention:

C:\Picarro\G2000\Log\Archive\DataLog_Private \[year]\[month]\[day]\[hour]

The archive files are in a more efficient HDF5 format, with extension .h5.

DataLog_EventLogs

Event logs contain records of the operation of the instrument, the performance of the wavelength monitor and lasers, and record exceptional events like pressure or temperature instability. This is also a critical resource for Support to diagnose or troubleshoot an issue with an analyzer. Files are stored by the convention:

C:\Picarro\G2000\Log\Archive\DataLog_EventLogs \[year]\[month]\[day]\[hour]

DataLog_Mailbox

The Mailbox folder contains individually zipped files which have been compressed to allow automated transfer via email. Unlike the folders above, this folder is not subdivided by year, month, and day. Email synching is described in greater detail in A Setup Tool and Communication.

14.4 User Data Folder

The User Data folder C:\UserData\ contains one or more subfolders associated with real-time instrument data.

14.4.1 DataLog_User (all instruments)

Raw user data is contained in the DataLog_User folder, with format:

C:\UserData\DataLog_User\[year]\[month]\[day]\hour

This is the most relevant folder for users of non-isotopic instruments, as this provides the real time data output in its most digestible form. These data files reflect the native time interval of the instrument, typically between 0.1 Hz and 10 Hz.

14.4.2 DataLog_Sync

Some instruments will also contain a (*C:\UserData\DataLog_Sync\...*) directory, which includes data that is evenly spaced in time as specified by the user in the Setup Tool, covered in A Setup Tool and Communication. This format is preferred by some users who need e.g., 1 Hz data exactly, or who prefer to record smaller data files with data spaced, e.g., every 60 seconds.

14.4.3 DataLog_GPS

Instruments may come with the ability to log GPS data, which can be found in this subdirectory.

14.4.4 DataLog_SFP

Instruments may come with the soil flux processor software. Associated data files may be found in this subdirectory.

14.5 Isotopic Data

Isotopic instruments use Coordinator programs to produce discrete isotopic values for individual samples or injections. Each time a Coordinator is opened, a data file will be produced in one of two places, depending on the peripheral used, either:

C:\IsotopeData (sometimes called ***C:\IsotopicData***)

or

C:\Picarro\IsotopicData (sometimes called *C:\Picarro\IsotopeData)*

While the coordinator program is running, individual sample value outputs will be populated as a new line into the coordinator window, and the respective data file.

14.6 File Archiving

Picarro instruments will not delete data. Some instruments will, however, compress and archive older data to conserve hard drive space. Raw data file archiving frequency and details can be modified in the file:

C:\Picarro\G2000\AppConfig\Config\Archiver\Archiver.ini.

⚠ CAUTION

To avoid losing data, discuss with Picarro support before attempting any changes to the Archiver.ini file.

For each file type, there are various items along with some recommended default settings which may vary by file type:

- **Directory = C:/UserData/DataLog_Sync**

Optionally specifies which directory to find files to archive.

- **MaxCount = -1**

Specifies how many files to keep. A setting of -1 indicates that there is no maximum number of files. Generally, -1 is used in conjunction with a maximum size limit, below.

- **MaxSize_MB = 1500**

Specifies that a maximum of 1.5 GB of data is to be kept before the system begins to archive old data.

- **Compress = True/False**

Specifies if archived files are to be zipped – recommended setting is true to save hard drive space. True means files are zipped, false means files are not zipped.

- **AggregationCount = 0**

If compression is set to TRUE, specifies how many files to be included in each zip archive.

- **StorageMode = FIFO**

First in first out. Specifies that old data is archived first.

- **Quantum = 4**

Generally, should not be changed. Specifies the files be sorted by year\month\day\hour in the archived directory structure.

14.7 Measuring Time in Picarro Data Files

Since measurements performed by Picarro analyzers are asynchronous (they require a variable and unpredictable amount of time to complete) data reported by the analyzer is time stamped. Each independent measurement is given a time derived from the Windows™ computer's system clock (reference http://en.wikipedia.org/wiki/System_time). This time can be reported by one or many of the following variables.

Table 14 - Time Measuring Variables

Variable Name	Description	Units
DATE	The calendar date formatted as YYYY-MM-DD **Example:** August 24, 2023 is formatted as 2023-08-24	-NA-
TIME	The time of day formatted as HH:MM:SS.SS on a 24-hour clock **Example:** 4:18:53.12 PM is formatted as 16:18:53.12	-NA-
FRAC_DAYS_SINCE_JAN1	The number of days since midnight January 1 of the current year **Example:** at 3:00:00 PM on January 12 the value is 11.625	days
FRAC_HRS_SINCE_JAN1	The number of hours since midnight January 1 of the current year **Example:** at 3:00:00 PM on January 12 the value is 279.0 (=FRAC_DAYS_SINCE_JAN1*24)	hours
JULIAN_DAYS	The number of the day of the current year **Example:** at 3:00:00 PM on January 12 the value is 12.625 (=FRAC_DAYS_SINCE_JAN1+1)	days
EPOCH_TIME	The number of milliseconds since midnight January 1, 1970 **Example:** at 3:00:00 PM on January 12 the value is 1421074800000 (= time)	ms
timestamp	The number of milliseconds since midnight January 1, 1 if the current Gregorian calendar was extended back to that time **Example:** at 3:00:00 PM on January 12 the value is 63556671600000	ms

Variable Name	Description	Units
time	The number of milliseconds since midnight January 1, 1970 **Example:** at 3:00:00 PM on January 12 the value is 1421074800000 (= EPOCH_TIME)	ms
ymd	The calendar date formatted as YYYYMMDD **Example:** August 24, 2023 is formatted as 20230824	-NA-

In the table above, all times are reported in GMT (also known as Zulu time and very closely related to UTC – reference: http://en.wikipedia.org/wiki/Greenwich_Mean_Time). We express these timestamps in GMT to avoid complications during Daylight Saving Time or when instruments are moved across time zones. The accuracy of the times are, of course, only as good as the accuracy of the Windows™ clock. To learn how to automatically synchronize the computer's clock to a time standard, see section A Setup Tool and Communication. There are many online calculators (for example, http://www.epochconverter.com) that convert Epoch Time to local time at any time zone, as well as many functions in commonly used data analysis programs that perform the same calculations.

15 Performance Verification

Performance verification through drift and precision testing is used to confirm that the analyzer is operating within specification over time. These tests provide a baseline for new installations, support ongoing performance monitoring as the instrument ages, and help identify developing issues before they impact data quality. Drift and precision testing is also recommended whenever data quality degrades unexpectedly or when evaluating whether a Factory Refresh is required.

The following sections describe the recommended procedures for performing drift and precision testing, along with additional diagnostic checks to assess analyzer and vaporizer performance.

15.1 Drift and Precision Testing

Precision and drift tests for $\delta^{18}O$ and $\delta^{2}H$ ($\delta^{2}H$) are recommended every 6 to 12 months throughout an analyzer's lifetime. This will allow you to verify a new installation, track performance as the instrument ages, determine if it is time for a Factory Refresh, and perhaps identify a small problem before it becomes a major setback. These tests can also be performed when data quality suddenly and inexplicably deteriorates.

The drift and precision test for a L2130-*i* and L2140-*i* is conducted by measuring water from the wash station, instead of vials. These analyzers are precise enough to detect small variability in the composition of water from individual vials, even if it was sourced from the same supply. By running the drift and precision test from the wash station, vial to vial noise is avoided.

The following instructions contain sections specific for each of the Picarro Autosamplers (model number A0340 or A0325), covering small setup and software settings differences.

1. Fill a wash station jar with water and screw on the cap. The water should be pure deionized water, with no organics or salts, although tap water, bottled water, or one of your secondary standards can be used. Because of the large volume required, we do not recommend using primary standards for this test. The sample should be filtered if it contains particulate matter.
2. **Autosampler (A0340)** – Users place the wash station jar in either one of the two wash station jar positions. (Picarro_DIW_Analysis_Station in the software) The software is instructed to pull from the correct jar.

   Note: In Autosampler (A0340) the was station are designated 1 and 2 from front to back. Contrary in older models this designation is reversed.

   Autosampler (A0325) – Users place the wash station jar in the rear wash station jar position (Wash Station 1).

3. Double-click on the desktop icon **Autosampler Control**. This opens the program that controls the Autosampler.
4. **Autosampler (A0340)** – Create a job with 210 injections from the position of the Picarro_DIW_Analysis_Station that you want to measure.

   Autosampler (A0325) – In the top row of the sample list, check the box to the right of the **Clear button**. Then use the keyboard command '**Ctrl** + **i**' to switch to the wash station test mode.

   Note: This is a run sequence that will only draw water out of wash station 1. Select the method **Picarro** from the drop down list and enter 210 into the box underneath the column '#Inj.'. This will set up a run of 210 injections from the wash station.

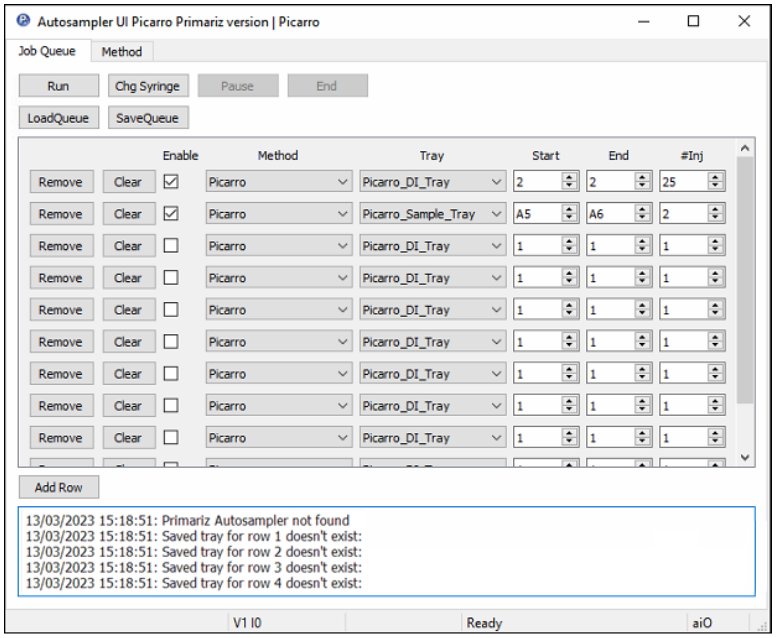


Figure 70 - Autosampler Control Window

5. Click **Run**.
6. Minimize the Autosampler window and double-click on the desktop icon **Coordinator Launcher**.

   This will open the window 'Picarro Coordinator Launcher' with a dropdown menu 'Select Coordinator.'

7. Select **High Precision** and click **Launch**.

   Once the 'CRDS Coordinator' window is open, it will start to run through a series of checks, which include cleaning the vaporizer by opening and closing valves.

8. Once the vaporizer cleaning has finished, the Coordinator will initiate the first injection from the Autosampler. Then it will run through the entire Autosampler queue that was set up in step 5. The complete Autosampler queue will include 210 injections and it will take approximately 24 hours.

   You can monitor the progress of the run in the **CRDS Coordinator** window. Please check to ensure that H_2O concentrations of the first few injections fall within about 15,000 to 20,000 ppm, and that the injection concentrations are within about ± 1,000 ppm of each other. You can now leave the system to run for 24 hours, during which time it will collect the necessary data to test the precision and drift of the instrument.

9. When the run is complete, navigate to the file C:\IsotopeData and identify the Coordinator output file. The correct file name can be found in the CRDS Coordinator window in the **Filename** box, and the file will have the format .csv (comma-separated values). Move this file to another computer with Microsoft Excel or similar spreadsheet program.

10. Open the .csv Coordinator output file. Then copy and paste data from the columns labeled **d(18_16)Mean** and **d(D_H)Mean** into a drift and precision test analysis spreadsheet that can be downloaded here:

    https://picarro.box.com/s/f660al39eiacqvmss40bt57tuq47dbfy

    The spreadsheet is set up to calculate precision and drift and record the values in table provided. Within the spreadsheet, you will find a table labeled **Report**. Review this table and check the cells underneath the column **State**. If these cells read **pass**, the instrument passed the standard drift and precision test. If any boxes are labeled **fail**, you should contact Picarro's Technical Support team at support@picarro.com. Please be prepared to provide the serial number of your analyzer.

15.2 Leak-Free Operation with a High Precision Vaporizer (A0211)

Following an injection of liquid into the water isotope analyzer, the shape of the square "pulse" in the water concentration versus time graph provides information about the quality of the injection and any potential problems that can lead to poor data.

One potential problem is a leak between the vaporizer and the analyzer. These leaks can be detected by plotting the water concentration along with the "outlet proportional valve" setting during the analysis. The outlet valve performance provides a way to identify unexpected pressure changes in the system, and it is a useful indicator of vaporizer performance. Here's why: The vaporizer converts a liquid sample into gas. At the beginning of sample analysis, one of the vaporizer valves is opened to the analyzer to allow gas to pass from the vaporizer into the analyzer cavity. During analysis, the pressure in the cavity steadily decreases because the gas is leaving the fixed volume of the vaporizer. To keep the cavity pressure constant, the outlet proportional valve slowly adjusts to compensate for the pressure change at the inlet.

For additional background on the operation of the High Precision Vaporizer, you can review the following Picarro Community post online: http://www.picarro.com/community/picarro_community/vaporizer_a0211_operation_schematic (Access requires user login; If you do not yet have an account, please send an email to: support@picarro.com to request access to documents and manuals.)

15.3 Viewing the Outlet Valve Position

To access the outlet valve position plot within the CRDS Data Viewer GUI, go to **Settings** > **Change GUI Mode**. When asked for a password, use the default Picarro password ("picarro"), and press **OK**. Now you can select the Outlet Proportional Valve plot.

The outlet valve position is also recorded in the Private Data Log files (see section 14 File Management for details on how to access these files). If you would like the data stored in the User Data, you can refer to A Setup Tool and Communication to include the outlet valve in your user data files.

15.4 Water Concentration and Outlet Proportional Valve Graphs

For all of the following plots, the water concentration is the top graph and outlet proportional valve position is on the bottom. Ideally, the water pulse should be square, and the outlet proportional valve position should gradually decrease at the flat top of the water pulse, as shown below. These features correspond to the outlet valve gradually closing during the analysis of the pulse.

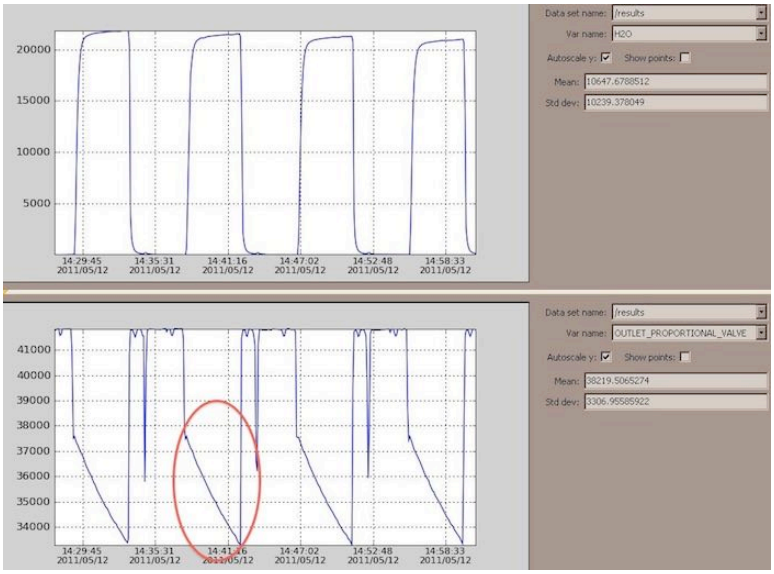


Figure 71 - Ideal Water Concentration and Outlet Proportional Valve Graphs

For a proper analysis, the concentration of the dry gas (between the pulses) should be < 500 ppm H_2O. The peak height of the pulse should be reproducible (within ± 1,000 ppm) and between approximately 17,000 and 23,000 ppm.

15.5 Graph Problems and Potential Causes

The water concentration and outlet proportional valve plots provide a primary diagnostic view of sample delivery, vaporizer performance, and system integrity during analysis. Under normal operation, the water concentration signal exhibits a stable, square-shaped pulse, while the outlet proportional valve position changes in a predictable manner to maintain pressure within the analyzer.

Deviations from these expected patterns can indicate issues such as leaks, inconsistent sample delivery, poor vaporizer mixing, or gas supply problems. Careful evaluation of both the water concentration trace and the corresponding outlet valve behavior allows users to distinguish between these conditions and identify likely causes.

The following examples illustrate common abnormal signal patterns observed during operation, along with their typical causes. These patterns are intended to support troubleshooting and help determine when corrective action or Technical Support assistance may be required.

15.5.1 Problem: Extra Pulses after the Main Sample Pulse

The image below shows extra little "pulses" after the main sample pulse. Note that the peaks for the main pulses appear normal, and the outlet valve is operating normally. The problem is during the cleanout cycle of the vaporizer, not during sample delivery.

There are three potential causes of this problem:

1. Leaky vaporizer septum. This should be changed after every ~ 300-400 injections.
2. Bad vaporizer vacuum pump. The pump may be starting to fail if it has more than 10,000 hours of use.
3. Bad connection between the vaporizer vacuum pump and the vaporizer. Check the tubing and swage connections for cracks near the metal connections. Be careful not to over-tighten the swage fittings.

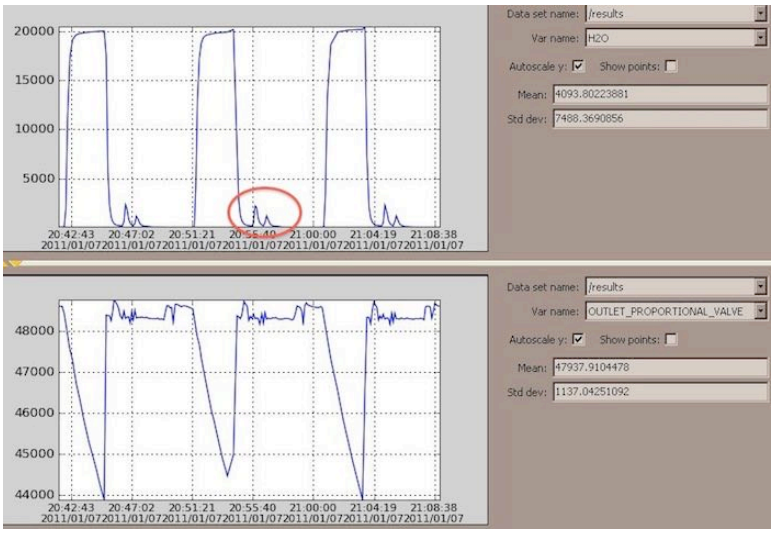


Figure 72 - Extra Pulses after the Main Sample Pulse

NOTE

When reattaching 1/4" Swagelok fittings, the nut should be hand-tightened and then turned an additional 1/8 of a turn using a wrench.

15.5.2 Problem: Extra Peaks Before and After the Main Sample Pulse

The water concentration graph below has two abnormalities: an extra little peak after the main peak, and a "spike" at the beginning of the main peak. Note also that the outlet proportional valve is flat. This indicates that the outlet valve is constant during the time the analyzer is drawing air from the vaporizer's internal fixed volume. Because the outlet valve is constant, the pressure on the inlet of the analyzer is not changing. This indicates there is a leak between the analyzer and the vaporizer.

The spike at the beginning of the main pulse could be moist ambient air entering through the leak. In this particular example, the spike peaks at ~ 12,000ppm. In a dry environment, a leak might look like a slope going upwards from left to right with a dependence on the ambient conditions relative to the nominal 20,000 ppm concentration of the vaporized sample. A very leaky septum could also look similar.

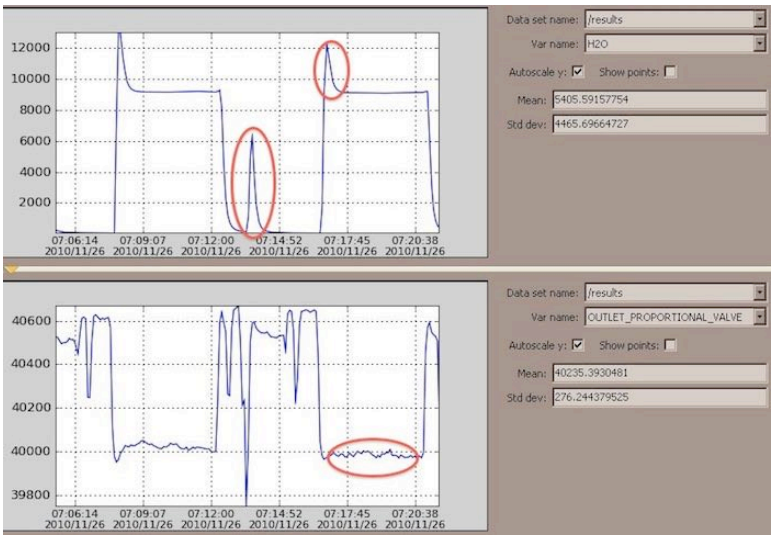


Figure 73 - Extra Peaks Before and After Main Sample Pulse

15.5.3 Problem: Decreasing Concentration in the Main Pulse

In this example, the outlet valve is constant during the pulse, but the pulse has a decreasing concentration. This is consistent with a leak of lower-concentration ambient air into the analyzer during analysis. This leak is likely at the connection from the vaporizer to the analyzer.

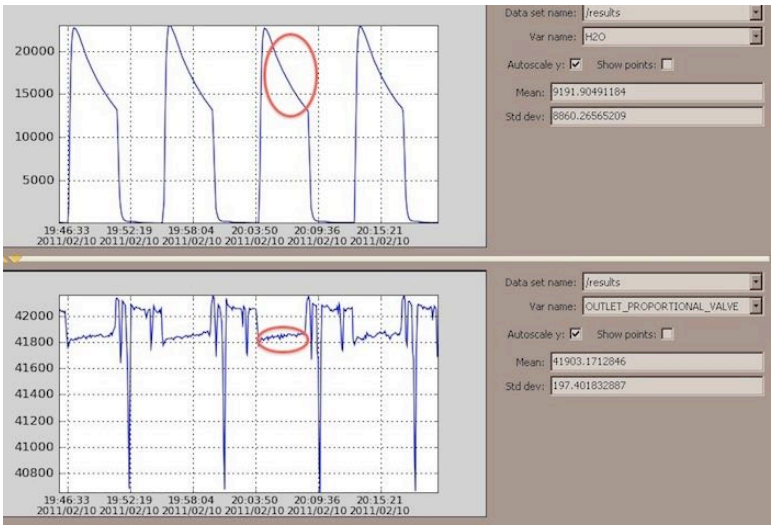


Figure 74 - Decreasing Concentration in Main Pulse

15.5.4 Problem: Water Pulse Is Sloped

The slope of the main pulse in the water concentrations, particularly one going upwards as in the first example shown below (Figure 75 - Water Pulse Sloped – Poor Mixing in Vaporizer), indicates poor mixing inside the vaporizer. This can happen if the valve that injects dry gas

into the vaporizer is not working perfectly. In this case, the outlet valve position is normal and therefore a leak between the vaporizer and analyzer is excluded as the cause of the problem.

In the second example (Figure 76 - Water Pulse Sloped – Inconsistent Filling of Vaporizer below) however, note the change in the nominal outlet valve position. This shows the vaporizer is filling to different pressures with each pulse, so there is inconsistent filling of the vaporizer.

If you see either:

- **Variation in the nominal stopping position of the outlet valve, or**
- **Large increases in water concentration during a pulse**

Contact Technical Support (support@picarro.com) and we can help diagnose and repair the fault, if necessary. Please always provide your analyzer and vaporizer serial number when contacting Picarro.

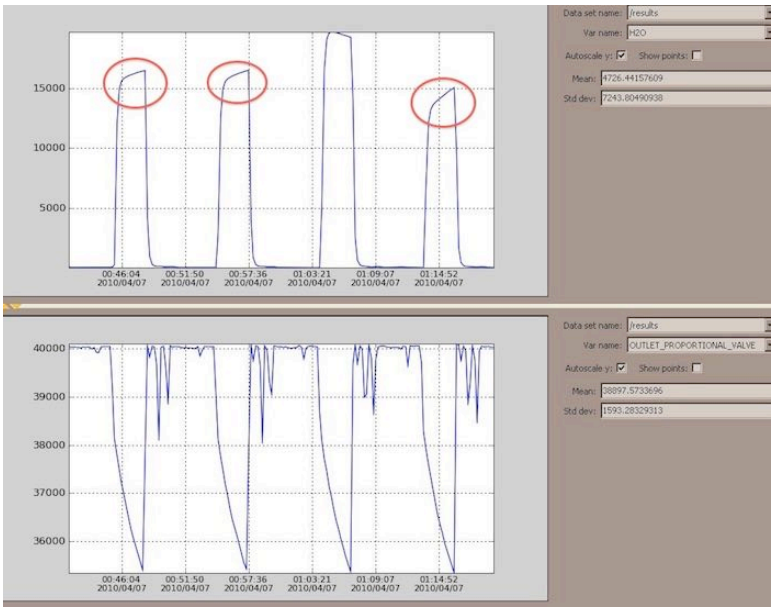


Figure 75 - Water Pulse Sloped – Poor Mixing in Vaporizer

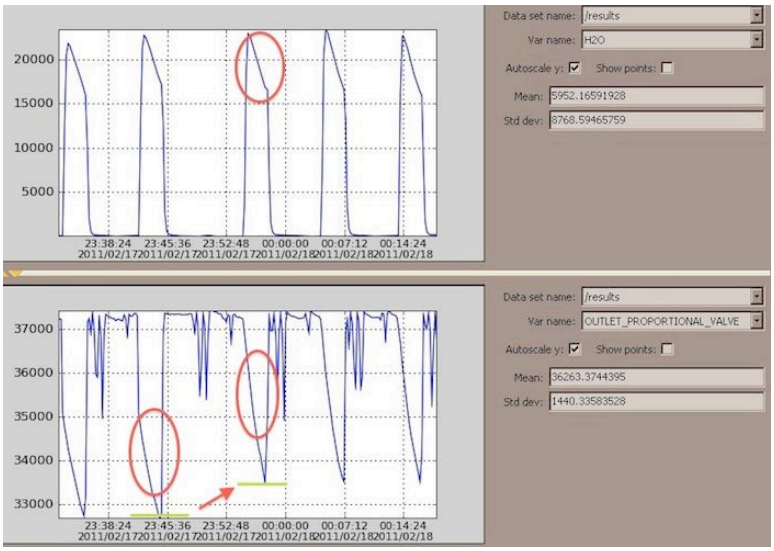


Figure 76 - Water Pulse Sloped – Inconsistent Filling of Vaporizer

15.5.5 Problem: Variability in Measured Water Concentration

The measured water concentration should consistently be near 20,000 ppm (±1000 ppm). The circled areas in the water graph below shows values that are higher or lower than expected. The outlet valve behavior is normal.

This can happen if the syringe is clogged, causing inconsistencies in the injected volume. Another problem is an inconsistent gas supply, perhaps due to a failing regulator or another piece of equipment using the same dry gas supply. This causes inconsistent pressure or flow at the inlet dry gas supply.

Other problems associated with sample delivery are:

- Overfilling or pressurizing the liquid in the vials
- Significant contamination of the samples
- Insufficient needle depth resulting in the collection of air, rather than liquid
- Variable volume bubble in the syringe

A test injection is recommended before each run, when you change a syringe, or if water concentrations during the pulse are consistently outside of the ideal ~ 17,000 to 23,000 ppm range. It is possible to scale the injection volume by the appropriate percentage to target the ideal water concentration range (see section).

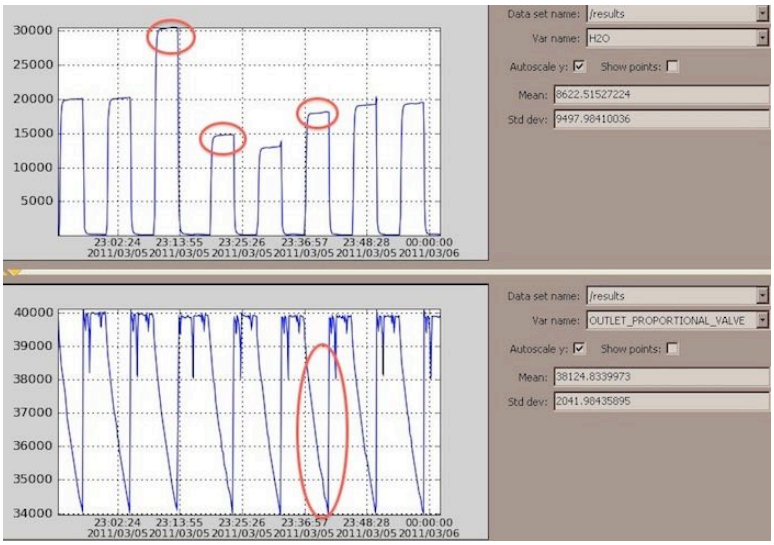


Figure 77 - Water Pulse Sloped – Water Concentration Variability

15.5.6 Problem: Water Concentration Suddenly Decreases

In this example, the measured water concentration drops to near the baseline. This can happen if the needle penetration depth into the vaporizer changes and is not deep enough to get the sample into the vaporizer. The tall peak at left is a partial injection, but the subsequent peaks indicate that little water was injected into the vaporizer.

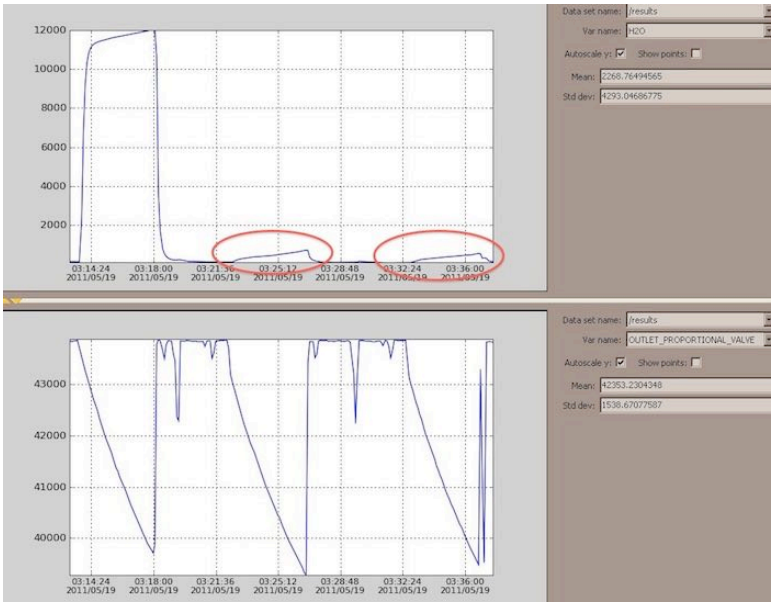


Figure 78 - Water Pulse Sloped – Sudden Decrease in Water Concentration

15.5.7 Problem: Baseline of Water Concentration and Outlet Valve Change

This is what happens when a normal analysis runs out of dry air from the dry air cylinder. The same behavior is also possible if there is a large gas leak in your cylinder. As the cylinder gas pressure goes to zero, the vaporizer is forced to take in moist room air, either from the leak or backwards through the Wavelength Monitor (WLM) purge line. The result is that the nominal dry baseline rises to the level of the room air. Also, the outlet valve position decreases since the vaporizer experiences less pressure from the cylinder gas.

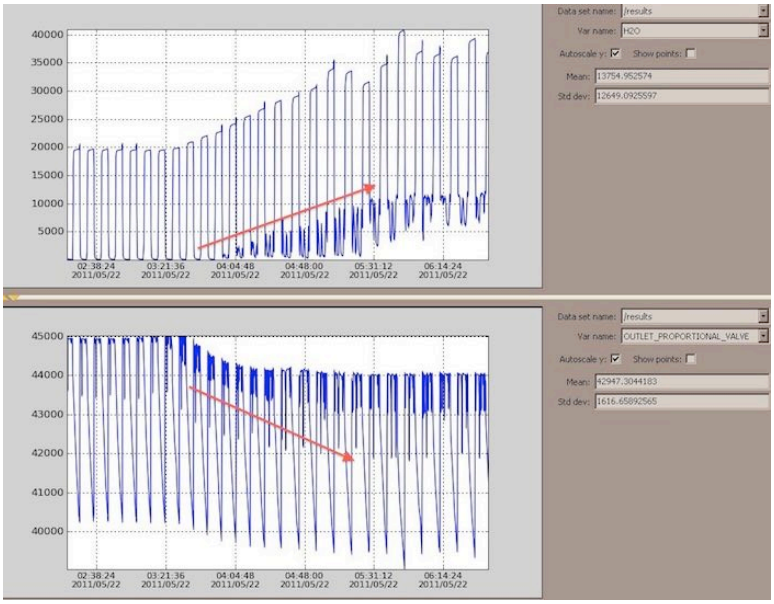


Figure 79 - Baseline of Water Concentration and Outlet Valve Change

15.5.8 Problem: Water Pulses Split Into Multiple Peaks

The final example shows what happens if the analyzer's solenoid valve sequencer is running at the same time the coordinator is. The solenoid valve sequencer should be disabled by default for Picarro water isotope analyzers. If the sequencer runs at the same time as the coordinator, the two components send conflicting signals to the valves that control the vaporizer. In this example, the sequencer is turned off following the third pulse, and the final pulse returns to normal.

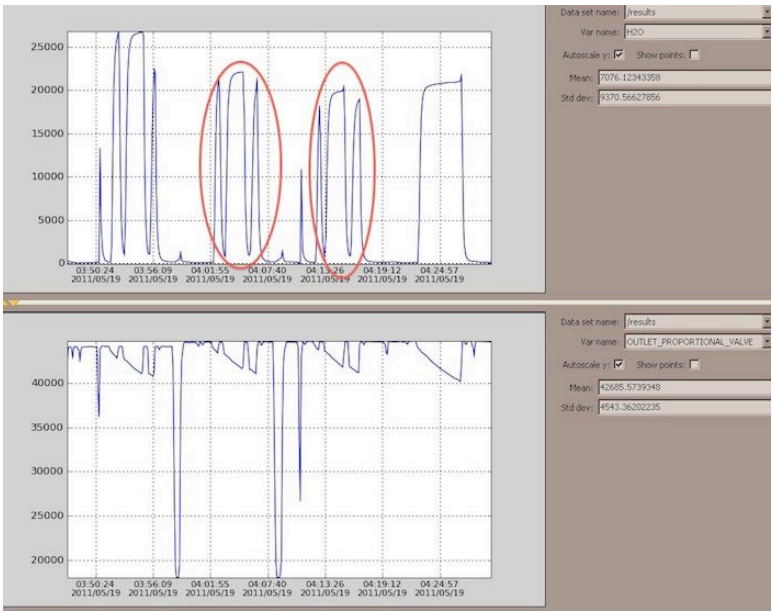


Figure 80 - Water Pulses Split Into Multiple Peaks

16 Best Practices and Operational Tips

This section provides recommended practices to help ensure reliable data quality, consistent instrument performance, and long-term system durability during liquid water analysis. The guidance in this section addresses common operational considerations, maintenance-related behaviors, and sampling strategies that can reduce downtime, minimize consumable wear, and prevent avoidable measurement issues.

16.1 Pulse Customization

Pulse customization allows experienced users to refine how the coordinator identifies and evaluates liquid injection pulses. While the default pulse analysis settings are suitable for most applications, certain workflows or sample types may benefit from adjusting pulse timing or trigger thresholds to better capture the most stable portion of each pulse. This section describes how pulse analysis parameters can be modified and outlines considerations for making these adjustments safely.

16.1.1 Pulse Analysis

There is a delay of a few seconds at both the beginning of the pulse and the end of a pulse where the pulse analysis ignores incoming data. Therefore, only the most stable center portion of the pulse is included in the pulse analysis. Although the default settings should be adequate for most uses, one can adjust the delays by editing the appropriate Coordinator .ini script. Please be sure to keep a copy of the original file in case of any mistake. The example below is for the High Precision Mode Coordinator on a L2130-i with a Picarro Autosampler.

- Edit the `validTimeAfterTrigger` or `validTimeBeforeEnd` fields in the following file: C:\Picarro\G2000\AppConfig\Config\Coordinator\CoordinatorLIMS_G2000_A0340.ini (**Note:** for A0325 Autosampler, find file "…G2000_A0325.ini")
  The default settings are: `validTimeAfterTrigger = 100, validTimeBeforeEnd = 15`
- One can similarly adjust the level that triggers a pulse analysis event by changing the 6500 value in the upslope or downslope trigger in the following file: C:\Picarro\G2000\AppConfig\Config\Coordinator\ CoordinatorLIMS_G2000_A0340.ini (**Note:** for A0325 Autosampler, find file "…G2000_A0325.ini")

The default settings are: thres1Pair = [6500, 30000] and thres2Pair = [5500, 30000] #this is the downslope trigger

16.2 Adjusting Injection Volume

For best results, liquid sample injections should be provided to the instrument at a concentration of **18,000 ± 3,000 ppmv (parts per million by volume)**. Each liquid injection will be labelled as "good" in the coordinator if this concentration is between **15,000 - 21,000**

ppmv. If the concentration is significantly above or below this range (i.e., < 15,000 ppmv or > 25,000 ppmv) or if the dry background is > 500 ppmv, the pulse will not be analyzed, and the data will not appear in the coordinator.

To achieve the appropriate injection concentration:

1. Dry nitrogen or zero air (< 50 ppmv water concentration) should be supplied to the instrument at 2.5 ± 0.2 psi (17.2 ± 1.4k Pa), with a flow of approximately 200 sccm (Standard Cubic Centimeters per Minute). If Drierite (or similar) is used for the dry air (rather than a nitrogen or zero air tank) supply, a measured background level of ~ 100-200 ppmv will produce satisfactory data. Remember to select the Measurement Mode appropriate to your background gas matrix (see the section8 Basic Operation).
2. Sample injection volume (controlled by utosampler) should be set at ~ 1.8 µL.

   If the resulting concentration peak after the 2nd or 3rd liquid injection is substantially different from 20,000 ppmv:

3. **The injection volume may need to be scaled appropriately:** For example, if the resulting concentration peak of an initial 'test' injection is 16,000 ppmv, then the injection volume needs to be adjusted by the factor 20,000/16,000 = 1.25. To accomplish this, multiply the current injection volume in the Autosampler method by 1.25.
4. **The injection quality may need improvement.** Bad Injections can cause incorrect injection concentrations. Bad injections can be from a clogged needle, damaged vaporizer septum, or incorrect dry gas pressure/flow restriction.

NOTE

Five failed injections will lead to a Time Out: Every time there is a liquid injection into a vaporizer by the Autosampler, a pulse of water vapor should enter the cavity and be analyzed. If something goes wrong (e.g., syringe breaks), and the pulse analysis fails, the software will try injecting five times in a row. After 5 failed injection pulses, the coordinator will time out. You will need to restart the coordinator to continue the experiment. This is a built-in safety mechanism that helps prevent un-intended sample contamination following multiple pierces of the vial septum.

16.3 Syringe Lifetime

Syringe breakage is a common failure mode in liquid water analysis. These consumable components are replaceable but can be costly. The following best practices help extend syringe lifetime and maintain consistent performance.

16.3.1 Recommended Practices

- **Use a 10 µL syringe**
- **Manually clean the syringe between each autosampler run using deionized water**

- Ensure the plunger moves smoothly within the barrel
- Apply a lubricant (e.g., N-Methyl-2-pyrrolidone [NMP]) if needed
- Use the Autosampler Training program (not the Autosampler Controller) when replacing the syringe
- Verify syringe injection speed, fill speed, and injection depth

16.3.2 Syringe Details

Picarro analyzers ship with 10 µL syringes from SGE Analytical Science (part number 002982, 10R-C/T-5/0.47C). The thicker plunger design provides improved durability compared to 5 µL syringes.

16.3.3 Samples with Precipitates

The High Precision Vaporizer can operate with liquid waters containing as much as approximately 200 g/kg total dissolved solids (TDS). In principle, water samples can be analyzed without filtration, especially if the precipitate has settled and the syringe is collecting water from near the top of the vial. However, running samples with high TDS will decrease syringe life, require more vaporizer maintenance, and possibly decrease the lifetime of the vaporizer valves.

Therefore, samples should be filtered or centrifuged when possible. The "purer" the liquid being injected into the vaporizer, the longer the syringe, septa, and vaporizer can go without replacement or maintenance.

Dissolving the precipitate by lowering the pH of the fluid is not recommended for these reasons: (1) the sample will fractionate, and (2) introducing acid to the vaporizer, stainless steel tubing, and potentially the cavity, may result in corrosion that requires repair.

16.4 Memory Effect

Memory refers to the effect of the previous sample on the current measurement due to carryover of trace amounts of the previous sample. Water is especially subject to this effect because it adheres to surfaces even at temperatures well above the boiling point. It is a common problem encountered by all methods of isotopic analysis.

In Picarro analyzers, the memory is a function of the entire assembly (vaporizer, connection to the analyzer, and the analyzer itself). It is commonly accounted for by performing multiple injections of the same sample.

The simplest way to correct for memory is to ignore the first 2 or 3 injections of a sample and only use the later injections. For waters with closely clustered isotopic values, this usually means running 6 injections per sample and ignoring the results of the first two injections. In more extreme cases, running 8 injections and ignoring the first 3 or 4 will yield better results.

The effect of memory is stable over time. This means that the same percentage of the previous sample is carried over to the new sample each time.

However, memory should be characterized every one to two months, particularly if samples with high levels of insoluble material or high dissolved solids are frequently analyzed. These materials build up in the vaporizer and can increase the retention of old sample.

This effect can be quantified using the following procedure:

1. Inject a sample of water at least 20 times (40-50 times is preferable).
2. Switch to a new sample with significantly different (> 100‰ for δ^2H) isotopic value and inject the new sample the same number of times as the previous sample.
3. Switch back to the original sample and again measure that multiple times.
4. Calculate the 'true' value of each sample by averaging the last 5 to 10 injections of that sample.
5. Then subtract an individual injection from the 'true' value of the previous sample and divide this by the difference in isotope space between the 'true' value of the current sample and the previous sample.

   This will yield a memory coefficient (in percent) for each injection, x, where, for example 99% means that 99% of the true isotope difference between two samples of water has been attained after x injections. The first injection of sample will be in the range of 94% to 97%. By the 4^{th} injection, it will be approximately 98% for δ^2H and 99% for $\delta^{18}O$. Typically, the memory effect is larger for δ^2H than for $\delta^{18}O$.

16.5 Analyzing Samples with High Total Dissolved Solids

Picarro's High Precision Vaporizer can be used to measure saline samples. However, these samples present two unique challenges to instrument performance and lifetime:

1. Salty samples generate residue in the syringe, which decreases syringe lifetime. See previous section Analyzing Samples with High Total Dissolved Solids for more information on increasing syringe lifetime when running salty samples.
2. Upon vaporization, dissolved solids create a residue in the vaporizer, which can increase the memory effect and influence data quality.

If you are running salty samples and you see a decrease in the memory coefficient, Picarro recommends cleaning the vaporizer. The vaporizer might need cleaning every 200 mg of salt injected, and the cleaning will take about 12 hours of downtime. Contact Picarro to receive instructions on cleaning the vaporizer, or to order the Vaporizer Cleaning Kit (part number C0211).

NOTE

vaporizer cleaning will improve the performance of your High Precision Vaporizer, salt build up can decrease the lifetime vaporizer valves and eventually lead to valve failure. This is particularly true if salts get into the valves themselves, preventing good seals at the valves.

16.6 Sample and Standard Handling

Proper handling and storage of samples and isotopic standards are critical for maintaining the integrity of isotope measurements. This section describes recommended practices for storing, transferring, and preparing samples and standards to minimize evaporation, contamination, fractionation, and memory effects. Adhering to these guidelines helps ensure measurement consistency and long-term traceability of analytical results.

16.6.1 Sample Storage

Whenever samples should be stored in sealed vial in a refrigerator or freezer. If samples are frozen prior to analysis, it is essential to have sufficient headspace in the vial to prevent breakage during phase change, and to ensure the entire sample is returned to liquid form prior to isotope analysis. Parafilming the cap of the storage container is also recommended. If samples are stored in 2 mL autosampler containers, the cap with septa should be replaced once pierced.

Two types of autosampler vial are recommended for use with your Picarro Autosampler:

- **2 mL glass vial with cap and septa (Picarro part number C0322, or as part of a consumables kit, C0328 or C0329)**
- **If samples or standards are limited, it is also possible to use 2 mL vials with 250 µL inserts. These vials act to limit headspace for small samples. Picarro recommends the use of fixed inserts to avoid water vapor passing between the insert and the wall of the larger 2 mL vial. For example, Agilent LS Screw Vial (Agilent part number 5188-6591, available from Fisher Scientific).**

16.6.2 Storage of Secondary Isotopic Water Standards

Selecting the proper containers for long term storage is critical to avoid any change of isotope composition with time due to evaporation or exchange. The following is a list of storage methods for isotope standards.

Glass ampoules: The most reliable containers are glass ampoules that are sealed with a gas torch, such as those provided by the International Atomic Energy Agency with VSMOW2 and SLAP2. After filling and sealing, ampoules can be sterilized by heating the ampoules to about 105°C overnight. This will eliminate the possibility of the growth of algae or other biological activities. Leaking ampoules should be discarded.

Stainless steel barrels: Internal laboratory standards can be stored in stainless steel barrels (25 to 50 liters). These barrels can be obtained from suppliers for the juice, wine, and beer processing industries. When using this method, water standards should be kept under a slight overpressure of argon or nitrogen gas. The dispensing system ideally consists of a valve with a tube down to the bottom of the barrel to extract the water and a second valve with a manometer and tube connector to keep a headspace overpressure of inert gas in the barrel. Due to the overpressure in the barrel, water can be dispensed by opening the first valve. The laboratory standard has no contact with the atmosphere and therefore no risk exists of any evaporation during storage.

Amber vials and glass bottles: For routine work, a 250 mL glass bottle can be filled from the appropriate internal laboratory standard barrel. 2 mL aliquots of these standards can then be moved to a standard autosampler vial with septa cap for routine, daily calibration. Glass bottles should be filled from their source on a regular basis (every few weeks), without discarding the remaining portion of the standards. This handling method minimizes isotope fractionation during evaporation and exposure to air while the bottle is open.

NOTE

Picarro recommends that once an autosampler vial is pierced by a needle, the vial should be discarded and not used repeatedly. For example, if a multi-day autosampler run is set up, the first standard water should not be used again for the last standard water in the sequence. Exceptions can occur if the cap with septa is replaced between the first and last analysis. Once a septa is pierced the sample is susceptible to isotopic fractionation due to evaporation and loss of the water through the cap.

Recommended Reading:

Groening, M. (2018) "TEL Technical Note No. 03 Stable Isotope Internal Laboratory Water Standards: Preparation, Calibration and Storage", Terrestrial Environment Laboratory, International Atomic Energy Agency, Vienna, Austria.

17 Troubleshooting

The following section lists problems that may be encountered during installation and operation of the analyzer. The corresponding step-by-step procedures provide resolution in most cases. If, after attempting these procedures, the problem remains unresolved, please contact Picarro Customer Service at (408) 962-3900 or techsupport@picarro.com.

17.1 Power LED on Analyzer Does Not Illuminate

Context: Turning on the analyzer by momentarily depressing its front panel power switch should apply power. The green power LED is illuminated when it detects the correct power levels.

1. Check that the AC power cord is attached and plugged into a working outlet.
2. Check that the rear on-off switch near the AC power cord is in the on position (**I**).
3. Press and hold the front panel power switch for at least 5 seconds as the analyzer may take several seconds to respond.

17.2 User Interface Program Does Not Start

Context: The computer may be configured to start the instrument and the associated user interface program automatically after it completes its boot-up sequence, or the program may be launched using the **Start instrument** icon on the desktop.

Communications problems with the analyzer may occur if the analyzer fails to initialize correctly on power up. Should the analyzer initialization process not complete correctly, shut down the instrument by shutting down the Windows operating system on the control computer:

1. Using the Start menu, select the red Shut Down button and select **Shut down** in the drop-down box under “What do you want the computer to do?”

   Wait for the shutdown to complete normally and for the computer and analyzer to turn off completely.

2. After a few seconds, restart the computer by momentarily depressing the power button.

NOTE

Do not simply restart Windows since this does not cycle the power to the analyzer.

17.3 Sample Pressure Can't Be Controlled to Appropriate Value for Concentration Measurements

Context: Under normal operation, the cavity pressure is automatically locked to the correct value by means of electronically controlled inlet and outlet valves. The message **Pressure Locked** on the front panel display and the user interface indicates that the cavity pressure is at the appropriate value. Should either of the messages **Pressure high** or **Pressure low** be displayed, the cavity pressure is out of its correct operating range.

1. The **Pressure low** message indicates that there is insufficient gas available at the inlet of the analyzer. Check the inlet plumbing to the analyzer and ensure that the pressure at the inlet is within the specifications.

   Check for blockages in the lines, or regulators that are turned off, especially by removing all items upstream of the inlet to see if the pressure returns to specification. If removing plumbing from upstream of the instrument inlet doesn't work, the inlet particulate filter may need to be replaced. See Maintenance for more information.

2. The **Pressure high** message indicates that gas cannot be removed from the analyzer at a sufficient rate. Check the vacuum line between the analyzer and the power vacuum unit for leaks. Failure of the vacuum pump, injecting dilution gas at excessive pressure, or excessive pressure at the inlet can also cause this problem.

17.4 User Interface Program Freezes / Won't Update Graphs as Data Are Collected

Context: The computer may become unresponsive causing the programs that control the analyzer to stop functioning. The computer and analyzer should be shut down and restarted.

1. Re-setting the computer and the instrument requires that the computer be shut down and restarted. If the computer responds to the mouse, a normal Windows shutdown may be carried out: use the Start menu, select the red Shut down button and select **Shut down** in the drop-down box under "What do you want the computer to do?"

   Wait for the shutdown to complete normally and for the computer and analyzer to turn off completely. After a few seconds, restart the computer by momentarily depressing the power button.

2. If the computer does not respond to the mouse, hold down the power switch on the front panel for a few seconds until the computer and the instrument turn off. After another few seconds, restart the analyzer by momentarily depressing the power button.

17.5 ChemCorrect Processing Software Hung Up (frozen)

Recommendation: Check that you ran a coordinator compatible with ChemCorrect. Coordinators for the ^{17}O-excess mode are not compatible with ChemCorrect. Coordinator output csv files should contain columns with baseline_shift for L2130-*i* and L2140-*i*.

If the above checked out, the other usual cause is syntax error and/or missing/empty rows in the coordinator output file. The three files listed below are user-editable:

- Instruction Set: *C:\Picarro\ChemCorrectExe\chemcorrect_inst xx.csv*
  The instruction set is usually not edited unless you're an avid user.
- Standard Library: *C:\Picarro\ChemCorrectExe\standards file.csv*
  The standards file syntax is not too complicated to follow.
- Coordinator Output csv file or source file: *HBDSxx _CC_IsoWater_xx.csv*

The most common errors occur in the Coordinator Output file. These are the items to check:

- The number of injections that you set ChemCorrect Analysis to ignore has to be less than the total injections/sample.
- There can't be any empty row or blank value (as a result of broken/bent needle, or sample ran out of liquid). This is not an issue if you have ChemCorrect version 1.2.0 or later.
- **Line** column has to be sequential and start at 1
- **Time Code** column has to be chronological.
- Port number should correspond with the correct sample number.

18 Maintenance

The advanced, rugged design of Picarro analyzers provides stable, long-term operation with minimal service or maintenance. With the exception of the following items, the analyzer and pump are not user serviceable. Should either appear to malfunction, please refer to the Troubleshooting Guide or contact Picarro Customer Support.

In the following sections, users may obtain preventive maintenance components as part of a service plan, as part of a designated PM kit, or individually from the Picarro store.

18.1 Service Plans

In addition to basic telephone and email support and remote diagnostics, service plans include an annual preventive maintenance kit and can be purchased by contacting sales@picarro.com. The three service plans are as follows:

- **W3101 Essential Service Plan** — Free yearly maintenance kit; 50% discount on Field Replaceable Parts; 10-20% Discounted factory repair. See data sheet for complete terms and conditions.
- **W3102 Premium Service Plan** — Free yearly maintenance kit; Extended warranty; Free factory repair; Free Field Replaceable Parts. See data sheet for complete terms and conditions.
- **W3103 Commercial Service Plan** — Free yearly maintenance kit; Extended warranty; Free factory repair; Free Field Replaceable Parts; Loaner instrument; Free yearly prevention maintenance visit; Complimentary remote refresher training. See data sheet for complete terms and conditions.

18.2 Preventative Maintenance Kits

Preventive maintenance kits can be purchased by contacting support@picarro.com. The maintenance kits all include the following elements:

Replacement CPU Fan; particulate filter (Stainless Steel or Teflon); dust filter; replacement screws for instrument cover panels; Ball-Point Hex L-Keys; Anti-Static Wrist Strap.

The kits come in three forms depending on the instrument being serviced.

- **S3092** — Yearly Maintenance Kit for GHG, L2xxx, and EtO
- **S3093** — Yearly Maintenance Kit for PI2114, PI2124
- **S3094** — Yearly Maintenance Kit for HAPs G2xxx User-Replaceable Hardware

18.3 User-replaceable Hardware

This section provides a list of components that are self-serviceable. These items can be purchased online through the Picarro store by using the links below.

18.3.1 Particulate Filter

The inlet particulate filter is user-replaceable. Use the following link to order replacements and to find the instructional video and supporting maintenance document.

Parts

- **Stainless Steel Filter (for all models except those that measure HF, NH_3, CH_2O, HCl and H_2O_2):**
  S1020 Particulate Filter Kit – If viewing this manual as a paper hard copy, enter the following URL in your browser:
  https://store.picarro.com/Particulate-filter-kit-all-models-except-HF-NH3
- **Teflon Filter: For models that measure NH_3, HF, CH_2O, HCl and H_2O_2**
  S1021 Particulate Filter Kit – If viewing this manual as a paper hard copy, enter the following URL in your browser:
  https://store.picarro.com/Particulate-filter-teflon-for-NH3-HF._3

Instructions

- **Video:**Replacing Your Inlet Particulate Filter
  https://www.picarro.com/environmental/videos/replacing_your_inlet_particulate_filter
- **Manual:**Inlet Particulate Filter Maintenance Guide
  https://www.picarro.com/environmental/inlet_particulate_filter_maintenance_guide

18.3.2 CPU Fan

The analyzer CPU fan is user-replaceable. Use the following link to order replacements and to find the instructional video and supporting maintenance document.

Parts

- **CPU Fan for MI990 Motherboards:**
  S3267: PI5000 CPU Fan Replacement Kit. Includes the S3263 (CPU Fan) and required tools for replacement.nstructions

Instructions

- **Video:**CPU Fan Replacement
  https://www.picarro.com/environmental/videos/cpu_fan_replacement
- **Manual:**CPU Fan Replacement for Picarro Analyzers

A2000 Pump Rebuild Kit

The pump rebuild kit is the only component not currently sold as part of a preventive maintenance kit because the replacement frequency is not strictly annual (frequency depends on pump usage).

The A2000 pump diaphragms and valves are user-replaceable. Use the following link to order rebuild kits and to find the instructional video and supporting maintenance document.

Parts

- **Pump Rebuild Kit — Used with SI2xxx, G2xxx analyzers (except Flight and Flux analyzers)**
  S2009 Rebuild Kit for A2000 Vacuum Pump – If viewing this manual as a paper hard copy, enter the following URL in your browser:
  https://store.picarro.com/Rebuild-kit-for-Picarro-A2000-vacuum-pump

Instructions

- **Manual:**A2000 Pump Maintenance Guide
  https://www.picarro.com/environmental/a2000_pump_maintenance_guide

18.4 A0211 Vaporizer Injection Port Septum Replacement

For instructions on replacing the injection port septum and salt liner (if used), refer to the Maintenance section in the A0211 High-Precision Vaporizer User Manual (PN 40-0044).

18.5 Cleaning

Clean the outside of the analyzer with a clean dry cloth. Only certified service technicians should access or clean the inside of the analyzer.

19 Transportation and Storage

If the analyzer will be transported or stored, use the following procedure to prepare and repack it into the original packaging.

⚠ CAUTION

When shipping or relocating the analyzer, it is important to protect it from mechanical shocks. Failure to do so can compromise its performance. When shipping the analyzer, use its original packaging only.

19.1 Shutdown and Preparation

⚠ CAUTION

A flow of clean, relatively dry gas should always be directed to the instrument for several minutes prior to shutting down. Trapping a high-moisture content gas sample in the cavity can cause condensation damage to the mirrors as the instrument cools from its operating temperature. See section 8 Basic Operation, for specific shutdown instructions.

1. Click on the **Shutdown** button located on the left side of the Data Viewer window.
2. A window will pop-up prompting the user to confirm the shutdown. Once confirmed, the analyzer software and hardware will turn off.

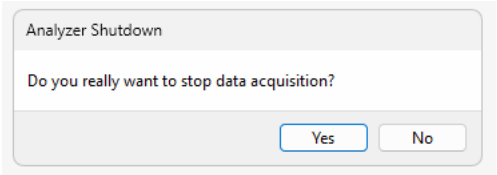


Figure 81 - Shutdown Confirmation Dialog

3. Manually turn off the pump(s) and dry gas (if used).
4. Disconnect all tubing and electrical connections from the analyzer.
5. To prevent contamination and possible damage to the connector threads, place protective caps on all gas connections.

19.2 Packing

1. Place the analyzer in a plastic bag with a package of desiccant. Seal the bags with tape. If shipping the pump, do the same for it.

2. Pack the analyzer and pump in the original shipping containers ensuring that all the foam pieces are in place to protect the analyzer during shipping.

A Setup Tool and Communication

The Setup Tool and Communication features provide the configuration and interface options required to manage how the analyzer records, outputs, and communicates data. The Picarro Analyzer Setup Tool enables users to customize data logging, digital communication interfaces, remote data delivery, and user interface behavior to meet specific operational and integration requirements.

In addition to local configuration, the analyzer supports multiple communication methods, including serial (RS-232), TCP/IP, and automated email delivery. These capabilities allow the analyzer to integrate with external systems, support remote monitoring, and enable automated data transfer and system time synchronization.

Before making changes using the Setup Tool, the analyzer software and drivers must be stopped to ensure that configuration settings are applied correctly. The following sections describe the Setup Tool interface, its available configuration tabs, and the communication options supported by the analyzer.

A.1 Setup Tool

In the desktop folder called **Picarro Utilities**, the **Picarro AnalyzerSetup Tool** can be launched by double clicking on its icon. This tool allows the user to configure data file saving details, including which data elements are written to data files, digital data output (via serial port or TCP/IP), remote data delivery (via email), and general GUI properties.

Seven tabs of the Setup Tool Window are explained in the next pages in brief. A more in-depth description of the material is provided in the subsequent section. If you have any questions about the Setup Tool, please contact Picarro or refer to Picarro Community for further details.

https://www.picarro.com/support/community

NOTE

Before running the Setup Tool, the instrument software and drivers must be stopped.

From the desktop, open the Diagnostics folder, double-click on the Stop Instrument icon. The Stop CRDS Software window appears. Select the radio button "Stop software and driver," then click the Stop button.

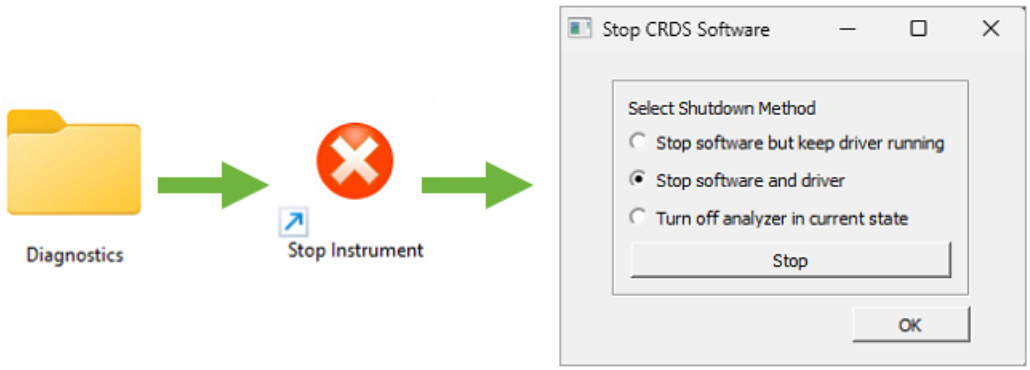


Figure 82 - Stop CRDS Software

A.1.1 Data Logger Tab

Configuring Data File Saving Details with Data Logger

The **Data Logger** tab (Figure 83 - Data Logger Setup Window) allows the user to configure various data file saving details, including which data elements are written to data files.

- **Data Columns:** Controls which data elements are written to data files.
- **Hours of Each Log File:** Controls the size of each data document.
- **Enable Mailbox Archiving:** Enables archiving of data in the mailbox folder – C:\Picarro\G2000\Log\Archive\DataLog_Mailbox
- **Archived Directory Structure:** Specifies part of naming convention for data documents.
- **Total User Log Storage Size (GB):** Specifies the size of storage allowed for User Data (Recent Data).
- **Mode:** Changes the way the analyzer fits and displays data in the data viewer on the basis of gas matrix, species reported, precision, and dynamic range.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

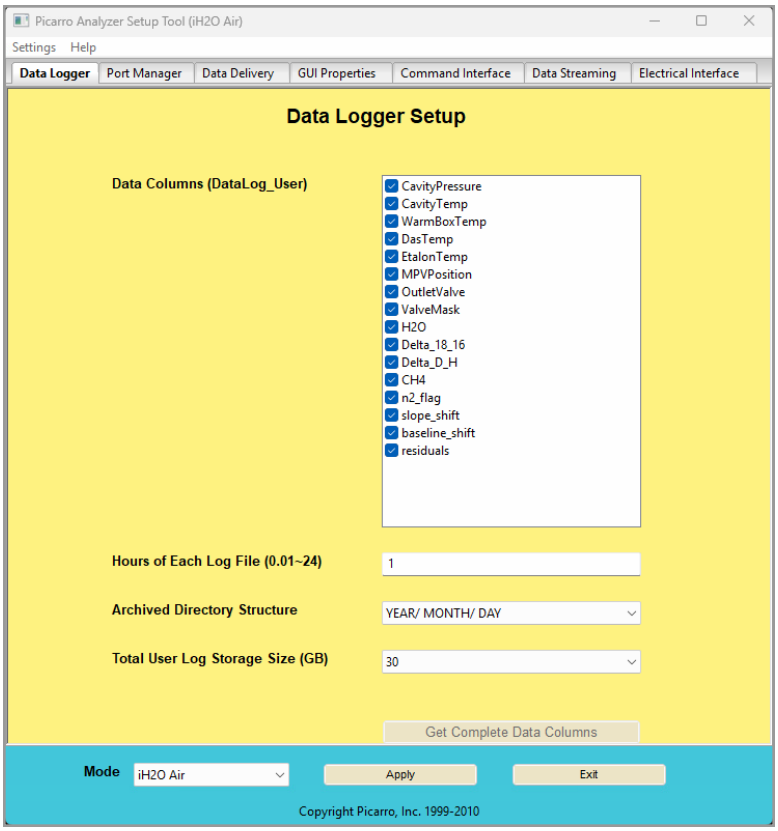


Figure 83 - Data Logger Setup Window

A.1.2 Port Manager Tab

Managing Ports for Digital Data Output/Input and Serial Communication with Port Manager

The **Port Manager** tab (Serial/Socket Port Manager Window) allows you to control digital data output/Input via serial port or TCP/IP.

On this window, you can specify:

- **Data Streaming:** The port you want your data to stream through (COM1/COM2/Off),
- **Valve SequencerMPV (Multi Position Valve):** The port you want to connect your MPV to (COM1/COM2/Off)

For more information on the configuring for external valves, contact Picarro Support.

- **Command Interface:** (COM1/COM2/TCP/Off).

Make sure there are no COM port conflicts before clicking **Apply**.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

To learn more about Serial Communication, see To learn more about Serial Communication, see To learn more about Serial Communication, see To learn more about Serial Communication, see To learn more about Serial Communication, see Remote Data Access in

Setup Tool and Communicationon page 1. in 1.0.1 Port Manager Tab*on page 1*. in A.1.2 Port Manager Tab*on the previous page*. in A.1.2 Port Manager Tab*on the previous page*. in A.1.2 Port Manager Tab*on the previous page*.

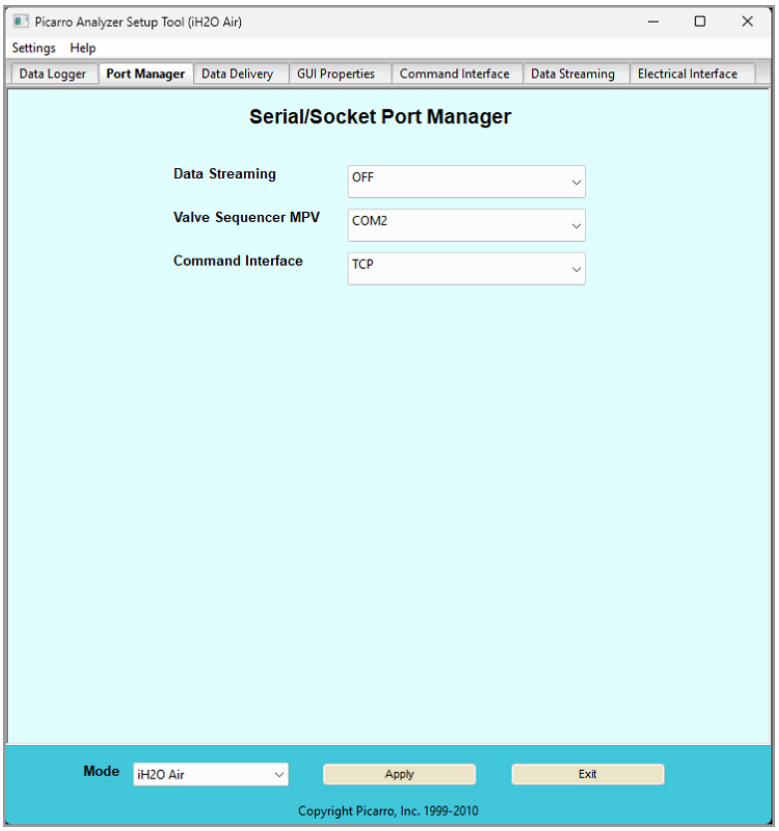


Figure 84 - Serial/Socket Port Manager Window

A.1.3 Data Delivery Tab

The **Data Delivery** tab (Figure 85 - Data Delivery Settings Tab) allows the user to schedule remote data delivery (email).

- **Delivery Start Time:** Time of the day when data will be sent.
- **SSL:** Depending on the sender's email server, the sender can activate the Secure Sockets Layer (SSL).
- **Use Authentication:** Turning this on will require the receiver to provide a password and a username to access data. Set up the password and Username from this window.
- **From:** Sender's email
- **To:** Receiver's email.
- **Subject:** subject line of the email.
- **Data Directory:** Location of the data you want email.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

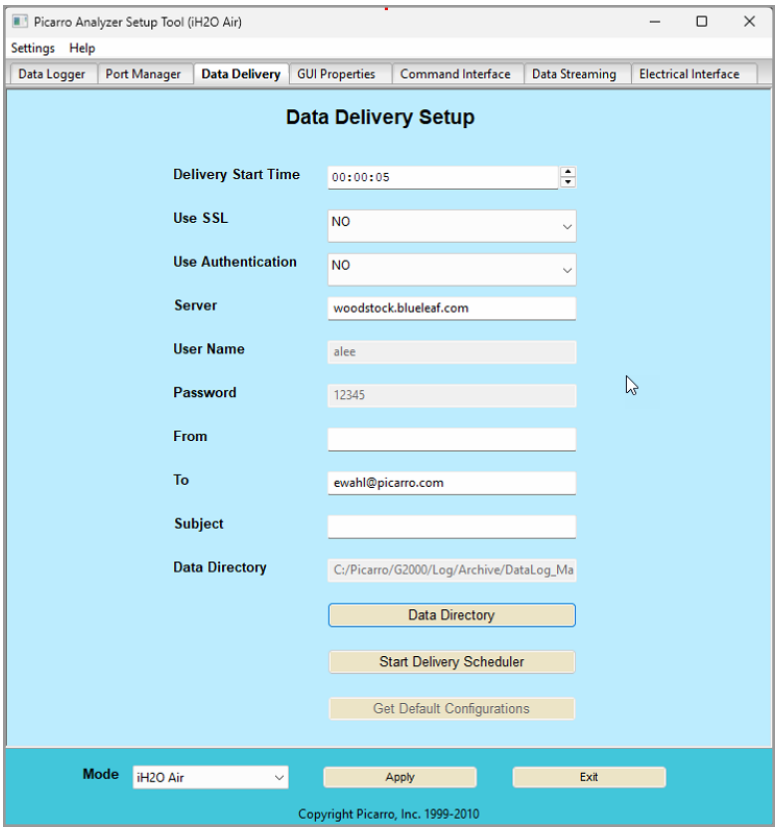


Figure 85 - Data Delivery Settings Tab

A.1.4 GUI Properties

The **GUI PROPERTIES** tab (Figure 86 - GUI Properties Settings Tab) allows you to set the number of graphs displayed and to enable the control of Valve Sequencer from the main GUI.

Number of Graphs: Set the desired number of line graphs to be visible on the main GUI.

Enable Control of Valve Sequencer: To make the Valve Sequencer menu item visible under the **Tools** menu of the main GUI:

1. Click on **Settings** of the **Setup Tool** window, and then **Switch to Service** mode.
2. Choose Yes next to Enable Control Valve Sequencer drop down menu on the GUI Properties tab.
3. Click **Apply** to put changes into effect and then **Exit** to close the window.

   You should now be able to access the **Show/Hide Valve Sequencer GUI** menu from the main GUI under the **Tools** menu.

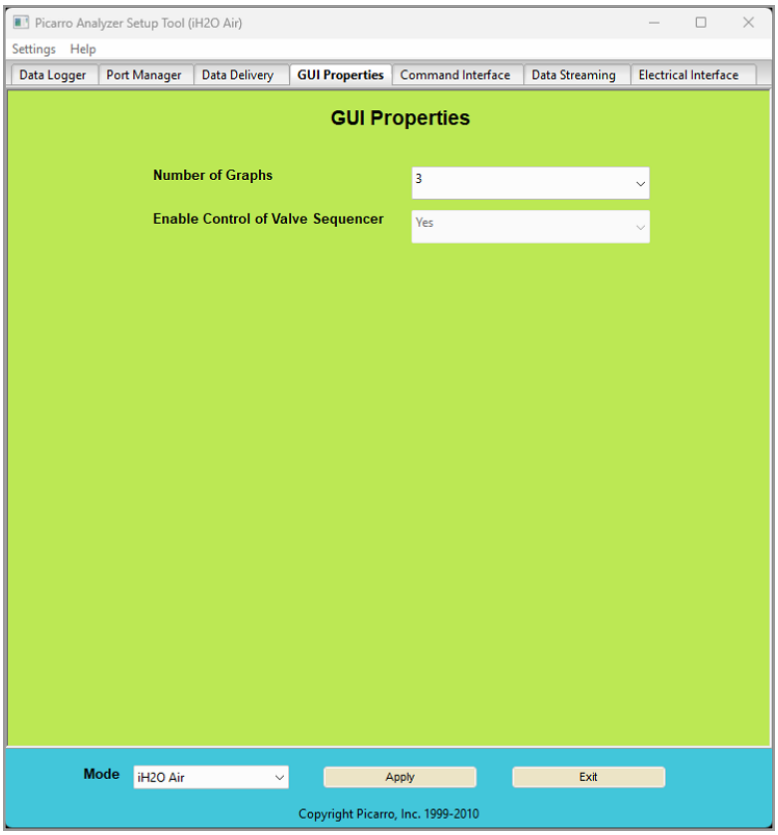


Figure 86 - GUI Properties Settings Tab

A.1.5 Command Interface – Specifying Digital Data Output

The **COMMAND INTERFACE** tab allows you to specify the data elements that are sent via COM port/TCP (specified in the **PORT MANAGER** tab). Two types of data can be specified here:

Output Data Source:

- Datalog_User
- DataLog_User_Sync (Relevant only for Flux G2311-f analyzers).

Output Data Columns:

- The data columns are output in the order they are checked, e.g., CH_4, comes before CO_2. Command Interface enables an external device to send a set of predetermined commands to a Picarro analyzer. The Picarro returns data or metadata on the basis of the command received.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

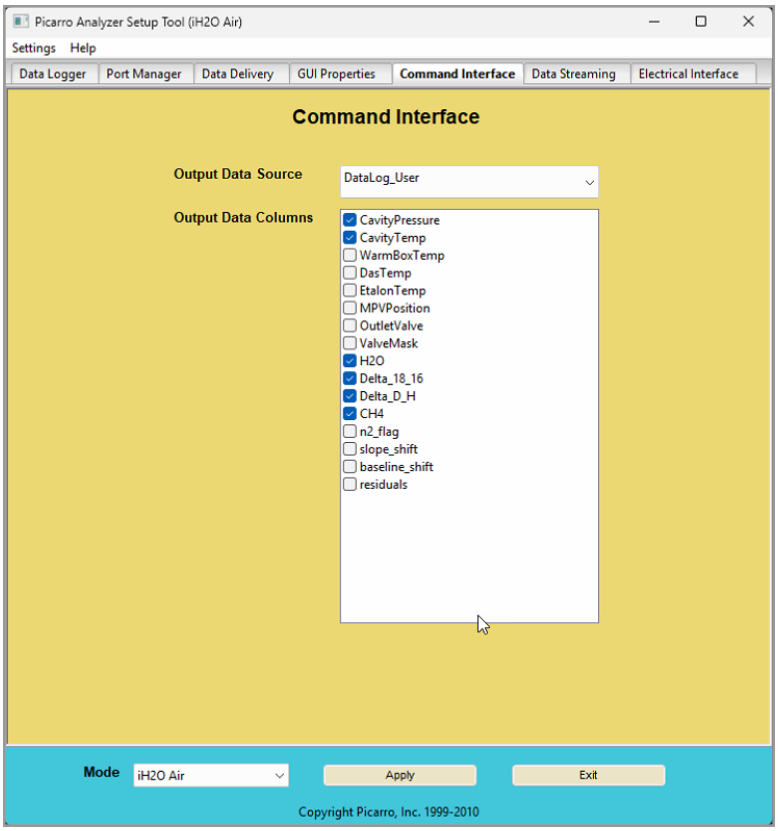


Figure 87 - Command Interface Settings Tab

A.1.6 Data Streaming – Specifying Digital Data Output

The **DATA STREAMING** tab allows you to specify the data elements that you want to send via COM port (specified from the **PORT MANAGER** tab). Two types of data can be specified here:

Output Data Source:

- Datalog_User
- DataLog_User_Sync (Relevant only for Flux G2311-f analyzers).

Output Data Columns:

The data columns are output in the order they are checked, e.g., CH_4, comes before CO_2. Command Interface enables an external device to send a set of predetermined commands to a Picarro analyzer. The Picarro returns data or metadata on the basis of the command received.

Data Streaming outputs data continuously, whereas the Command Interface needs commands to output data.

After making the appropriate edits, click **Apply** to put changes into effect and then **Exit** to close the window.

Figure 88 - Data Streaming Settings Window

A.1.7 Electrical Interface – Customizing Analog Output Channels

The Picarro analyzer may be optionally configured with an **Electrical Interface Card** (EIC) that provides up to 8 analog signals available to the user for monitoring various measurements results and analyzer parameters.

The **ELECTRICAL INTERFACE** tab (Figure 89 - Electrical Interface Settings Window) allows you to customize each analog output channel.

After making the appropriate edits, click Apply to put changes into effect and then **Exit** to close the window.

⚠ CAUTION

This tab will be disabled if your analyzer was not configured to work with an analog peripheral.

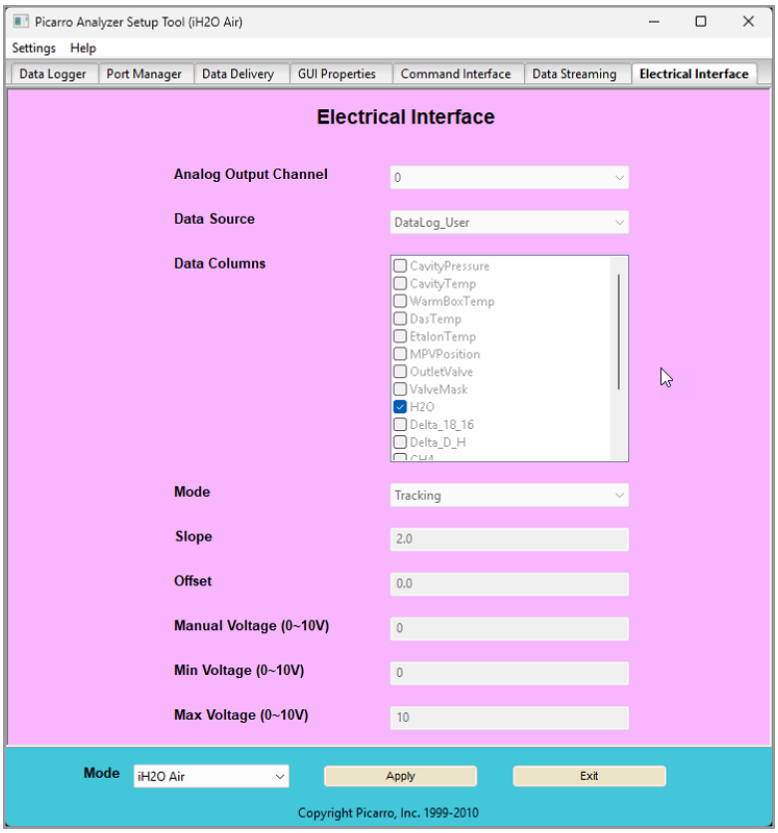


Figure 89 - Electrical Interface Settings Window

A.2 Remote Data Access

The analyzer supports remote data access capabilities that allow users to retrieve instrument data, configure remote communications, and automate data delivery. Through the RS-232 serial interface or Ethernet connection, users can remotely control the analyzer and retrieve concentration data using Picarro's supported command set. For complete command syntax, configuration details, and supported functions, refer to the Remote Interface Programming Guide 40-0063 available through Picarro's Document Library.

In addition to direct communication, the analyzer can be configured to automatically send data files to designated email recipients and synchronize the host computer clock with internet time servers using the RemoteAccess.ini configuration file. These functions are managed through the RemoteAccess.exe utility and can be scheduled to run automatically at user-defined intervals. This section explains how to access the remote interface documentation and configure remote data transfer, email notifications, and time synchronization settings.

A.2.1 Picarro Serial Communication

The analyzer supports an RS-232 physical command interface, which can be used to control the instrument and to retrieve concentration data. Not all features of the instrument are available on the serial interface.

For details on using the serial command interface, please see the Picarro analyzer **Remote Interface Programming Guide**.

To Download:

1. Go to https://www.picarro.com/.
2. Under the **Support** tab (near the home page upper-right corner), select **Document Library**.

   ⚠ CAUTION

   Registration/Login Required: Access to online User Manuals is available to all registered Picarro customers with login credentials. If you do not yet have an account, please email us at support@picarro.com to request access to the document library.

3. When the Document Library page opens, enter the search terms, "Remote Interface" in the **Search** field.
4. In the results, click on the link titled "**Remote Interface Programming Guide 40-0063**" to open the manual in your browser. From there you can also download and save it to your PC.

   This command set may also be used across a TCP/IP interface through an Ethernet connection. Please contact Picarro for further details if needed.

A.2.2 Remote Data Access

Using the RemoteAccess.ini file, the analyzer can be configured to automatically:

- Send data from the instrument to a list of e-mail accounts.
- Measure the offset of the host computer system clock from a set of Internet time servers and (optionally) to resynchronize the clock based on this information.

The Internet connection need not be permanent and may be a dial-up connection accessible via a user-supplied USB modem. The task of sending data and/or synchronizing the clock on the analyzer is performed using the C:\Picarro\G2000\HostExe\RemoteAccess.exe program. This program can be set up to run periodically using the Windows task scheduler at a user-configurable frequency. If a dial-up connection to the Internet is employed, it is used only on demand to minimize the connection time.

Each time that the RemoteAccess.exe program runs, it appends information to a log file, which keeps a record of the results of the time synchronization and of the files sent by e-mail. The RemoteAccess.exe program is configurable by means of an initialization file, which includes information such as the login credentials for the dial-up connection, the e-mail account, and the list of time servers.

The initialization file is:

C:\Picarro\G2000\AppConfig\Config\UtilitiesRemoteAccess\RemoteAccess.ini

It should be placed in the same directory as the executable RemoteAccess.exe. The file has one required section named **LOGGING** and optional sections named **NTP** and **EMAIL**. The logging section has a single key Logfile whose value is the path to the log file. Once this log file exceeds 64 Kbytes in length, it is backed up, appending a numeric extension to the file name, and a new file is opened. A total of ten backup log files are kept.

A.2.3 NTP

The NTP section controls querying the Internet time servers using the SNTP protocol (RFC4330) and the resetting of the clock on the host computer. If the section is not present, time synchronization is not carried out. The keys Server1, Server2, etc., are used to specify the URLs of the time servers. If the UpdateClock key is set to “true,” the offset is applied to the host clock. Otherwise, the offset is recorded, but the host clock is not changed.

A.2.4 Email

The EMAIL section controls the sending of the data files as e-mail attachments. If the section is not present, e-mail messages are not sent. The key Directory specifies the directory that contains the data files. When the program is run, files in this directory are sent to the specified recipients and the files are deleted. To avoid problems with incomplete files, programs that place files into this directory should do so using an atomic operation, such as a rename. The Server key is set to the name of an RFC2821- compliant SMTP server that sends the e-mail messages.

The From key is the e-mail address from which the messages are sent. Note that some SMTP servers check that the source is permitted to send email while others allow any name in this field. The collection of e-mail addresses to which copies of the e-mail is sent is specified by the keys To1, To2, etc. The Subject key is used to fill the subject field in the email header and may be set to any string. Depending on the SMTP server, it may be necessary to use authentication before e-mails can be sent, as described in RFC2554. If such authentication is not needed, the key UseAuthentication is set to false. If this key is set to true, two additional keys Username and Password must also be specified for the e-mail account.

B Data File Viewer

The Data File Viewer is a software tool used to visualize, analyze, and manage instrument data collected over time. This Quick Start Guide introduces a common workflow for viewing data trends by converting, concatenating, and plotting measurement files, allowing users to efficiently examine data spanning multiple hours or days. Subsequent sections describe additional features of the Data File Viewer in greater detail, including statistical analysis, data transformation, and advanced plotting options.

B.1 Quick Start Guide

The following sections introduce the user to all functions of the Data File Viewer in detail. This section describes the most common, simple use case.

The Data File Viewer software allows the user to concatenate multiple one-hour files into one larger file, enabling the user to observe trends over several days of measurements.

1. To start, translate the UserData files from DAT to H5. The **Batch Convert option (B)** allows users to select any folder containing instrument data from a given day.

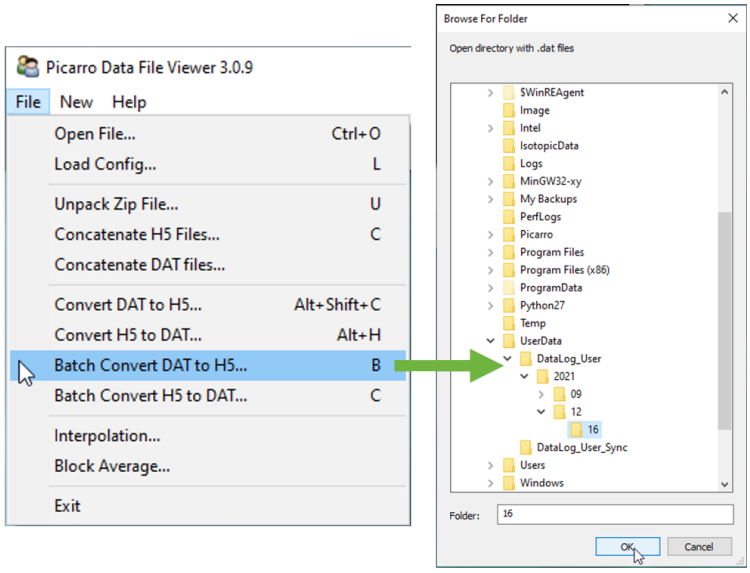


Figure 90 - Batch Convert DAT to H5 – Navigation

2. In the source folder there are now copies of the original files translated into the H5 format.
3. From **File** menu select **Concatenate H5 Files** (C) to combine the H5 files into a time series. Take care to select exactly the same folder in the file viewer window.
4. In the Select Variables window, click **All** to move over all variables for concatenation. If concatenating very long records, the user can instead select only a few variables by clicking the variable name on the left dialogue, and clicking the double arrow button. Confirm by clicking **OK**.

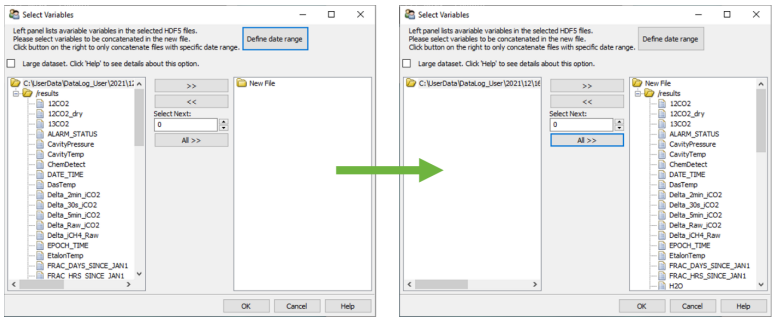


Figure 91 - Selecting Variables for Concatenation

5. The user will then be asked to confirm the file name for the concatenated data. The default location will be in the parent folder for the selected day, and the filename will by default describe the time span of the measurements within. Successful concatenation will lead to the filename automatically being displayed in the main data file viewer window.

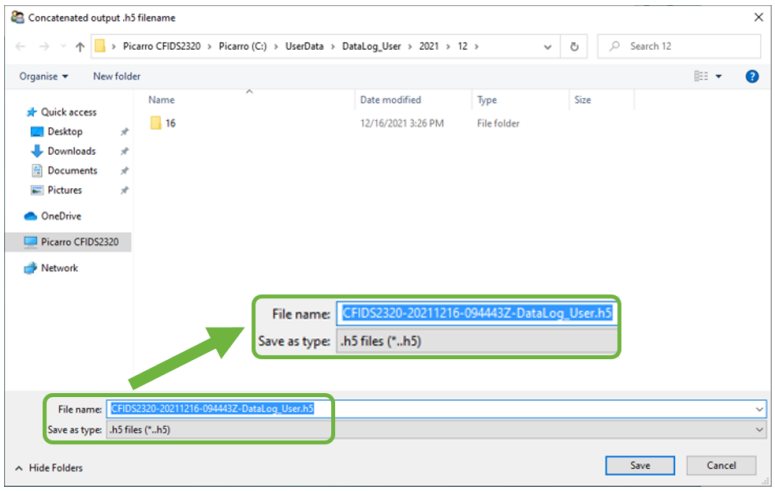


Figure 92 - Concatenated Output .h5 Filename

NOTE

You can concatenate several days into one larger file, either by following steps 1-3 for selected folders, or by copying all their DAT files into a new folder and performing steps 1-5 just once.

6. With the file now opened, the user can select how many **Time Series** to display on the screen.

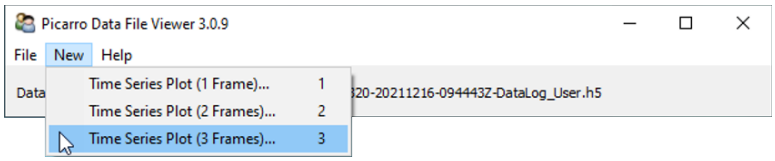


Figure 93 - Time Series Selection Options

7. In the new window that appears, select the variables from the **Var Name** dropdown on the right of each plot. Deselect **Autoscale y** if the data stream has a large amount of variability in the Y-axis.
8. Please read the following sections to learn more about features of the Data File Viewer.

B.2 Data File Viewer Overview

The Picarro Data File Viewer software is located on the desktop of the Picarro instrument. The software allows the user to graph and to conduct statistical analysis of the raw data. Additional functions include Allan Variance plot and quadratic or polynomial fittings. The Picarro Data File Viewer includes two main menus: **File** and **New.**

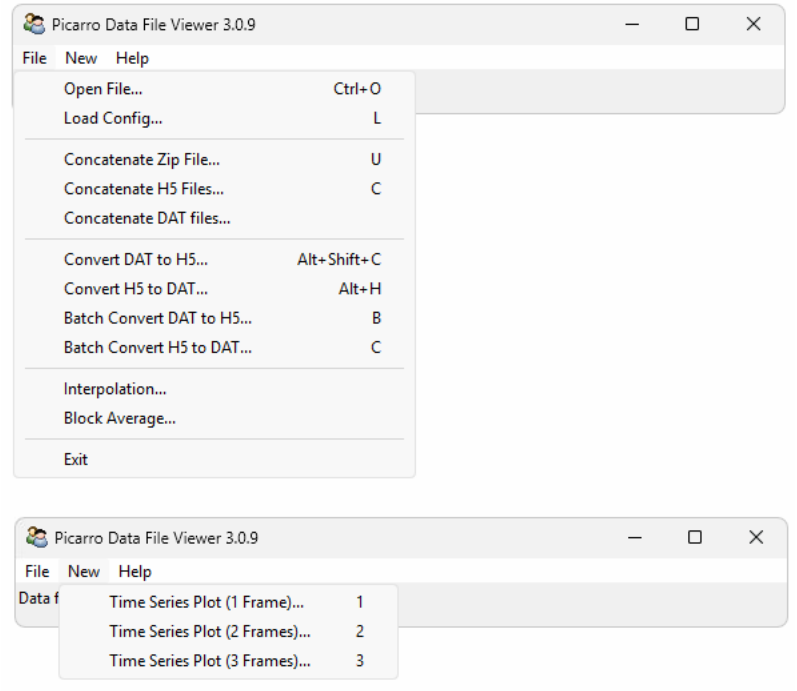


Figure 94 - Picarro Data File Viewer – File and New Menus

B.3 File Menu

This section describes the functions available from the Data File Viewer File menu.

B.3.1 Open H5

File > Open H5 File: Opens a Picarro data file (HDF5 format) for data analysis and visualization. After opening the data file, you can create a new time series plot. Refer to section B.3 File Menu for more information.

B.3.2 Load Config

File > Load Config: Loads a configuration file (ini format) to restore parameters of a workplace. Refer to B.3 File Menu for more information.

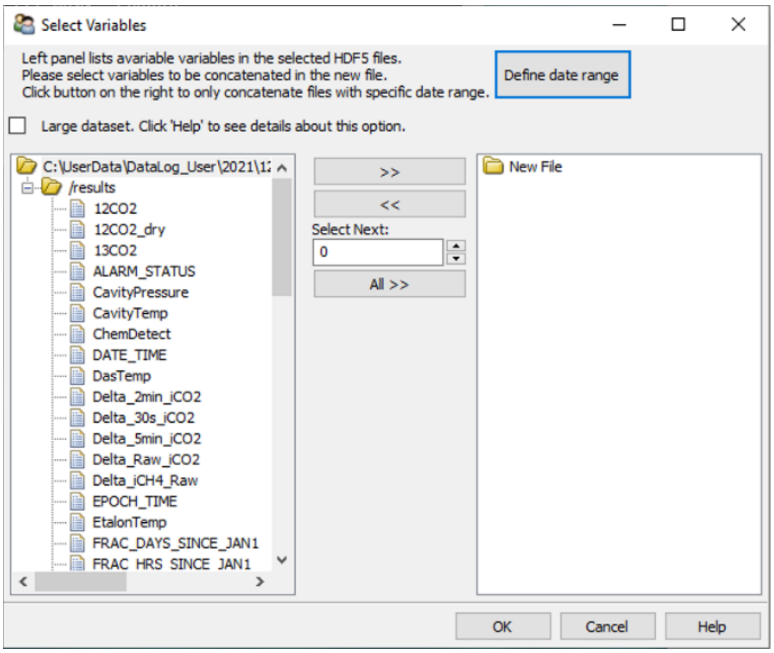
B.3.3 Unpack Zip File

File > Unpack Zip File: Use to concatenate all H5 files inside the zip file into a single H5 file. Refer to Concatenate H5 Files below for details.

B.3.4 Concatenate H5 Files

File > Concatenate H5 Files: Use to concatenate multiple files and zip archives of H5 files into a single H5 file. Navigate to the desired folder or use the **Define Date Range** button to specify a date range of files to concatenate. (See next section.)

After selecting the path of the data files, Data File Viewer will automatically search an H5 file in the specified zip/folder and look for all available variables in the H5 file. The variables are then listed in the **Select Variables** window in the left panel (as shown in Figure 95 - Select Variables Form), and users can use the "**>>**" button to move variables to the right panel for concatenation.



Note: This screenshot is for example only. The species selections shown on your analyzer may vary.

Figure 95 - Select Variables Form

B.3.5 Define Date Range

Data File Viewer can search data files within the desired date range and then concatenate such files into an H5 file.

By default, TimeZone is set to your local time zone. However, if data were taken elsewhere, select the time zone where data were taken.

Select File > Concatenate H5 Files, then click **Define Date Range** to specify the desired date range as shown in Figure 96 - Define Date Range Dialog.

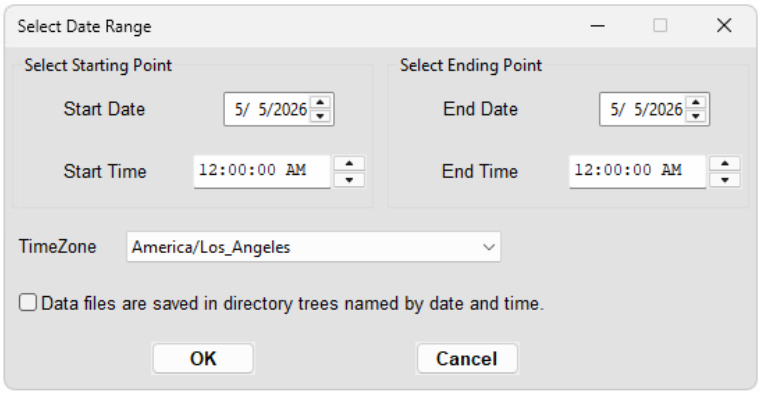


Figure 96 - Define Date Range Dialog

Data files are saved in directory trees named by date and time option.

Picarro software saves data in a directory tree that is named by the creation year, month, and day as shown in Figure 96 - Define Date Range Dialog. Select this option if the target folder has this file structure. This way, Data File Viewer will only search folders within the desired date range, which can substantially reduce processing time.

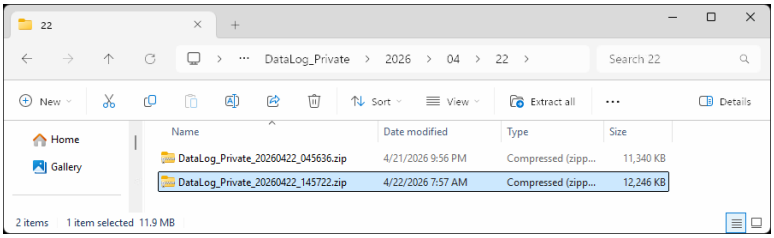


Figure 97 - File Structure of Data File Viewer

NOTE

To save processing time, Data File Viewer does not open data files, but only determines data acquisition time based on the file name.

CAUTION

Do not define a time range for data files whose names have been changed.

NOTE

Data File Viewer does not concatenate data files exactly within the defined time range. This is because the time extracted from file name is different from the data acquisition time. To not miss data points, Data File Viewer expands the specified time range, so the resulting dataset normally has a wider time range than the user specification.

B.3.6 Convert DAT to H5

Select File > Convert DAT to H5 to convert a file in DAT format to HDF5 format. These formats are described below:

- DAT format: DAT files accepted by DatViewer store tabular data (numbers and text) in plain text.
- Each line of the file is a data record. Each record consists of one or more fields separated by whitespaces.
- The first line of the data file indicates column names.

- There must be a field “EPOCH_TIME” to store the acquisition epoch time (expressed as seconds since Jan 1, 1970) of the data. Otherwise, the first and second fields must be “DATE” and “TIME.” The “DATE” field must have the format “mm/dd/yyyy” or “yyyy-mm-dd,” and the “TIME” field must have the format “HH:MM:SS(.sss)” where (.sss) is an optional fraction of seconds.
- **HDF5 Format:** HDF5 is a data model, library, and file format for storing and managing data. (See the HDF5 Home Page on the HDF Group website https://www.hdfgroup.org/ for more information.) When converting DAT to HDF5 format, Data File Viewer creates a table named “results” to the contained data.

B.3.7 Convert H5 to DAT

Select **File > Convert H5 to DAT** to convert a file in a HDF5 format to DAT. These formats are described in Convert DAT to H5.

NOTE

Data File Viewer does not concatenate data files exactly within the defined time range. This is because the time extracted from file name is different from the data acquisition time. To not miss data points, Data File Viewer expands the specified time range.

B.3.8 Interpolation

Interpolation describes the method for constructing data points with a range of a discrete set of known data points. Select **File > Interpolation** to perform interpolation on a time grid with a constant interval.

B.3.9 Block Average

Select File > Block Average to divide a dataset into small blocks based on a user-defined block size. The average is calculated for data in each block, and the results are saved in a new H5 file.

NOTE

The specified block size must be greater than the average data interval.

Because the data interval is normally not a constant (unless interpolation is performed), fluctuations in the data interval will affect block averaging if the block size is comparable to the average data interval.

B.4 Time Series Plot

You can create a time-series plots with one, two, or three frames. The additional plots display in the Time Series Viewer.

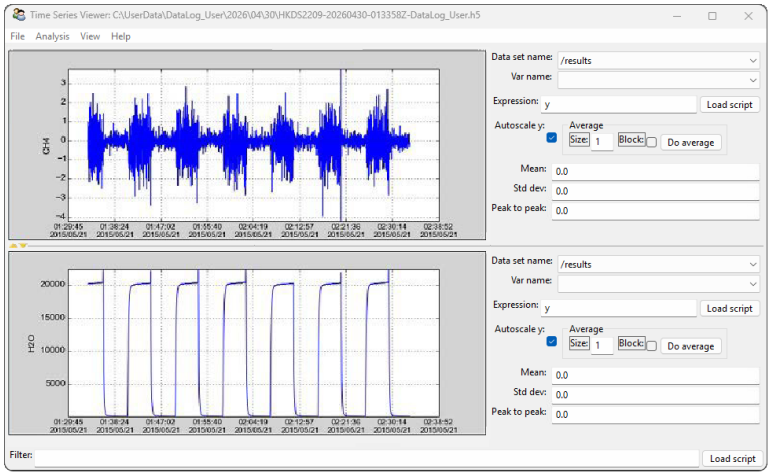


Figure 98 - Time Series Viewer

NOTE

This screenshot is for example only. The species shown on your analyzer may vary.

The next section describes the options available on the Time Series Viewer menu bar. Refer to The Time Series Viewer Canvas on Page 89 for more information on the Time Series Viewer UI features and options.

B.5 Time Series Viewer Menus

The Time Series Viewer includes menu options that allow users to save display settings, export images, and manage visualization configurations. These menus provide quick access to common actions used during data review and analysis.

B.5.1 Time Series Viewer File Menu

The File menu contains options for saving the current visualization setup and capturing images of the data display. These functions are particularly useful for preserving analysis settings and documenting results.

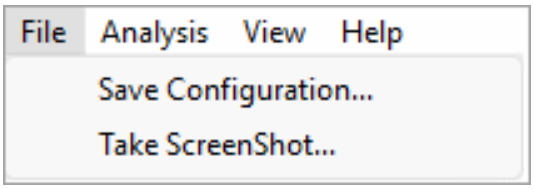


Figure 99 - Time Series Viewer – File Menu

Save Configuration

Select **File > Save Configuration** to open the Feature Capture dialog. This dialog allows you to save the current viewer configuration, including plot properties, applied expressions, filters, axis ranges, and other display settings, into a configuration (.ini) file. This file can be reloaded later to restore the same analysis environment.

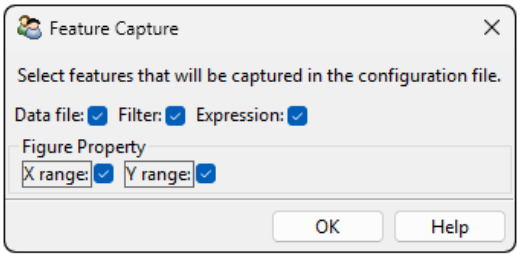


Figure 100 - Time Series Viewer – Feature Capture

NOTE

The options selected in the Feature Capture dialog determine which elements are saved. Any features not selected during capture will not be included when the configuration is reloaded.

Depending on the features captured, loading a configuration file can have different effects. For example:

- If all features are captured, a saved workplace is reproduced.
- If Data file is not captured, saved parameters will be applied to the data file in memory.
- If Expression is not captured, plots will not be transformed.
- If X (Y) range is not captured, figures will be auto-scaled on the x (y) axis.

Take Screenshot

Select File > Take Screenshot to capture the current Time Series Viewer display as an image file. The screenshot is saved in PNG format to a user-specified location and can be used for reporting, documentation, or sharing analysis results.

B.5.2 Time Series Viewer Analysis Menu

Use the Analysis menu to calculate statistics, generate a histogram, and to plot correlations and Allan Standard deviations.

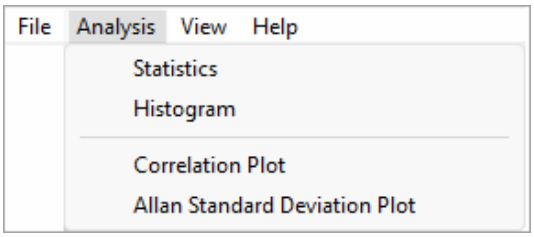


Figure 101 - Time Series Viewer – Analysis Menu

Statistics

Use **Analysis > Statistics** to calculate mean, standard deviation, and peak to peak for all plots in the current window.

Histogram

Use **Analysis > Histogram** to generate a histogram of data as shown in Figure 102 - Histogram Window – CH4 below.

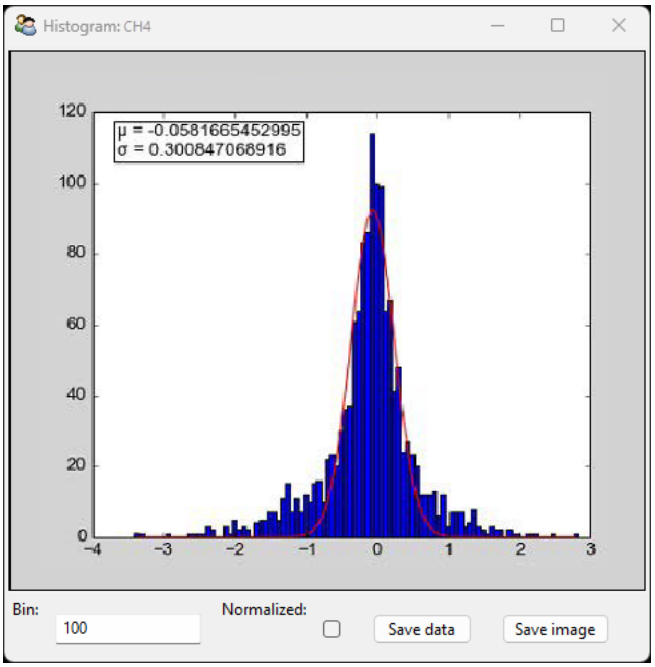


Figure 102 - Histogram Window – CH4

Histogram Window Features

- **Red Line:** A Gaussian function fitted to the histogram. Fitting results of μ and σ are shown in the top-left corner of the plot.
- **Bin:** Specifies the number of intervals that the range of values is divided into.
- **Normalized:** When selected, the sum of the histograms is normalized to 1.

- **Save data:** Saves histogram data to a CSV file.
- **Save image:** Saves the histogram image as a JPEG/PNG/PDF file.

Correlation Plot

Use **Analysis > Correlation Plot** to plot Y-axis data in one frame versus that in the other. This can be used when two or more frames exist in the current Time Series Plot window. See the section, Correlation/XY Plot.

Allan Standard Deviation Plot

Use **Analysis > Allan Standard Deviation Plot** to create an Allan Standard Deviation plot (versus a standard deviation plot) for data in the current window. See Allan Variance Wikipedia page for more information.

B.5.3 Time Series Viewer View Menu

Use the View menu to view X-axis information in date-time, minute, or hour format.

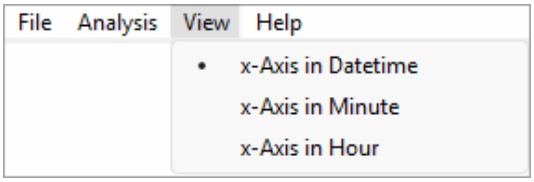


Figure 103 - Time Series Viewer – View Menu

NOTE

When switching from Datetime to Minute or Hour, the X-axis data is subtracted from the earliest point shown in the panel and then converted to the desired unit.

B.5.4 The Time Series Viewer Canvas

The Time Series Viewer canvas (Figure 104 - Time Series Viewer Canvas below) is comprised of interactive graphs and a variety of configuration options.

B.5.5 Mouse Options and Graph Transform

The following mouse actions can be used in the canvas graphs:

- Left click and drag: Zooms into the selected area of the plot.
- Left click and drag with the SHIFT key down: Pans the plot.
- Left click and drag with CTRL key down: Zooms out from the plot.
- Left click and drag with ALT key down: Stretches the plot.
- Right-click: Opens an additional menu. Refer to the Right-click Menu below in the next section.

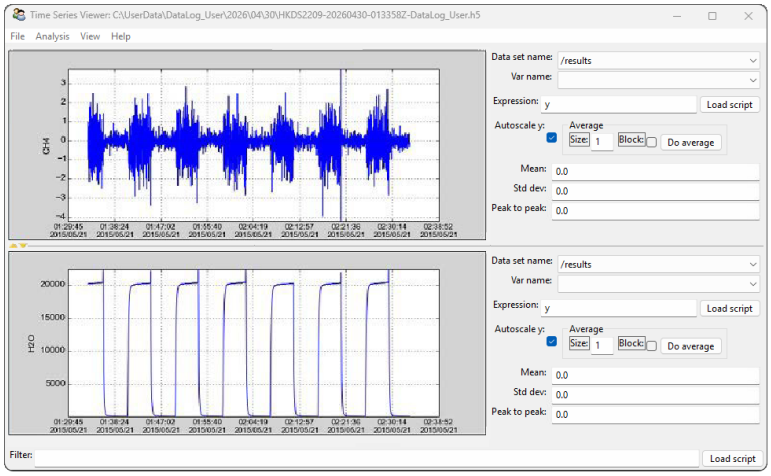


Figure 104 - Time Series Viewer Canvas

NOTE

This screenshot is for example only. The species shown on your analyzer may vary.

B.5.6 Right-click Menu

Right-clicking on the canvas opens a pop-up menu:

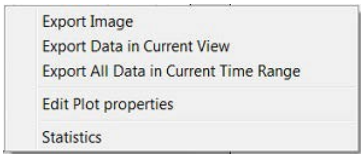


Figure 105 - Canvas Right-click Pop-up Menu

The following menu options include:

- **Export Image:** Exports the current plot as a jpeg, png, or pdf file.
- **Export Data in Current View:** Exports only date/time and the selected variable in the current view to an HDF5 or CSV file.
- **Export All Data in Current Time Range:** Exports all variable columns of the selected dataset in the current time range to an HDF5 file. Refer to Concatenate H5 Files on Page 81 for more information.

- **Edit Plot properties:** Opens the **ImageEditor form** (Figure 106 - Image Editor Form below), where the following options can be specified.

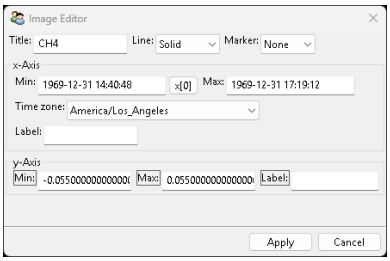


Figure 106 - Image Editor Form

Image Editor Form Options:

- **Title:** Edits the title of the plot.
- **Line:** Specifies the line pattern of the plot. If None is selected, the data points will be plotted without connecting lines.
- **Marker:** Specifies the marker type to indicate data points. If None is selected, data points will not be shown.
- **x-Axis: Min and Max:** Specifies the minimum and maximum of date range for the X-axis.
- **x[0]:** Sets the earliest time of the dataset as the minimum of the X-axis.
- **Time zone:** Sets the time zone for date/time variables. This defaults to the local time zone.
- **Label:** Specify labels for the X-axis and the Y-axis.
- **y-Axis: Min and Max:** Specifies the minimum and maximum of data displayed on the Y-axis.

B.5.7 Dataset Name and Var Name

An HDF5 file can store one or more tables. Each of these tables is called a Dataset. A table can contain one or more columns. Each column is called a variable (Var).

Use the **Dataset name** drop down (Figure 107 - Time Series Viewer Dataset Options) to select the dataset that will be used for this time series graph. Use the **Var name** drop down to select the column in the dataset to use in the graph.

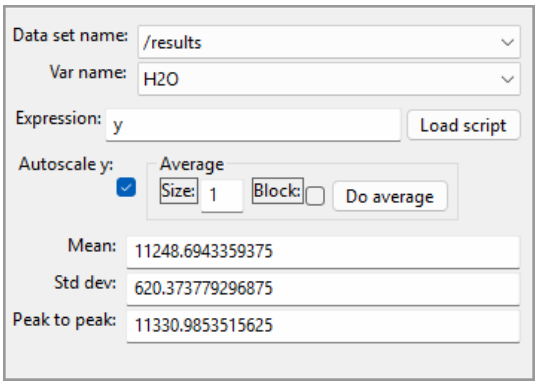


Figure 107 - Time Series Viewer Dataset Options

B.5.8 Autoscale Y

When the **Autoscale Y** option is selected, the Time Series Viewer will autoscale on the Y-axis to make sure that all data within the range of the X axis is displayed. This feature can make it hard to see small signals when large signals blow the Y axis out, so it is often advisable to deselect this checkbox for dynamic or spikey datasets.

B.5.9 Average

If **Block** is selected, a block average is calculated when you click the **Do average** button. Otherwise, a moving average is calculated.

For a block average, **Size** specifies block size in unit of a minute. For a moving average, **Size** specifies subset size in unit of data points.

REMINDER

Averaging is performed after the Filter and Expression are performed.

B.5.10 Mean, Std Dev, and Peak to Peak

The **Mean, Std dev** (Standard deviation) and **Peak to peak** fields (Figure 107 - Time Series Viewer Dataset Options) provide all the statistical information of data in the current view.

B.5.11 Correlation/XY Plot

The Correlation/XY Plot window (Figure 108 - Correlation XY Plot) includes two menu items: File and Analysis. For details about the File menu, see Save Configuration on page on page 182.

REMINDER

The canvas in this plot is interactive. For details about the plot canvas, see B.5.4 The Time Series Viewer Canvas on Page on page 184.

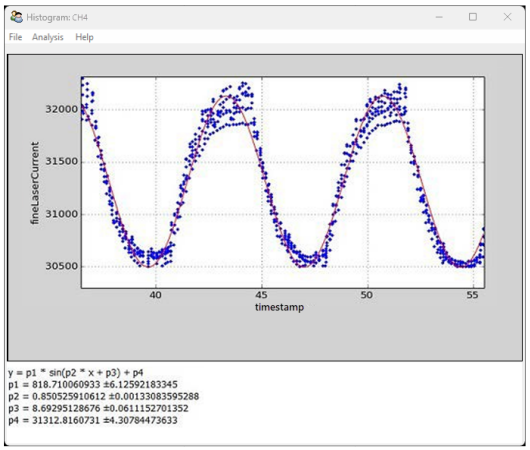


Figure 108 - Correlation XY Plot

B.5.12 Analysis Menu

The Analysis Menu includes three options: **Fitting, Integration**, and **Statistics.**

Fitting allows you to specify one of four fitting methods to include in the Correlation/XY plot:

1. **Linear fit:** Specifies to fit to linear function:

   y = c1x + c0

2. **Quadratic fit:** Specifies to fit to quadratic function:

   y = c2x2 + c1x + c0

3. **Polynomial fit:** Specifies to fit polynomial function of degree n:

   y = Σcnxn

4. **Curve fit:** Specifies to use non-linear least squares to fit an arbitrary function to data.

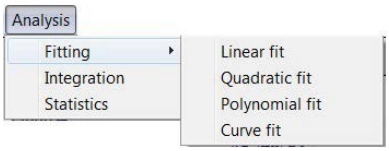


Figure 109 - Analysis Menu

Integration calculates area under the curve using the composite trapezoidal rule.

Statistics calculates mean, standard deviation, and peak to peak for data in the current view.

After applying any of the above Analysis options, the results, statistics, or fitting function with coefficients are displayed in the lower portion of the Correlation Plot window.

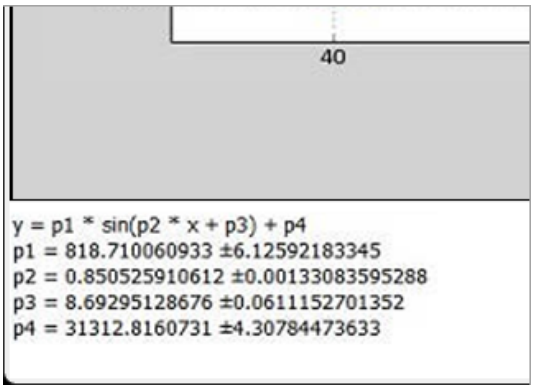


Figure 110 - Results of Quadratic Fitting

C Introduction to Technology

Picarro analyzers use time-based, optical absorption spectroscopy of the target gases to determine concentration. They are based on wavelength-scanned cavity ring-down spectroscopy (WS-CRDS), a technology in which light re-circulates many times through the sample, creating a very long effective path length for the light to interact with the sample, thus, enabling excellent detection sensitivity in a compact and rugged instrument.

The Picarro analyzer is comprised of two modules:

- The analyzer contains the spectrometer, sample chamber, and a computer with a hard drive to store and analyze data. The single analyzer module controls the operation of the system and converts spectroscopic measurements into gas concentration data.
- The external vacuum pump draws the sample gas through the instrument.

The following sections describe the key components and functions of the analyzer system.

C.1 Cavity Ring-Down Spectroscopy (CRDS)

Nearly every small gas-phase molecule (e.g., CO_2, H_2O, H_2S, NH_3) and isotopologue (e.g., $H_2{}^{18}O$, $^{13}CO_2$, $^{15}N^{14}N^{16}O$) uniquely absorb specific wavelengths of near-infrared light. The strength of the light absorption is related to the concentration of a molecule in a sample and the distance that light travels through the sample, called the path length.

Conventional infrared spectrometers are typically only sensitive enough to detect trace gases at levels in the part-per-million. Cavity Ring-Down Spectroscopy (CRDS), on the other hand, is one thousand to one million more times sensitive.

The increased sensitivity of CRDS is due to the design of the sample cavity and the time-based measurement. In the cavity, a series of mirrors reflects the infrared light through the sample, increasing the path length. For a Picarro cavity of only 25 cm in length, the effective path length of the cavity can be over 20 kilometers.

In Picarro analyzers, light from a single-frequency laser enters a cavity where three mirrors reflect the laser light as seen in Figure 111. The light enters through the mirror closest to the laser, bounces off the angled mirror in the lower right corner of the cavity, travels to the hemispherical mirror at the top of the cavity, bounces toward the mirror in the lower left corner of the cavity, and then returns to the first mirror. This motion becomes a continuous traveling light wave, which is represented by the dark orange path in Figure 111.

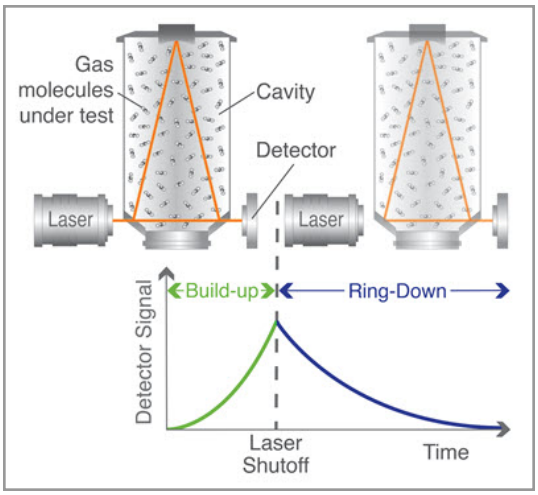


Figure 111 - Schematic of the Picarro CRDS analyzer cavity

When the laser is on, the cavity quickly fills with laser light. A small amount of the laser light is transmitted through the mirror closest to the photodetector, which turns the incident light into a signal that is directly proportional to the light intensity in the cavity.

When the photodetector signal reaches a threshold level (in a few tens of microseconds), the laser is turned off. The light contained within the cavity continues to bounce between the mirrors (about 40,000 times). Since the mirrors have slightly less than 100% reflectivity (99.999%), the light inside the cavity steadily leaks out of the cavity. The intensity of the light reaching the detector decreases, falling exponentially until it reaches zero. This decay, or "ring-down," is measured in real time by the photodetector.

C.2 Relating Ring-Down Time to Absorption Intensity

The time it takes to ring-down is inversely related to the total optical loss in the cavity, including the strength of molecular absorption at a given wavelength of light. For an empty cavity, the time it takes for the intensity to decrease by a given percent is determined solely by the reflectivity of the mirrors. A cavity containing gas that absorbs light will have a shorter ring-down time than an empty cavity. As the light circulates in a cavity with a gas sample, the molecular absorption by the gas results in a decrease of the light intensity.

Determining absorption intensity at a specific wavelength requires comparing the ring-down time of an empty cavity to the ring-down time of a cavity that contains gas. A cavity can be empty if it contains no gas; it will also appear empty if the molecules of the sample inside the cavity do not interact with the specific wavelength of light.

Picarro instruments gather measurements from an “empty” cavity by switching the light to wavelengths that are not absorbed by the target molecules. The analyzer subsequently measures ring-down times at wavelengths that are absorbed by the target gas. The analyzer automatically and continuously compares these two types of ring-down times, and the software uses those comparisons to calculate absorption intensities.

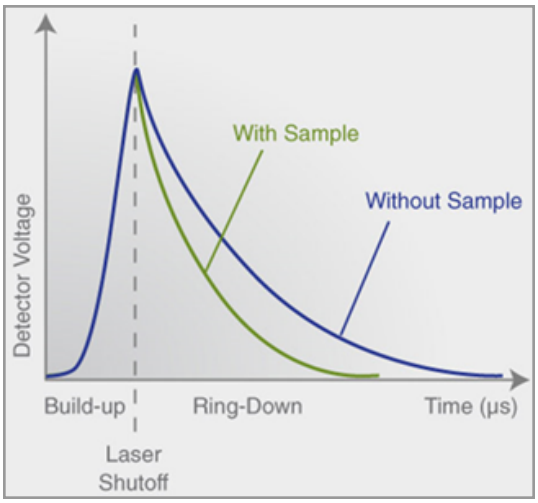


Figure 112 - Light intensity as a function of time in a CRDS system

C.3 Converting Absorption Intensity to Concentration

Plotting the absorbance at each measured wavelength generates an optical spectrum. This spectrum contains absorbance peaks that are unique to each molecule in the sample. The height of a particular absorption peak is proportional to the concentration of a molecule that generated the signal.

The height of the peak is calculated by subtracting the maximal absorbance from the baseline absorbance. Figure 113 shows a plot of ideal optical spectra with a clean, uniform baseline on either side of the absorption peak.

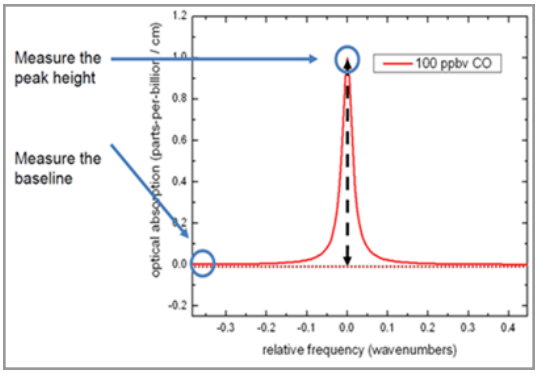


Figure 113 - Absorption Spectral Curve

However, optical spectra often contain several absorption lines, nested closely together. A particular absorption peak may be visible between lines, but the absorption may not return to the baseline before it rises in response to another molecule. Picarro analyzers calculate the baseline underneath a poorly resolved peak by modeling the absorption peaks from other surrounding molecules and subtracting contributions from neighboring peaks to the absorption intensity.

C.4 Spectral Precision and High Sensitivity Measurements

Picarro analyzers contain two features that provide high spectral precision:

- Proprietary wavelength monitor (WLM) that measures the absolute laser wavelength to a precision that is a few orders of magnitude narrower than the spectral linewidth: Picarro's patented WLM measures absolute laser wavelength to a precision more than 1,000 times narrower than the observed Doppler-broadened linewidth for small gas-phase molecules. The instruments lock the laser to the WLM, and then the monitor tunes to wavelengths known to be maximally and minimally absorbed by the target molecule. The result is closely clustered absorption intensities, measured at wavelengths just before peak absorption, at peak absorption, and just after peak absorption, as the absorbance returns to the baseline.
- Precise temperature and pressure control in the sample cavity: Accurate absorption measurements at precisely known wavelengths account for little unless the temperature and pressure of the CRDS measurement cavity are known. The observed line intensity and shape depend on the temperature and pressure inside the sample cavity. Small temperature and pressure instabilities can result in large concentration errors due to fluctuating peak heights and baselines. To completely minimize instrument measurement drift, temperature and pressure must be actively stabilized to constant values.

For precise temperature control, the sample cavity is surrounded by layers of thermally insulating material to provide a high degree of passive thermal stability. The cavity is further actively stabilized by means of a solid-state heating system locked to the output of a thermal sensor. This enables the temperature of the cavity to be within 20 mK of the set temperature.

For precise pressure control, the cavity pressure is monitored using a high-linearity pressure transducer. The system computer uses this pressure data in a feedback loop to control proportional valves that adjust the inlet and outlet gas flow of the cavity.

D 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: Picarro disclaims all other warranties, either express or implied, including 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.

Picarro Document Library
Picarro Community (Forums)
Picarro Software Downloads
Picarro Literature (Scientific Resources)
Picarro Web Store

Contact Picarro for questions regarding specific applications and additional information.

Picarro Customer Support (USA)		Picarro Customer Support (International)	
Email:	support@picarro.com	Email:	support@picarro.com
Phone:	+1 408 962 3991	Phone:	+31 85 888 1650