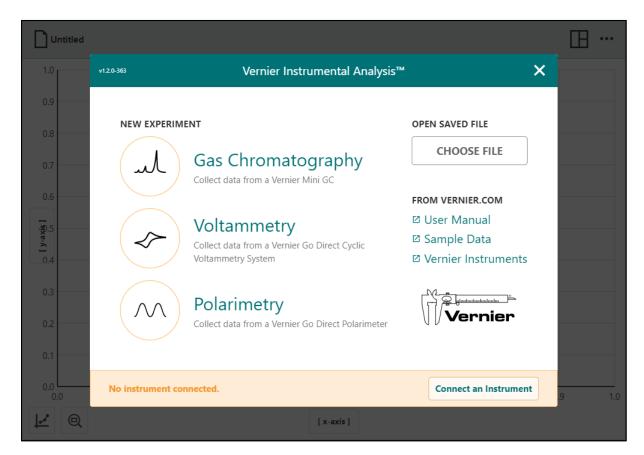
# Vernier Instrumental Analysis™ User Manual



Version 1.2.0 January 2021

#### **ABOUT THIS GUIDE**

The Vernier Instrumental Analysis User Manual is an extended guide detailing the features of the Instrumental Analysis app. This guide can be used with any platform-specific version including the versions for Windows® and macOS® computers, Chromebook $^{TM}$  notebooks, and iOS, iPadOS®, and Android $^{TM}$  devices.

This is the initial release of this document. It reflects features available in Instrumental Analysis version 1.2.0.

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### **CHAPTER 1—GETTING STARTED**

### I. Downloading Instrumental Analysis

Download Instrumental Analysis from the Vernier website or the appropriate web store.

- Windows and macOS computers—download from the Vernier website
- Chrome<sup>TM</sup> computing devices—download from the Chrome Web Store
- iOS, iPadOS devices—download from the App Store
- Android devices—download from Google Play

For up-to-date system requirements, visit www.vernier.com/instrumental-analysis

### **Licensing Information**

Vernier Instrumental Analysis is free and can be installed on an unlimited number of computers.

Instrumental Analysis is a free app for Chrome, iOS, iPadOS, and Android distributed through the respective web stores. Terms and licensing are thus determined entirely by these stores.

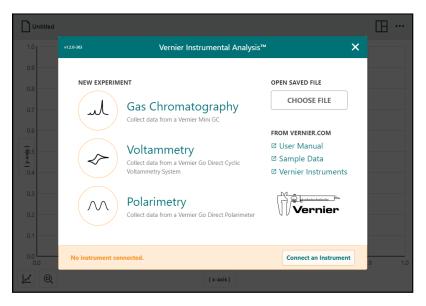
### Privacy Statement

#### COPPA, SOPIPA, and FERPA Compliance

Instrumental Analysis complies with federal regulations pertaining to student privacy and safety in the following ways:

- Instrumental Analysis does not collect, request, share, or store any personal information from students or instructors.
- Instrumental Analysis does not display advertisements in the app.

### II. Launching Instrumental Analysis for the First Time



When Instrumental Analysis is launched, the New Experiment box displays the experiment options available in the Instrumental Analysis app. The options are specific to the instrument you are using and provide access to instrument configuration, data-collection settings, and data displays optimized for that instrument. From here, you can also open saved experiments, access online tutorials, and view sample data.

**TIP!** If a supported instrument is connected via USB when Instrumental Analysis is launched, only the experiment option associated with the connected instrument will be active.



### **Gas Chromatography**

In gas chromatography, you are investigating or utilizing the properties of a substance related to how they interact with a chemically-coated column. This interaction causes each compound traveling through the column to elute at a different time, known as the retention time of the compound. The comparison of retention times is what gives a gas chromatograph its analytical usefulness.

The Gas Chromatography experiment option is used when collecting data with a Vernier Mini Gas Chromatograph. Supported instruments include the following:

- Go Direct<sup>®</sup> Mini GC<sup>TM</sup>
- Vernier Mini GC<sup>TM</sup> Plus
- Vernier Mini GC<sup>TM</sup>



### ✓ Voltammetry

Voltammetry experiments investigate the half-cell reactivity of an analyte. Information about an analyte is obtained by measuring the current as the potential is varied. The analytical data for a voltametric experiment comes in the form of a voltammogram, which plots the current produced by the analyte versus the potential of the working electrode. The voltammetry modes supported in Instrumental Analysis are Cyclic Voltammetry, Open-Circuit Potentiometry, and Bulk Electrolysis.

The Voltammetry experiment option is used when collecting data with the following instrument:

• Go Direct® Cyclic Voltammetry System



### **Polarimetry**

Polarimetry is a technique for measuring the chiral properties of optically active samples without chemically modifying or destroying the sample. A polarimeter is used to detect changes in rotation of plane polarized light passing through an optically active compound. The amount of optical rotation is determined by the molecular structure and concentration of chiral molecules in the test sample.

The Polarimetry experiment option is used when collecting data with the following instrument:

• Go Direct® Polarimeter

### **Other Options**

#### **Open Saved Files**

Click or tap \_\_\_\_\_ to open saved Instrumental Analysis files (.imbl) or comma separated value (.csv) files.

#### Sample Data

Choose Sample Data to access sample data files for Instrumental Analysis. Sample data files include the following:

- Separation of Toluene and Cyclohexane
- Detection of Chemical Isomers with Gas Chromatography
- Distillation of Banana Oil
- Exploring RuHex and Sweep Rate in Quantitative Cyclic Voltammetry
- Measuring Acetaminophen Using Cyclic Voltammetry
- Food Chemistry: Inversion Reaction of Sucrose and Invertase Enzyme
- Exploring Natural Products with Polarimetry

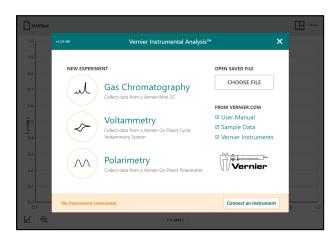
### III. Connecting an Instrument using Bluetooth Wireless Technology

The Go Direct version of instruments supported by Instrumental Analysis can be connected using Bluetooth® wireless technology. The wireless connection is one-to-one meaning that only one device (computer, Chromebook, smartphone, or tablet) can connect to that instrument at a time. *TIP!* The following directions describe connecting the instrument prior to selecting the experiment type. You can also connect to an instrument after selecting the experiment type as described in the instrument user manuals.

1. Launch the Instrumental Analysis app.

TIP! If Instrumental Analysis is already running, click or tap the file menu icon,

Untitled, and choose New Experiment. You may be prompted to save or discard the current file.



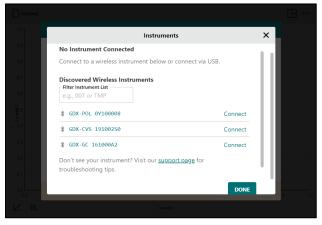
2. If required, connect your instrument to AC power. Turn the instrument on (the Bluetooth LED will flash red). Click or tap Connect an Instrument to access the Instruments connection screen.

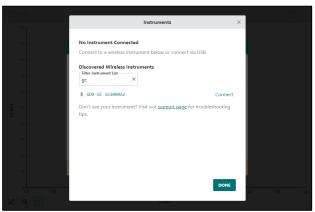
TIP! If the Bluetooth LED is flashing green, the instrument is already connected to a device. To force the instrument to disconnect, turn the unit off and then power the unit back on to continue.

3. Locate your instrument in the Discovered Wireless Devices list. The serial number, located on each instrument, represents the instrument name.

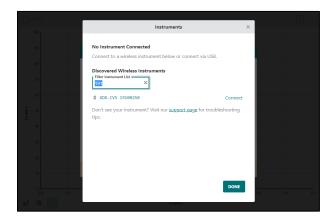
### **Using the Instrument List Filter**

You can use this filter to help locate your instrument in the list. Enter part of the instrument order code to look for all instruments of a certain type (e.g., enter "gc" to find all gas chromatographs in the list).



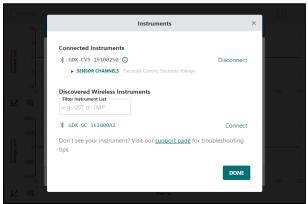


You can also enter part of the instument's serial number to show only instruments with that particular character or characters (e.g., type "19" to find all of the instruments with 19 in their serial number).



4. Click or tap the Connect button next to the instrument to which you want to connect. Note that the Bluetooth LED on the connected instrument will now flash green.

TIP! If you accidently connect to the wrong instrument, click or tap Disconnect, then select the correct instrument to continue. If someone accidently connects to your instrument, power off your unit, then power it back on to continue.

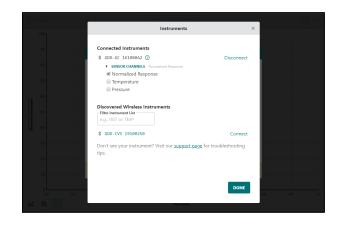


### **Setting Up Sensor Channels**

Vernier Go Direct instruments utilize multiple sensors when taking measurements. The outputs from these sensor channels are not all displayed by default but can be manually set up to display if desired. In most cases, the default configuration will display the necessary data.

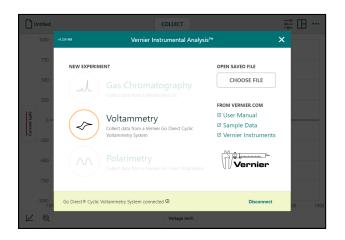
5. After connection to your instrument, click or tap Sensor Channels to modify the default instrument configuration. Modify the sensor channel configuration as needed for your experiment.

TIP! In some cases, deactivating the default channels can prevent Instrumental Analysis from working as designed.



6. Once your instrument is configured as desired, click or tap DONE to exit the Instruments dialog, then select the appropriate experiment option to continue with your experiment.

**TIP!** Click or tap ① to access the instrument details, such as battery level, for the connected instrument.



### IV. Connecting an Instrument using USB

All Vernier Instruments that work with Instrumental Analysis can be connected to a computer or Chromebook using a USB connection.

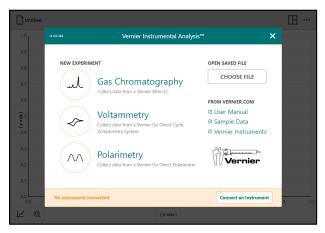
**TIP!** The following directions describe connecting the instrument prior to selecting the experiment type. You can also connect to the appropriate instrument after selecting the experiment type as described in the instrument user manuals.

1. Launch the Instrumental Analysis app on your computer or Chromebook.

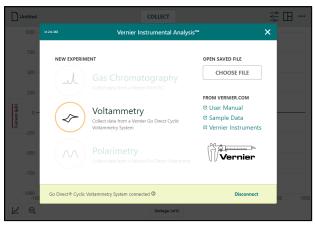
TIP! If Instrumental Analysis is already running, click or tap the file menu icon,

untitled, and choose New Experiment.

You may be prompted to save or discard the current file.



- 2. If required, connect your instrument to AC power.
- 3. Connect the included USB cable to the instrument and then to the computer or Chromebook.
- 4. Turn the instrument on, if necessary. The instrument will automatically be identified.
- 5. Select the appropriate experiment option to continue with your experiment.



### Setting up Sensor Channels on a Go Direct Instrument Connected via USB

Vernier Go Direct instruments utilize multiple sensors when taking measurements. The outputs from these sensor channels are not all displayed by default but can be manually set up to display if desired. In most cases, the default configuration will display the data you need.

1. Launch the Instrumental Analysis app on your computer or Chromebook.

TIP! If Instrumental Analysis is already running, click or tap the file menu icon,

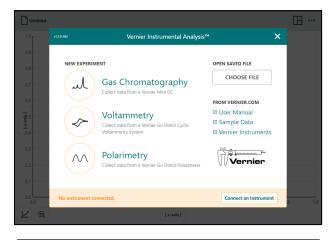
untitled, and choose New Experiment.

You may be prompted to save or discard the current file.



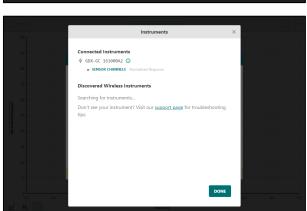


- 3. If required, connect your instrument to AC power.
- 4. Connect the included USB cable to the instrument and then to the computer or Chromebook.
- 5. Turn the instrument on, if necessary. The instrument will automatically be identified.



No Instrument Connected

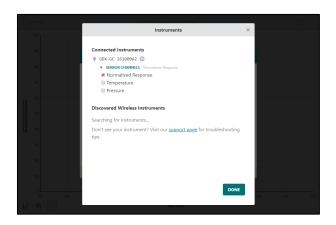
Discovered Wireless Instruments

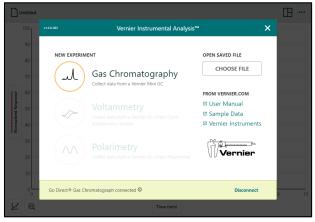


6. Click or tap Sensor Channels to modify the default instrument configuration. Modify the sensor channel configuration as needed for your experiment.

TIP! In some cases, deactivating the default channels can prevent Instrumental Analysis from working as designed.

7. Once the instrument is configured as desired, click or tap DONE to exit the Instruments dialog, then select the appropriate experiment option to continue with your experiment.

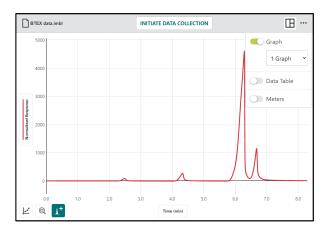




## V. Adjusting the Display

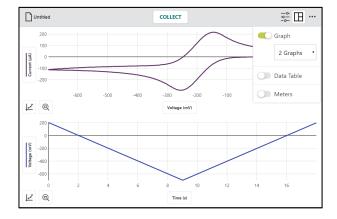
Instrumental Analysis automatically displays a single-graph view optimized for the selected experiment type. You can use this recommended view or modify the view using the options provided.

Click or tap the view options button,  $\square$ , then modify the view as desired. You can use the graph, table, and meter options individually or together as needed.



### **Multiple Graphs**

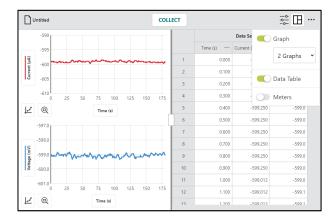
For some experiments, it may be desirable to show more than one graph. You can show up to three graphs.



#### **Data Table**

You can view the data table by itself or alongside a graph.

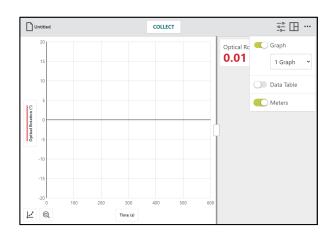
**TIP!** When displaying multiple elements, you can adjust the split by dragging the handles located on the separating lines.



#### Meter

You can view a live reading of the connected instrument by itself or alongside a graph or data table.

**TIP!** When displaying multiple elements, you can adjust the split by dragging the handles located on the separating lines.

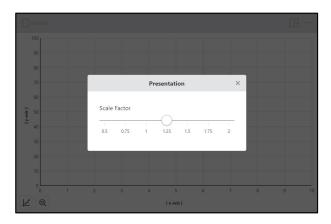


### **Modifying the Font-Size with Scale Factor**

You can modify the font size used in the app. This is particularly useful when presenting the app with a projector or viewing the app on a device with a high-resolution screen.

Click or tap ••• and choose Presentation to modify the font-size scale factor used in Instrumental Analysis.

**TIP!** Reduce the Scale Factor when viewing multiple graphs to see more detail on each graph.



## CHAPTER 2—(J) GAS CHROMATOGRAPHY

In gas chromatography, you are investigating or utilizing the properties of a substance related to how they interact with a chemically-coated column. This interaction causes each compound traveling through the column to elute at a different time, known as the retention time of the compound. The comparison of retention times is what gives a gas chromatograph its analytical usefulness.

The Gas Chromatography experiment option is used when collecting data from a Vernier Mini Gas Chromatograph. Supported instruments include the following:

- Go Direct Mini GC
- Vernier Mini GC Plus
- Vernier Mini GC

### I. Connecting your Mini GC

Launch Instrumental Analysis to view the New Experiment box.

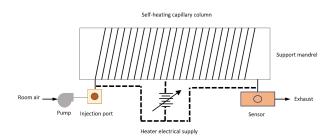
TIP! If Instrumental Analysis is already running, click or tap the file menu icon, Untitled, and choose New Experiment. You may be prompted to save or discard the current file.

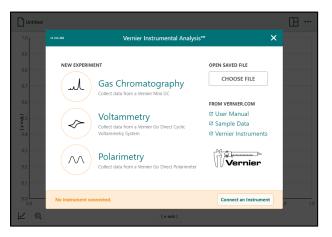
Connect your Vernier Mini GC to AC power and turn the instrument on.

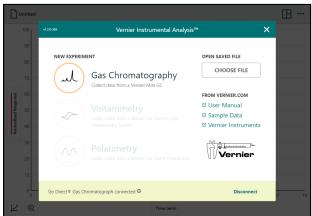
Connect your Gas Chromatograph to your device. For detailed instructions see the following Chapter 1 sections:

- Connecting Instruments using Bluetooth Wireless Technology
- Connecting Instruments using USB

**TIP!** If you are using a Go Direct Mini GC, vou may want to enable the Temperature sensor channel to compare the temperature of the column to the chromatogram.



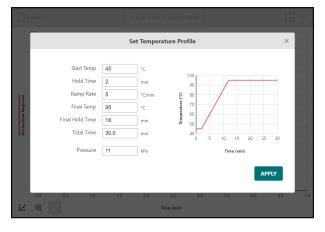




Select Gas Chromatography to display the default Temperature Profile settings. The default values depend on the Mini GC you are using and are designed to give you a chromatogram with many compounds you might inject. The different default values reflect the changes in the instrument design between versions.

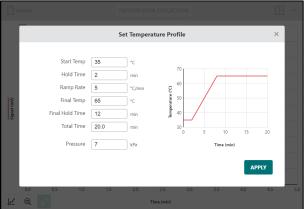
#### Go Direct Mini GC

The values shown to the right are for the Go Direct Mini GC.



#### Vernier Mini GC

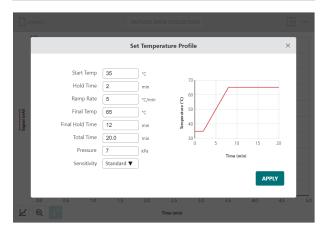
If you are using the Vernier Mini GC, the default values are slightly different as shown here.



#### Vernier Mini GC Plus

If you are using the Vernier Mini GC Plus, the default values are as shown here.

For the Vernier Mini GC Plus, there is also a Sensitivity field with Standard as the default.



### II. Adjusting the Temperature Profile

The default temperature and pressure settings can be used to detect a wide range of chemicals and are a good place to start. The values can be adjusted as needed for your specific experiment.

The graphic representation of the profile updates automatically as you modify the settings.

TIP! If the profile is not shown, click or tap INITIATE DATA COLLECTION to access it again.

#### **Start Temp**

This is the temperature, in °C, at which the column starts.

• Minimum temperature: 30°C

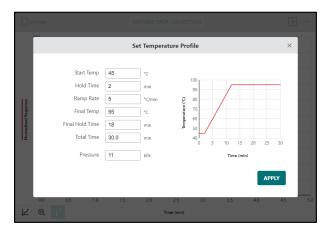
Maximum temperature: 160°C
 (120°C for the Vernier Mini GC)

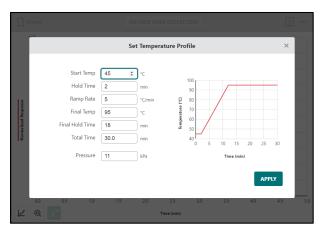
#### **Hold Time**

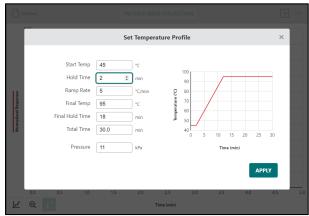
The time, in minutes, in which the column stays at the Start Temp before the column begins to warm.

• Minimum hold time: 0 minutes

• Maximum hold time: 450 minutes



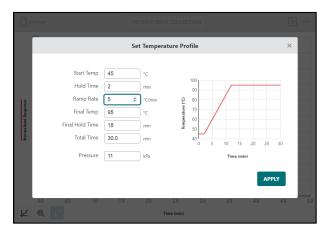




#### Ramp Rate

This is the rate, in °C/min, at which the column warms. The value must be greater than zero.

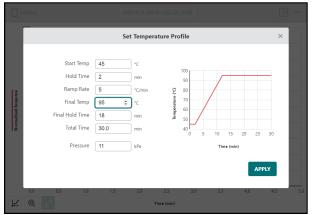
• Maximum ramp rate: 10°C/min



#### **Final Temp**

This is the temperature the column warms to during data collection. The Final Temp must be equal to or greater than the Start Temp.

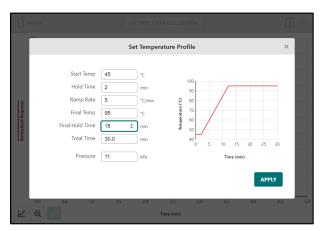
- Minimum temperature: ≥ Start Temp
- Maximum temperature: 160°C
   (120°C for the Vernier Mini GC)



#### **Final Hold Time**

The time, in minutes, in which the column stays at the final temp before data collection ends.

- Minimum hold time: 0 minutes
- Maximum hold time: 450 minutes



#### **Total Time**

This value updates automatically as you adjust the other parameters. You can change this value directly if desired. Doing so also changes the Final Hold Time to compensate for the change.

The Total Time cannot exceed 450 minutes and cannot be set such that the Final Hold Time is less than zero.

#### **Pressure**

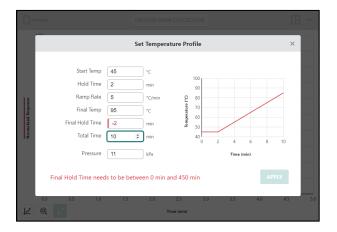
This is the operating pressure, in kPa above ambient pressure, the GC maintains during data collection.

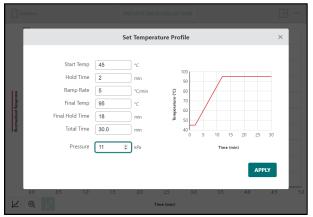
Minimum Pressure: 1 kPaMaximum Pressure: 21 kPa

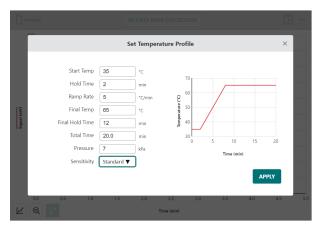
**TIP!** If your instrument is having trouble reaching high pressures, try changing the septum.

#### Sensitivity—Mini GC Plus Only

This is the sensitivity of the detector. Standard is appropriate for highly polar compounds. If you would like to increase your signal or investigate less polar compounds (for example, halogenated hydrocarbons) use the High Sensitivity setting.

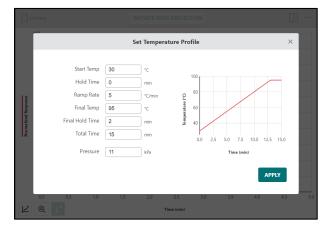






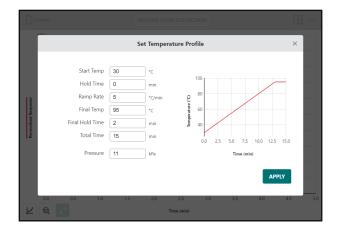
Once you have entered your changes, you are ready to send the profile to the GC and start data collection.

TIP! Changes made to this dialog are not saved when the dialog is closed. If you need to reset the default values, close the dialog, then click or tap INITIATE DATA COLLECTION .



### III. Initiating Warm Up

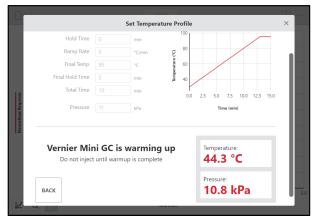
Once you have set the temperature and pressure profile as desired, you are ready to collect data.



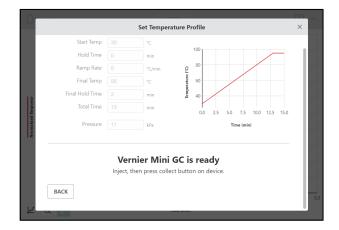
Click or tap APPLY to transfer the profile to your GC, which starts the warmup process.

While the GC is warming up, the current temperature and pressure are displayed in the dialog.

TIP! You can click to tap to cancel the warmup and modify your temperature and pressure profile.



The dialog displays a warmup is complete message when the GC is ready for injection.



### IV. Preparing for Data Collection

### **Preparing the Syringe**

While the Mini GC is equilibrating, clean and flush the syringe.

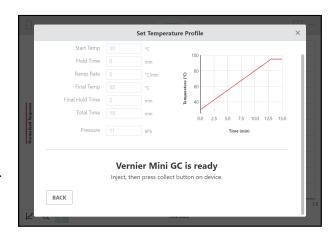
- 1. Depress the plunger fully.
- 2. Submerge the tip of the syringe needle into the vial of acetone or n-hexane.
- 3. Pull back the plunger to fill the barrel about 1/3 full of acetone or n-hexane. Examine the barrel of the syringe and estimate the amount of liquid in the barrel.
- 4. Expel the liquid onto a lint-free tissue or a paper towel.
- 5. Repeat steps 1–4 at least two times, until you are comfortable pulling up a liquid into the syringe and measuring the volume in the syringe barrel. Use a lint-free tissue or a paper towel to carefully pat around the tip of the syringe needle.

**Important:** The glass syringe is fragile and can be easily damaged.

- Be careful not to bend the needle or bend the plunger. If the plunger is accidentally pulled out of the glass barrel, reinserting it is extremely difficult, sometimes impossible.
- Never pull the plunger back more than 50% of its total volume.
- Be careful not to bend the plunger as you press it down.
- Do not remove the plastic spacer on the needle.

When the Mini GC is ready for data collection, you see the following:

- The dialog displays a warmup is complete message.
- The indicator LED on the Mini GC turns green.
- The status message on the Mini GC states the Mini GC is ready for injection.



### **Preparing the Sample**

Follow the process in Section IV to clean and flush the syringe using the sample to be injected into the Mini GC.

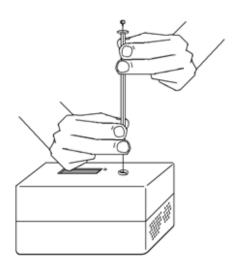
Collect about 0.2 to 0.4 µL of your sample in your syringe.

### **Inserting the Syringe**

Insert the needle of the syringe into the injection port of the Mini GC. Be sure to hold the syringe with one hand and steady the needle with your other hand.

### Do not move the plunger yet.

TIP! Supporting the needle guard and the lower part of the needle with two fingers, as shown, can prevent the possible bending of the needle. Insert the needle into the injection port until the needle stop is fully seated. If the needle sticks, rotate it slightly while inserting.



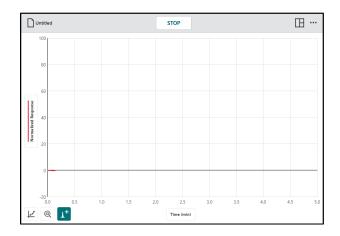
### V. Collecting Data

### Go Direct Mini GC Only

Depress the syringe plunger; be careful not to bend the plunger as you press it down.

Immediately following, press the white Collect button on the Go Direct Mini GC to begin data collection.

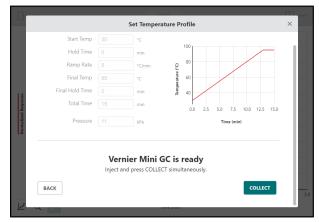
Pull the needle out of the injection port immediately. As you withdraw the syringe needle, lift straight up to avoid bending the needle.



### Vernier Mini GC and Mini GC Plus Only

When using a Vernier Mini GC or Vernier Mini GC Plus, a collect button, collect, is shown in the dialog.

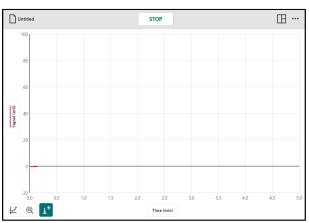
You will need to click or tap **COLLECT** at the same time you inject your sample.



Simultaneously depress the syringe plunger and click or tap COLLECT.

Be careful not to bend the plunger as you press it down.

Pull the needle out of the injection port immediately. As you withdraw the syringe needle, lift straight up to avoid bending the needle.



#### All Mini GC Models

While the data collection proceeds, clean the syringe as described in Section IV. It may take more than three flushes to feel the syringe plunger move smoothly again, which is your indicator that the syringe and needle are both suitably clean.

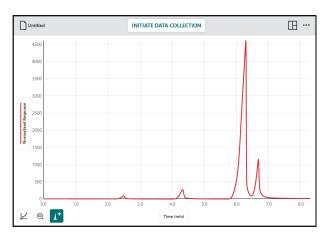
Data collection will automatically stop after the allotted time.

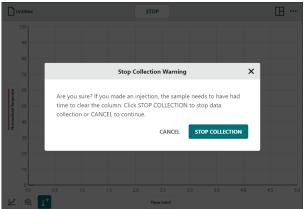
If needed, click or tap to scale graph to fit your data.

You can click or tap stop to end collection early if you are satisfied that all analytes have eluted completely.

Stopping data collection early will generate a warning. To confirm, click or tap

STOP COLLECTION





### VI. Analyzing Your Data

You can use the chromatogram to determine the retention time associated with the peaks of the eluded samples.

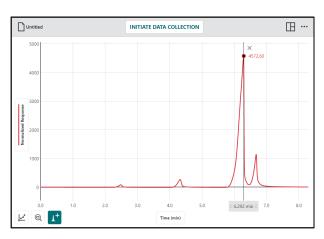
#### **Examine Tool**

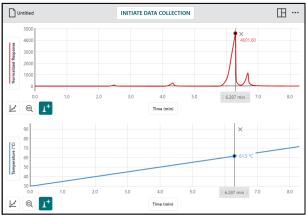
Click or tap the graph to examine a point of interest. The coordinates of the point are shown. Click or tap a different point or drag the examine line to further examine your data.

To remove the examine line, click or tap the close button, ×, displayed next to the line.

If you had collected temperature data using a Go Direct Mini GC, you can use the examine tool to determine the temperature of the column of a specific peak.

For more information, see Using the Go Direct Mini GC Sensor Channels.

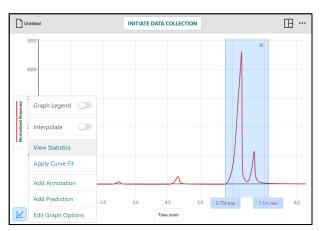




#### **Statistics Tool**

If desired, select a region of data. If a region of data is not selected, the statistics tool uses all data in the calculation.

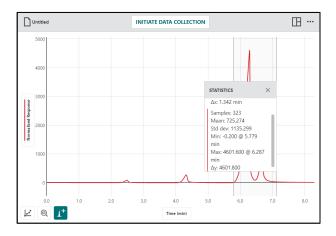
Click or tap and select View Statistics.



Statistics for all plotted columns on the graph are calculated and displayed in the Statistics details box.

The time associated with the Maximum (Max) is the data point of interest as it corresponds to the retention time of the eluded sample.

To dismiss the Statistics box, click or tap the close button, ×.



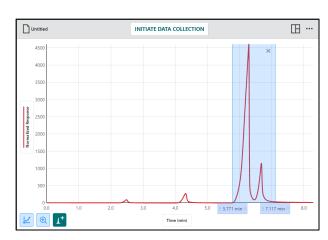
### **Peak Integration**

Integration of chromatographic peaks, which includes determination of height, area, and retention time, is an important step in data analysis of chromatograms. The information is used for identification of unknown substances, construction of calibration curves, and calculation of unknown concentrations.

Peak Integration differs from the Integral tool in that it does not use the x-axis as the baseline. Instead, the integral for Peak Integration is evaluated using the minimum y-values to the left and right of a selected peak.

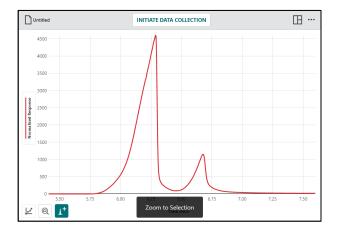
While not required, it can be easier to isolate peaks by zooming in on that section of the data.

Click-and-drag or touch-and-drag to select the peak or peaks you want to analyze.

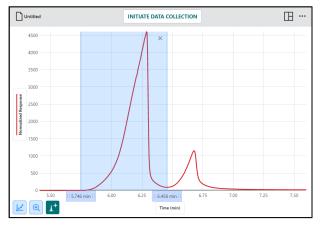


Click or tap (to zoom to the selection.

TIP! Click or tap or double click or double tap the graph to zoom to fit all data again.

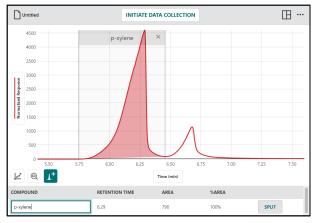


Click-and-drag or touch-and-drag to select the peak you want to analyze.

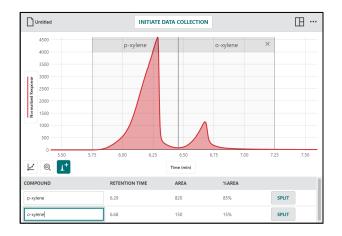


Click or tap 1<sup>+</sup>. Enter the compound information in the table below the graph.

TIP! You can drag the boundaries of the region to refine the area.



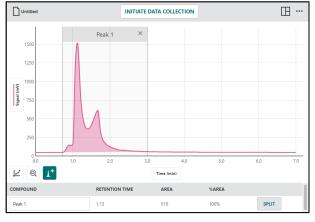
Repeat as needed for other peaks in your sample.

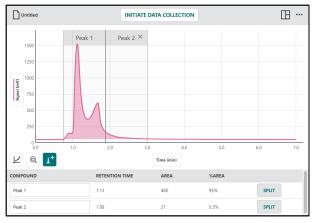


### **Split Peaks**

Some data may have peaks that overlap. To analyze overlapping peaks, drag across the graph to select the region containing both peaks, then tap 1<sup>+</sup>.

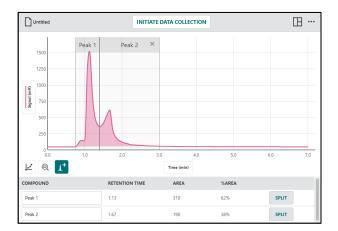
Click or tap split to divide the region into two equal-width sections.





Drag the separating line to the appropriate separation point for your data.

Label the two regions as desired.



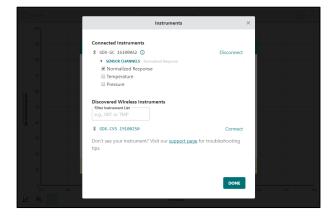
For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

### VII. Using the Go Direct Mini GC Sensor Channels

In addition to the normalized response data, the Go Direct Mini GC also has Temperature and Pressure sensors that can report data during data collection.

To use these sensors, they need to be activated when connecting your Go Direct Mini GC. For detailed instruction on how to set up sensor channels, see the following Chapter 1 sections:

- Connecting an Instrument using Bluetooth Wireless Technology
- Setting up Sensor Channels on a Go Direct Instrument Connected via USB



### **Displaying the Temperature and Pressure Data**

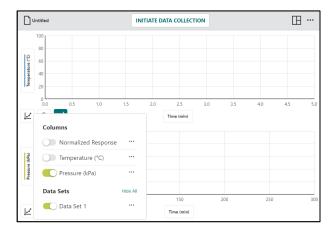
You can set up your graphs to display the Pressure and Temperature data during data collection.

**TIP!** You can change the graph data after data collection if desired, but the sensor channels must be active prior to data collection.

Click or tap  $\times$  to close the Temperature Profile Settings.

Click or tap View Options, , and select to show 2 Graphs.

Click or tap Normalized Response, and select the data you wish to plot. You can change one or both graphs.

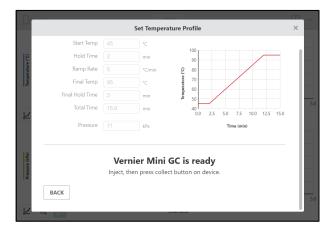


If necessary, click or tap and select Edit Graph Options to modify x-axis range so both graphs match.



Click or tap INITIATE DATA COLLECTION and set up your profile as described in Section I.

Send the profile to the Mini GC and collect data as described in Sections III–VI.

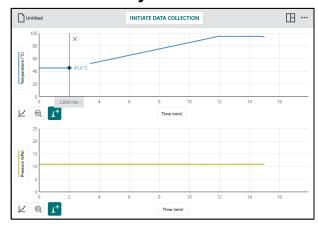


### Analyzing the Pressure and Temperature Data to Verify the Profile

#### **Examine Tool**

Click or tap the Temperature data to verify the temperature values and hold times are applied correctly.

**TIP!** If graphing the Chromatogram instead of the Pressure, examine is very helpful to determine how the chromatogram changes with the Temperature.

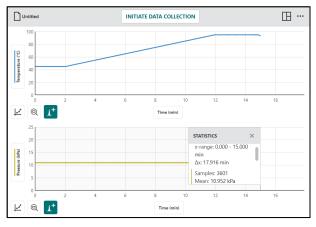


#### **Statistics**

Using the Pressure data, click or tap and select View Statistics. **NOTE:** Since no region is selected, all data are used in the statistics calculation.

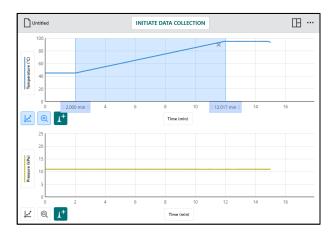
The mean of the pressure data should match the pressure value you set in the profile.

TIP! You can also select the constant temperature regions of the temperature graph to calculate the average temperature of those sections.

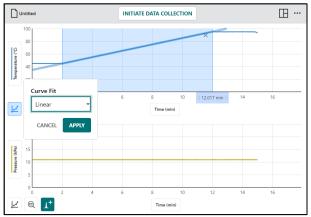


#### **Curve Fit**

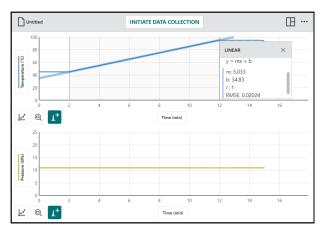
Select the region of the temperature data where the GC is warming.



Click or tap and select Apply Curve Fit, then click or tap apply to select a linear fit.



The slope of the curve fit should match the Ramp Rate of the profile.



For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

## CHAPTER 3— VOLTAMMETRY

Voltammetry experiments investigate the half-cell reactivity of an analyte. Information about an analyte is obtained by measuring the current as the potential is varied. The analytical data for a voltametric experiment comes in the form of a voltammogram, which plots the current produced by the analyte versus the potential of the working electrode. The voltammetry modes supported in Instrumental Analysis are Cyclic Voltammetry, Open-Circuit Potentiometry, and Bulk Electrolysis.

The Voltammetry experiment option is used when collecting data with the following instrument:

• Go Direct Cyclic Voltammetry System

### I. Connecting your Go Direct Cyclic Voltammetry System (CVS)

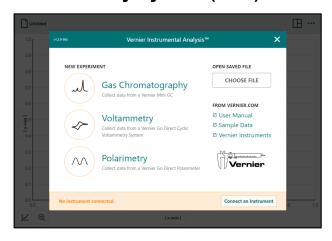
Launch Instrumental Analysis to view the New Experiment box.

TIP! If Instrumental Analysis is already running, click or tap the file menu icon,

untitled, and choose New Experiment. You may be prompted to save or discard the current file.

Insert a screen-printed electrode (SPE) into the connector on the Go Direct Cyclic Voltammetry System as shown. Avoid touching the black electrode part of the SPE.

Fill the scintillation vial about halfway full (~10 mL) with your sample. Insert the scintillation vial into the clip on the stand. Carefully guide the Go Direct Cyclic Voltammetry System with the SPE attached downward into the vial and snap the instrument into place.





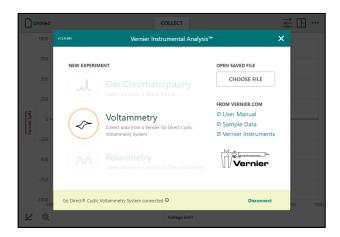


Press the power button to turn on the Go Direct Cyclic Voltammetry System.

Connect your instrument to your device. For detailed instructions see the following Chapter 1 sections:

- Connecting an Instrument using Bluetooth Wireless Technology
- Connecting an Instrument using USB

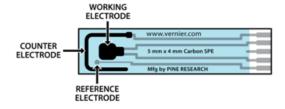
Select Voltammetry to continue with your experiment.





### **II. Using Cyclic Voltammetry Mode**

In the Cyclic Voltammetry mode, the electrode potential ramps linearly with time following a preset waveform, often through the electroactive species' standard potential, which allows for the investigation of the resulting electrochemical species generated at the electrode surface. The rate of voltage changes over time during each of the segments in the waveform is known as the experiment's sweep rate. The potential is measured between the working electrode and the reference electrode on the screen-printed electrode (SPE), while the current is measured between the working electrode and the counter electrode on the SPE.



### Adjusting the CV Profile

From the Voltametric Settings, ensure the Cyclic Voltammetry (CV) mode is selected.

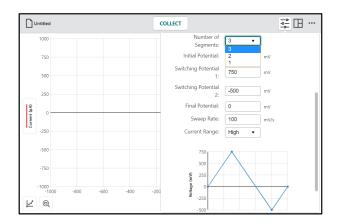
Change the CV Profile values as required for the analyte you are studying.



#### **Number of Segments**

This is the number of segments in the potentiostat's waveform and determines the number of potentials you must set.

- One segment is a linear sweep voltammetry with only an initial and final potential setting.
- A two segment CV has an initial and final potential, along with one switching potential.
- A three segment CV has an initial and final potential, along with two switching potentials.



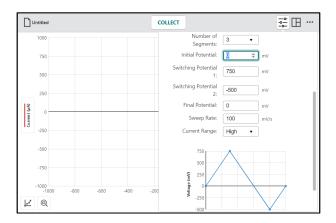
#### **Potentials**

Next, set each potential to dictate the potentiostat's waveform, including the Initial and Final Potentials, along with applicable Switching Potentials. To illustrate the importance of these settings, consider this example of a 3-segment CV.

#### Initial Potential

The Initial Potential is the potential at which the voltammogram will start. In this example, the Initial Potential is set to 0 mV.

**TIP!** Profile values are applied as they are entered.

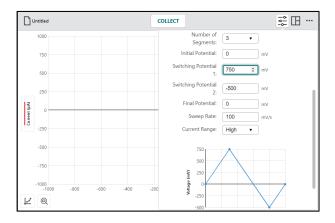


#### • Switching Potential 1

From here, the potential must sweep in either a negative or positive direction from the initial potential; therefore, in this case, Switching Potential 1 cannot be 0 mV.

Setting Switching Potential 1 to +750 mV means the CVS will sweep in a positive direction from 0 mV to +750 mV.

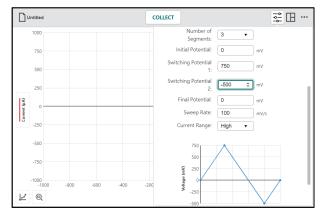
**TIP!** You cannot sweep more than 2000 mV in one direction and it is not recommended to sweep more than 1600 mV in one direction.



### Switching Potential 2

From Switching Potential 1, the CVS must sweep in a positive or negative direction to Switching Potential 2.

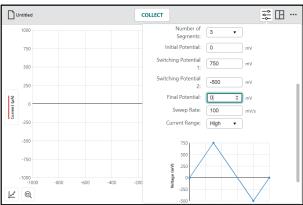
Setting Switching Potential 2 to -500 mV means the CVS will now sweep from +750 mV to -500 mV.



#### Final Potential

The Final Potential is where the CVS concludes the experiment acquisition.

Setting the Final Potential of 0 mV means the CVS will sweep from -500 mV to 0 mV, then data collection will end.

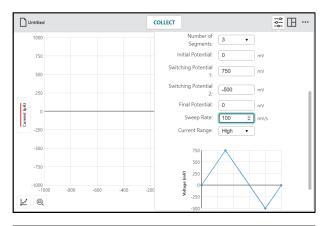


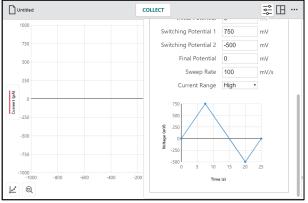
#### **Sweep Rate**

The Sweep Rate is the rate at which the segments sweeps will occur in mV/s.

A graph of the voltage (mV) vs. time (s) waveform that will be applied during data collection is shown at that bottom of the Voltametric Settings dialog.

You can use this graph to determine the time required for data collection to complete. For this example, data collection takes approximately 25 seconds to complete.



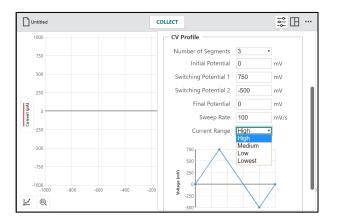


### **Current Range**

This entry sets the allowed current range for the CV. The current range values are as follows:

- High is  $\pm 1000 \, \mu A$ .
- Medium is  $\pm 100 \, \mu A$ .
- Low is  $\pm 10 \, \mu A$ .
- Lowest is  $\pm 1 \mu A$ .

Setting to a lower current range increases resolution of your CV; however, if the current range is set too low, the CV cannot proceed.



**NOTE:** The range values are not absolute. You may be able to get some additional current on any particular setting, but this varies from instrument to instrument.

# **Collecting Data**

Once you have set the CV profile as desired, click or tap to dismiss the voltammetry settings dialog. You are now ready to collect data.

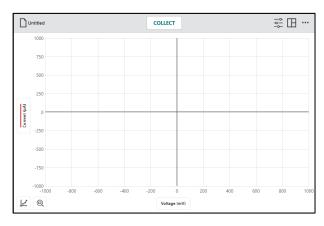
Click or tap collection to start data collection.

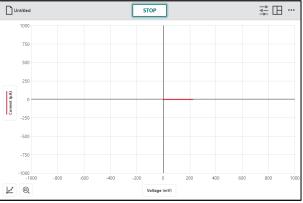
The sweeps follow the waveform profile you

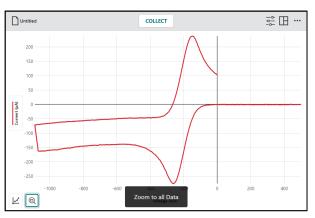
TIP! Notice that the collect button is replaced by a stop button while data are being collected. You can click or tap to end data collection early.

Wait for the data collection to complete. How long this takes depends on the range and speed of the sweeps you defined in the profile.

If needed, click or tap to scale graph to fit your data.







Often it is necessary to repeat data collection using different CV profiles to obtain the desired voltammogram.

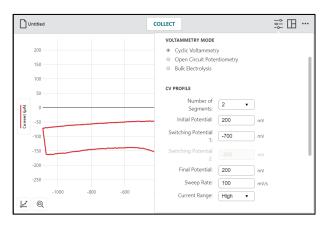
To collect additional data using a different profile, click or tap and modify the CV profile as desired.

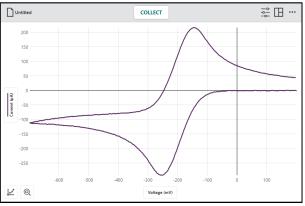
Click or tap collect additional data using the modified profile.

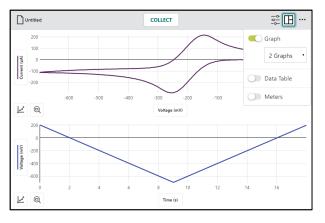
**TIP!** Data previously collected are saved with the file. You can repeat data collection as often as needed to get the desired voltammogram.

You can view a graph of potential vs. time and/or current vs. time along with the voltammogram.

Click or tap and select to show more than one graph. Tap the axis labels and select the desired columns to plot.







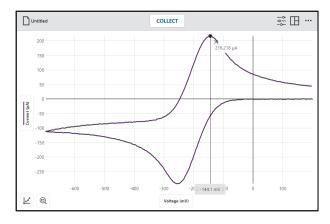
## **Data Analysis**

You can use the voltammogram to determine the anodic and cathodic peak currents ( $\mu A$ ) of your sample analyte. This can be done in two ways.

#### **Examine Tool**

Click or tap the graph to examine a point of interest. The coordinates of the point are shown. Click or tap a different point or drag the examine line to further examine your data.

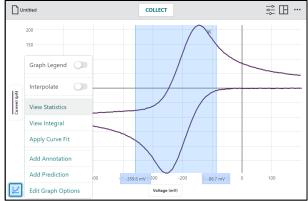
To remove the examine line, click or tap the close button, ×, displayed next to the line.



#### **Statistics Tool**

If desired, select a region of data. If a region of data is not selected, the statistics tool uses all data in the calculation.

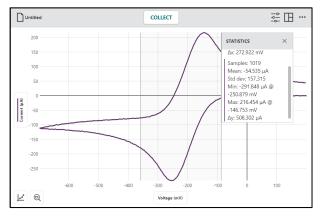
Click or tap and select View Statistics.



Statistics for all plotted columns on the graph are calculated and displayed in the Statistics details box.

The Minimum (Min) and Maximum (Max) points are the data of interest for this example as they correspond to the anodic and cathodic peak currents.

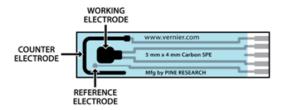
To dismiss the Statistics box, click or tap the close button, ×.



For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

## **III. Using Open-Circuit Potentiometry Mode**

The Open-Circuit Potentiometry (OCP) mode is a passive mode whereby the counter electrode circuitry of the potentiostat is bypassed. In this mode, only the resting potential, measured between the reference and working electrode, is measured. What makes OCP unique is that is a purely electrolytic measurement, thermodynamically.



OCP mode is typically used to determine the experimental parameters for more advanced CV experiments, or it could simply be looking at the stability of the chemical system in question. Values obtained from these measurements can be used in calculations for the standard potential of a reaction (Nernst studies).

## **Adjusting the OCP Profile**

From the Voltametric Settings, change the voltammetry mode to Open-Circuit Potentiometry.

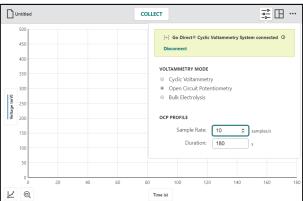
The experimental parameters to set for OCP are the Sample Rate and Duration.



Change the OCP Profile values as required for the analyte you are studying.

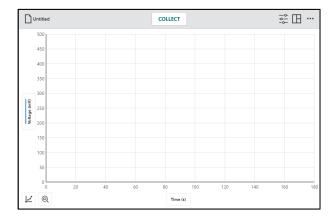
- Sample Rate values can be between 2 and 200 samples per second.
- Duration values can be between 1 and 40,000 seconds.

**NOTE:** The number of data points collected (Sample Rate × Duration) cannot exceed 20,000 points.



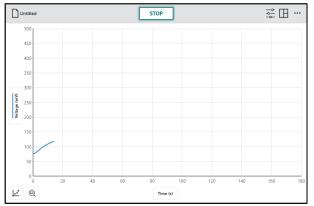
# **Collecting Data**

Once you have set the OCP profile as desired, click or tap to dismiss the voltammetry settings. You are now ready to collect data.



Click or tap collection to start data collection.

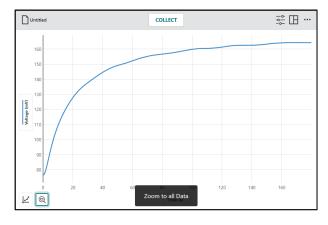
TIP! Notice that the collect button is replaced by a stop button while data are being collected.



Wait for the data collection to complete. You can click or tap stop to end data collection early.

If needed, click or tap to scale graph to fit your data.

**TIP!** You can repeat data collection if necessary. Your previously collected data will be saved with the file.



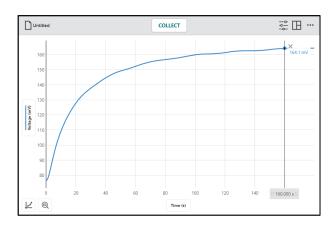
## **Data Analysis**

From this data you may want to note when that potential is steady for your analyte as it may be an important value to include in a CV sweep. Finding the related potential can be done in two ways.

#### **Examine Tool**

Click or tap the graph to examine a point of interest. The coordinates of the point are shown. Click or tap a different point or drag the examine line to further examine your data.

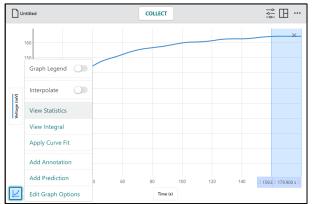
To remove the examine line, click or tap the close button, ×, displayed next to the line.



#### **Statistics Tool**

If desired, select a region of data. If a region of data is not selected, the statistics tool uses all data in the calculation.

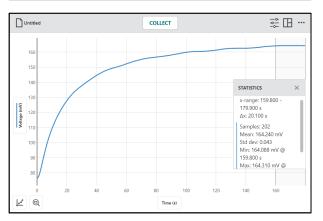
Click or tap and select View Statistics.



Statistics for all plotted columns on the graph are calculated and displayed in the Statistics details box.

The mean potential is the important statistic in this example as it denotes the average potential over the selected region.

To dismiss the Statistics box, click or tap the close button, ×.



For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

## IV. Using Bulk Electrolysis Mode

In the Bulk Electrolysis (BE) mode, the potentiostat holds the potential of the working electrode at one value and measures the resulting current over time. In this type of experiment, the analyte is converted from its original oxidation state to a new oxidation state either through reduction or oxidation. Analyzing the resulting data can help determine the electric charge passed over time.

This mode can be used to determine what current range to set when performing a cyclic voltammetry experiment.

## Adjusting the BE Profile

From the Voltametric Settings, change the voltammetry mode to Bulk Electrolysis.

The experimental parameters are Sample Rate, Duration, Electrolysis Potential, and Current Range.

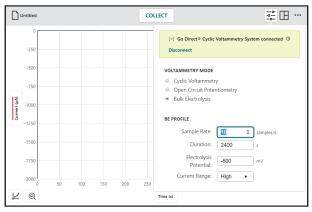


Change the BE Profile values as required for the analyte you are studying.

#### **Sample Rate and Duration**

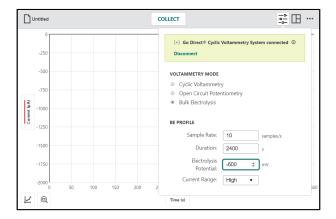
- Sample Rate values can be between 2 and 200 samples per second.
- Duration values can be between 1 and 40,000 seconds.

**NOTE:** The number of data points collected (Sample Rate × Duration) cannot exceed 20,000 points.



## **Electrolysis Potential**

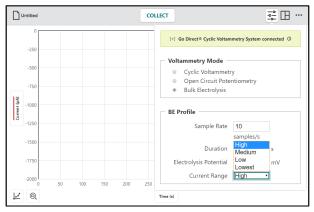
This is the constant potential the working electrode will be held at during data collection.



#### **Current Range**

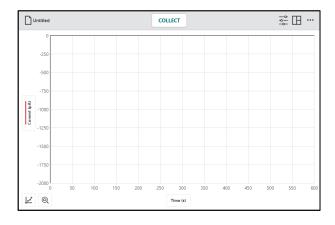
This entry sets the allowed current range for the CV. The current range values are as follows:

- High is  $\pm 1000 \, \mu A$ .
- Medium is  $\pm 100 \, \mu A$ .
- Low is  $\pm 10 \, \mu A$ .
- Lowest is  $\pm 1 \mu A$ .



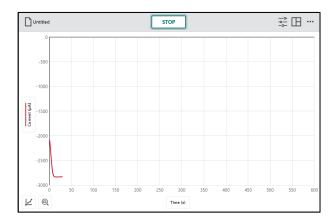
# **Collecting Data**

Once you have set the OCP profile as desired, click or tap to dismiss the voltammetry settings. You are now ready to collect data.



Click or tap **COLLECT** to start data collection.

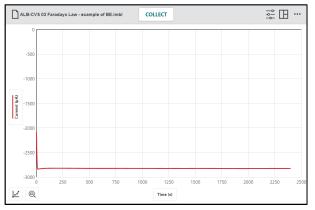
TIP! Notice that the collect button is replaced by a stop button while data are being collected.



Wait for the data collection to complete. You can click or tap stop to end data collection early.

If needed, click or tap to scale graph to fit your data.

**TIP!** You can repeat data collection if necessary. Your previously collected data will be saved with the file.



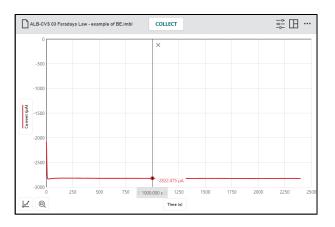
# **Data Analysis**

From this data you may want to note the value of the stable current and how long it is stable. Finding the current can be done in two ways.

#### **Examine Tool**

Click or tap the graph to examine a point of interest. The coordinates of the point are shown. Click or tap a different point or drag the examine line to further examine your data.

To remove the examine line, click or tap the close button, ×, displayed next to the line.



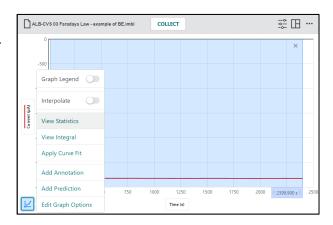
#### **Statistics Tool**

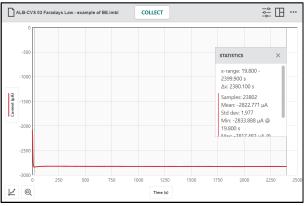
If desired, select a region of data. If a region of data is not selected, the statistics tool uses all data in the calculation.

Click or tap and select View Statistics.

Statistics for all plotted columns on the graph are calculated and displayed in the Statistics details box.

The mean current is the important statistic in this example as it denotes the average current over the selected region. Also,  $\Delta x$  represents the duration over which the average current is applied. The product of the mean and  $\Delta x$  relate to the charge transfer during the experiment.





To dismiss the Statistics box, click or tap the close button, ×.

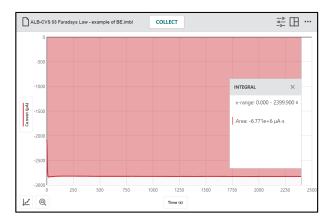
#### Integral Tool

The area under the current vs. time graph relates to the charge transfer during the experiment. Use the Integral tool to find the area.

**TIP!** If desired, select a region of data before selecting the integral tool to find the integral of only a selected region of your data.



The integral of this data is typically used to determine the quantity of material electroplated on an SPE to determine further characteristics about the chemical system.



For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

# V. Using the Cyclic Voltammetry System Without an External SPE

The Go Direct Cyclic Voltammetry System (CVS) has an internal resistor that can be used to verify that the CVS is properly applying the profile you have set up. This is an internal test of the CVS; no analyte is used. **Do not use the internal resistor with a Screen-Printed Electrode** (SPE) attached.

The example that follows describes testing a Cyclic Voltammetry (CV) profile.

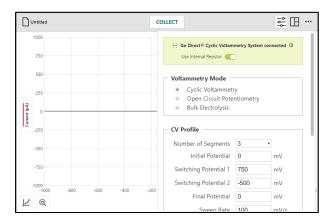
## **Setting up the Internal Resistor and CV Profile**

If you have a Screen-Printed Electrode (SPE) attached to the Go Direct Cyclic Voltammetry System, remove it before continuing. You should not use an SPE and the internal resistor at the same time.

From the Voltametric Settings, olick or tap [+] in the connected device box at the top of the dialog.

Select to use the internal resistor.

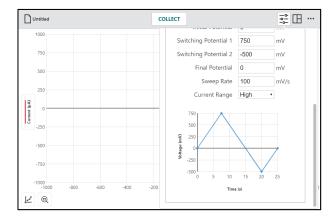




Setup the CV profile as desired.

Scroll to the bottom of the dialog to view the voltage *vs.* time waveform graph. Note the minimum and maximum voltages and the time required to complete the sweeps.

In this example the minimum voltage is -500 mV, the maximum voltage is 750 mV, and the duration of the sweeps is 25 seconds.



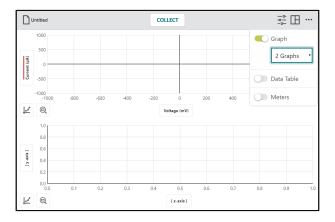
## **Modifying the View**

To assist with troubleshooting, you may want to add additional graphs and/or a data table.

For this example, set up a voltage vs. time graph to monitor the changes in voltage during the sweeps.

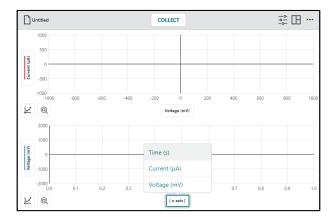
Click or tap View options,  $\square$ , and select to show 2 Graphs.

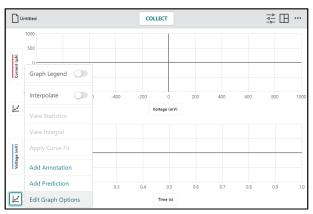
Click or tap the y-axis label, [y-axis], for the second graph and select to plot Voltage from Data Set 1.





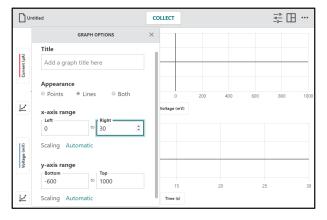
Click or tap the x-axis label, [x-axis], for the second graph and select to plot Time.



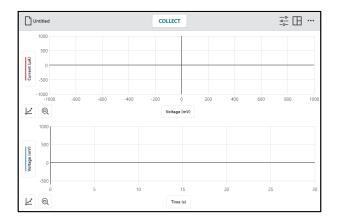


Modify the x- and y-axis ranges to replicate the waveform graph determined by the CV profile.

TIP! Set the time and voltage ranges to be slightly larger than the values of the waveform graph to ensure the data will show during data collection.

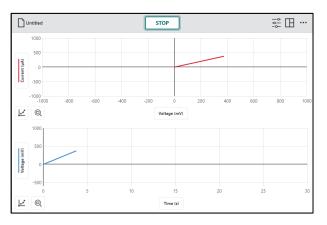


Click or tap close, ×, to dismiss Graph Options. You are now ready to collect data.



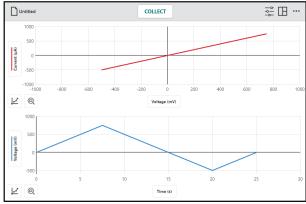
## **Collecting Data**

Click or tap collection to start data collection. The collection will follow the profile you set.



Wait for the data collection to complete.

**TIP!** You can repeat data collection if necessary. Your previously collected data will be saved with the file.



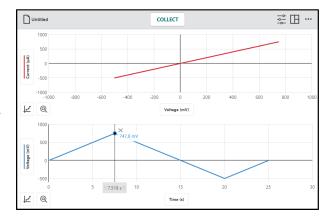
## **Data Analysis**

There are various things you can check to determine if the CVS is functioning as expected.

#### **Examine**

Tap the Voltage vs. Time graph to determine if the starting, stopping, and switching potentials have the appropriate values.

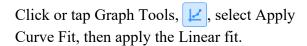
TIP! The values should be close but will not be an exact match.



#### **Curve Fit**

You can verify the sampling rate by doing a linear fit one of the regions of the voltage *vs.* time graph.

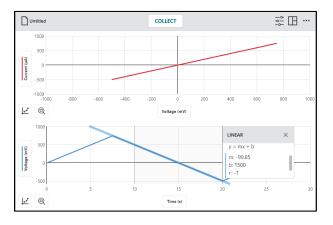
Click-and-drag or touch-and drag to select a region of the graph.



The absolute value of the slope of the linear fit should match the CV sweep rate.

**TIP!** You can also apply a linear curve fit to the Current vs. Voltage data, where the slope is related to the resistance of the internal resistor [Resistance  $(\Omega) = 1/\text{slope} \times 1000$ ].





#### **Calculate Column**

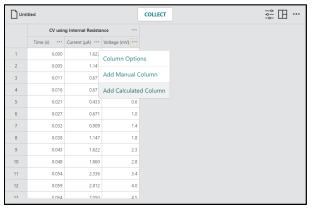
You can verify the relationship between the Voltage and Current (based on Ohm's law) by using a calculated column to calculate resistance.

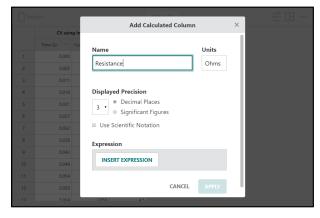
Click or tap View Options, , and change the view to show the table.

Click or tap the column options button, ..., next to the Voltage column header, then select Add Calculated Column.

Modify the column Name, Units, and Displayed Precision as desired for the new column.







Click or tap INSERT EXPRESSION to view the expression options.

For this application, choose the expression

A\*X^B\*Y^C

.

A, B, and C represent constants. X and Y represent data columns.

Resistance ( $\Omega$ ) can be calculated by dividing Voltage ( $\mu$ V or mV×1000) by Current ( $\mu$ A).

Enter the following for the expression:

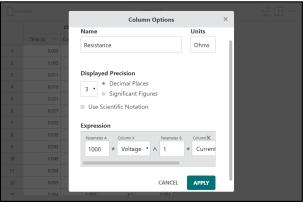
- A = 1000
- X = Voltage
- $\bullet$  B = 1
- Y = Current
- $\bullet$  C = -1

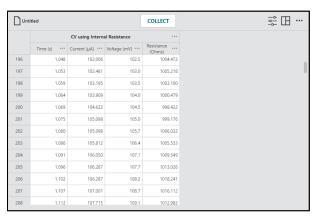
Click or tap APPLY to create the data column.

The resistance in this circuit is the 1,000  $\Omega$  internal resistor. Overall, the resistance values in the data table should match this value.

TIP! You can plot the resistance vs. time data and use the statistics tool to calculate the average resistance over the entire data collection.







For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

# **Using other Voltametric Modes**

## **Open Circuit Potentiometry**

From the Voltametric Settings, click or tap [+] in the connected device box, located near the top. Select to use the internal resistor.

Set up the OCP profile as desired.

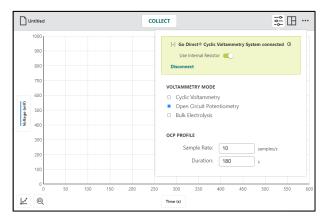
Add a second graph displaying Current vs. Time data. After collecting data, check the following:

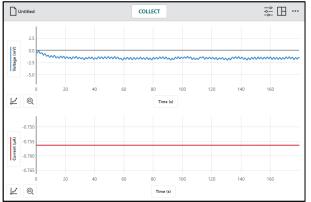
- Voltage and Current should stay relatively constant during data collection.
- View the data table to ensure the selected sampling rate is used.
- Create a calculated column to determine the resistance during data collection.

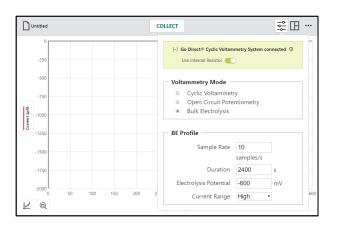
#### **Bulk Electrolysis**

From the Voltametric Settings, click or tap [+] in the connected device box, located near the top. Select to use the internal resistor.

Set up the BE profile as desired.

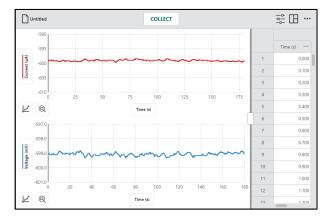






Add a second graph displaying Voltage *vs.* Time data. Check the following:

- Voltage and Current stay relatively constant during data collection.
- Check to see that the desired Electrolysis Potential is used.
- View the data table to ensure the selected sampling rate is used.
- Create a calculated column to determine the resistance during data collection.

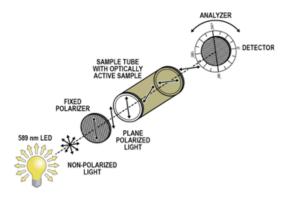


# CHAPTER 4— POLARIMETRY

Polarimetry is a technique for measuring the chiral properties of optically active samples without chemically modifying or destroying the sample. A polarimeter is used to detect changes in rotation of plane polarized light passing through an optically active compound. The amount of optical rotation is determined by the molecular structure and concentration of chiral molecules in the sample being tested.

This experiment option is used when collecting data with the following instrument:

• Go Direct Polarimeter

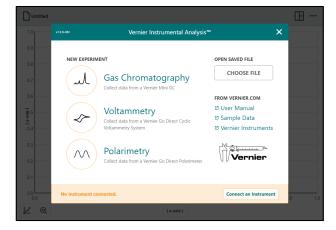


## I. Connecting your Go Direct Polarimeter

Launch Instrumental Analysis to view the New Experiment box.

TIP! If Instrumental Analysis is already running, click or tap the file menu icon,

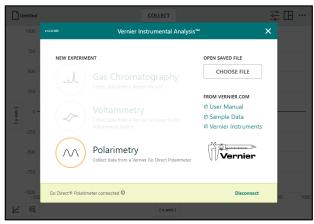
Untitled, and choose New Experiment. You may be prompted to save or discard the current file.



Turn on your Go Direct Polarimeter and connect your polarimeter to your device.

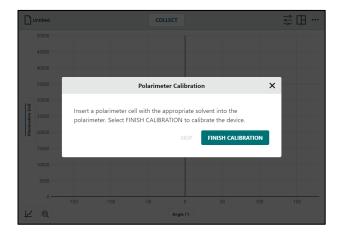
For detailed instructions see the following sections in Chapter 1:

- Connecting an Instrument using Bluetooth Wireless Technology
- Connecting an Instrument using USB



Select Polarimetry to continue with your experiment.

You will be required to calibrate your Go Direct Polarimeter before continuing.



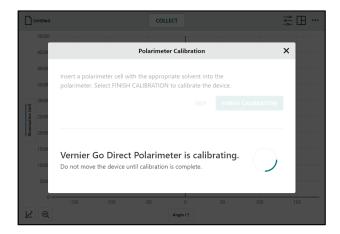
## **II. Calibrating your Polarimeter**

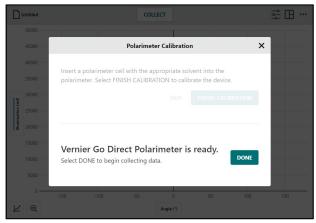
Pour the appropriate solvent in the Go Direct Polarimeter cell to a height of 10.0 cm. It is important to read the height to the nearest 0.1 cm, reading the bottom of the meniscus.

Place the cell in Go Direct Polarimeter, then click or tap FINISH CALIBRATION

When the Polarimeter Calibration is complete, click or tap DONE. You are now ready to continue your experiment.

TIP! The Polarimeter Calibration finds the angle where illumination is at a minimum and sets this angle to zero degrees. You can recalibrate your polarimeter at any time from the Polarimeter Settings,





# **III. Investigating Optical Rotation**

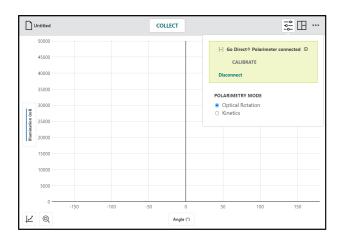
In the Optical Rotation mode, the Polarimeter collects data as the detector rotates at a fixed rate reporting measurements 50 times per second.

## **Preparing for Data Collection**

Rinse the polarimeter cell with a few milliliters of your optically active sample. Pour your sample into the polarimeter cell to a height of 10.0 cm (1.00 dm). It is important to read the height to the nearest 0.1 cm. Read to the bottom of the meniscus.

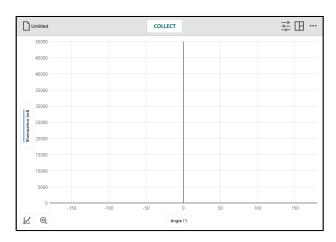
Place the sample cell in the polarimeter.

From the Polarimetry Settings, ensure the Optical Rotation mode is selected.



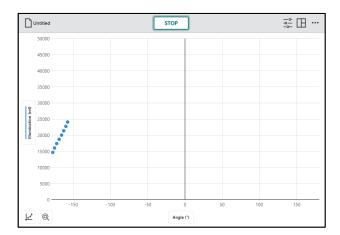
# **Collecting Data**

Click or tap to dismiss the polarimetry settings. You are now ready to collect data.



Click or tap **COLLECT** to start data collection.

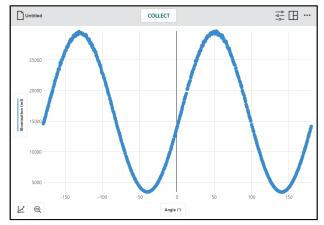
TIP! Notice that the collect button is replaced by a stop button while data are being collected.



Wait for the data collection to complete. You can click or tap stop to end data collection early.

If needed, click or tap to scale the graph to fit your data.

**TIP!** You can repeat data collection if necessary. Your previously collected data will be saved with the file.



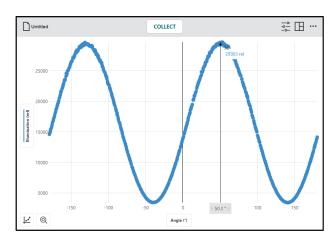
# **Data Analysis**

From this data, you are looking for the angle associated with the peak illumination closest to 0°. This can be found in different ways, using the examine tool, statistics, or a curve fit.

#### **Examine Tool**

Click or tap the graph to find the data point associated with the peak of the Illumination vs. Angle graph that is closest to 0°.

*TIP!* To remove the examine line, click or tap the close button, ×, displayed next to the line.



#### **Statistics**

To ensure you find the data point with the maximum illumination for this peak, click-and-drag or touch-and-drag to select a region of the graph that includes this peak.

Click or tap and select View Statistics.

Statistics for all plotted columns on the graph are calculated and displayed in the Statistics details box.

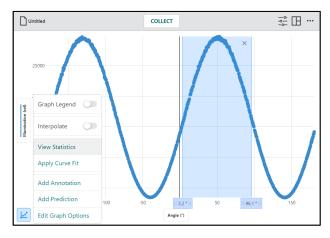
You are looking for the angle associated with the maximum illumination of the selected data.

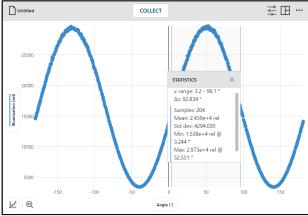
**TIP!** To dismiss the Statistics box, click or tap the close button, ×.

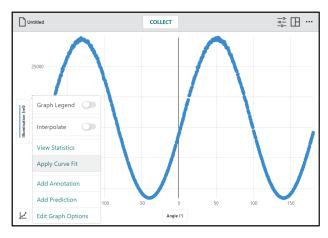
#### **Curve Fit**

Click or tap 🗾 and select Curve Fit.

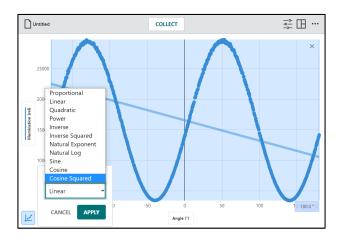
TIP! While you can, select a region of data before selecting the curve fit tool. In this situation you want to use all data points.







The function that bests models this type of data is a Cosine Squared function. Select that option from the Curve Fit dropdown menu.



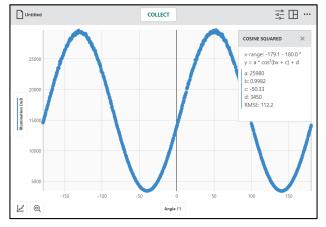
Click or tap to view the Curve Fit parameters.

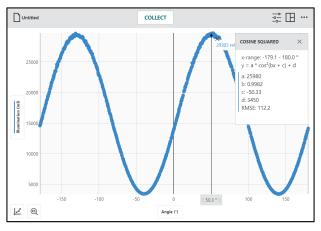
The data are modeled by the following function:

 $Illumination = a \cdot \cos^2(b \cdot angle + c) + d$ 

The parameter, -c, represents the angle associated with the peak in which you are interested as it represents the phase shift of the cosine squared function.

**TIP!** The curve fit is the preferred method for finding the angle of rotation since all data are used to find this value and not just a single data point.



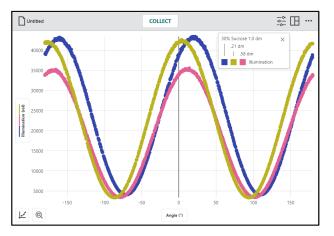


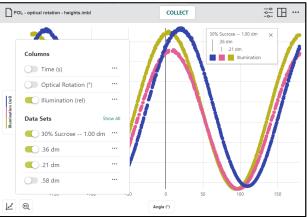
For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

# **Collecting Additional Data**

It is common to collect multiple runs of data varying experimental parameters such as concentration of the solution or solution height.

TIP! Data previously collected are saved with the file. You can repeat data collection as often as needed to get the desired voltammogram.





# IV. Exploring Kinetics

The kinetics mode is used to determine how the rotation angle of an optically active solution changes over time during a reaction.

# **Adjusting the Kinetics Collection Options**

From the Polarimetric Settings, select the Kinetics Polarimetry Mode.

Untitled

COLLECT

Collection

CALIBRATE

Disconnect

POLARIMETRY MODE

Optical Rotation

Kinetics

Kinetics

Kinetics Collection Settings

Sample Rate 1 samples/s

Find Collection

After 600 s

End Collection

Manually

Immedia

Change the Kinetics Collection Settings as required for your experiment.

### Sample Rate

Select the number of samples per second you what to collect.

• Minimum: 1 sample per second

• Maximum: 50 samples per second



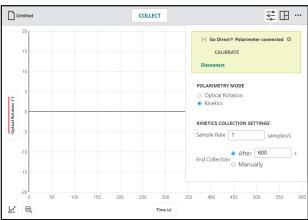
## **Ending Collection**

Set the End Collection duration as needed for your experiment.

• Minimum: 1 second

• Maximum: 86,400 seconds

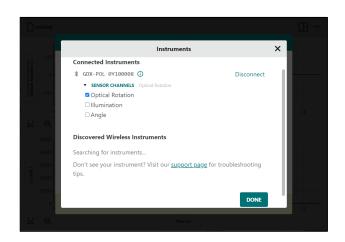
If you are not sure how much time is needed, you can choose to end collection manually.



**NOTE:** Collecting more than 10,000 points can impact performance of the app. You can improve performance of the application by turning off the Illumination and Angle sensor channels when connecting your instrument.

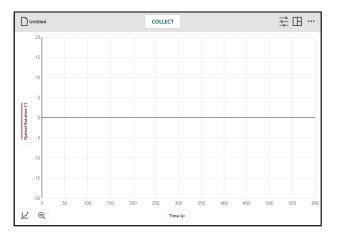
For detailed instruction on how to set up sensor channels, see these sections in Chapter 1:

- Connecting an Instrument using Bluetooth Wireless Technology
- Setting up Sensor Channels on a Go Direct Instrument Connected via USB

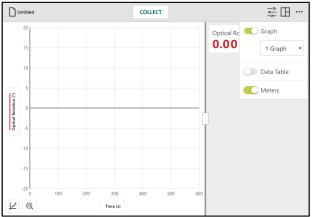


## **Preparing for Data Collection**

Click or tap to dismiss the polarimetry settings.



For this collection it can be helpful to include a live meter readout of the Optical Rotation sensor. Click or tap and select to show Meters.



Click-and-drag or tap-and-drag the handle on the separator line and adjust the split as desired.

## **Preparing the Sample**

Remove the solvent from the cell. Mix your two reactants together in a beaker. Pour this mixture into the polarimeter cell. Place the sample cell in the polarimeter.

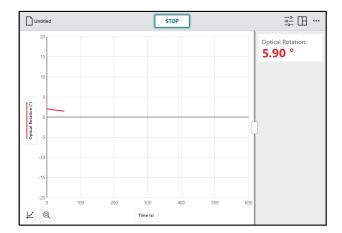
You are now ready for data collection.



# **Collecting Data**

Click or tap **COLLECT** to start data collection.

TIP! Notice that the collect button is replaced by a stop button while data are being collected.



Wait for the data collection to complete. If you selected to end collection manually, click or tap stop to end data collection.

If needed, click or tap to scale the graph to fit your data.

**TIP!** You can repeat data collection if necessary. Your previously collected data will be saved with the file.



COLLECT

Optical Rotation:

<u>≅</u> ⊞ …

**1.72** °

## **Data Analysis**

From this data, you are looking for the rate of the reaction. This is best done using a curve fit.

Apply Curve Fit

Edit Graph Option

Untitled

#### **Curve Fit**

Click or tap 🗾 and select Curve Fit.

TIP! While you can select a region of data before selecting the curve fit tool, in this situation you want to use all data points.

The typical functions used to investigate the reaction rate are linear and exponential. Choose the model that best fits your data.

Optical Rotation:

1.71 °

Proportional Linear Quadratic Power Inverse Squared Natural Log Sine Cosine Cosine Cosine Squared Linear Cosine Cosine Squared Linear Cosine Squared Linear Cosine Squared Linear Time (a)

Time (s)

Click or tap to view the Curve Fit parameters.

- For linear curve fits, the slope, m, is of interest.
- For exponential curve fits, the exponent, c, is of interest.



For a complete list of data analysis tools available in Instrumental Analysis, see Chapter 6—Analyzing Your Data.

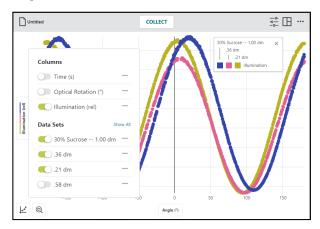
## **CHAPTER 5—CUSTOMIZING THE GRAPHS**

## I. Changing What is Plotted on the Graph

Click or tap the vertical-axis (y-axis) label to change the data that are plotted on the graph.

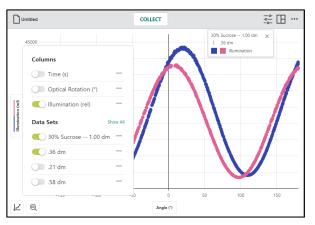
Click or tap a column name to add or remove the column data from the graph.

**TIP!** Column data for all selected data sets are shown on the graph.



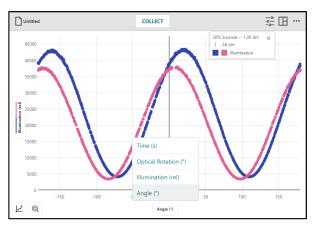
Click or tap a data set name to show or hide the column data for a specific data set.

**TIP!** Use the Show All and Hide All options to quickly show or hide data from every data set.



Click or tap the horizontal-axis (x-axis) label to select the desired independent variable for your graph. Only one column can be used as the independent variable for any graph.

TIP! You cannot plot a column vs. itself. If the column you select for the independent variable is already plotted on the vertical axis (y-axis), that column is removed from the graph.



# II. Changing the Graph Style

Click or tap (2) and choose Edit Graph
Options to access the graph configuration tools.

Adjust the appearance as desired. Click or tap the close button, ×, to dismiss Graph Options.

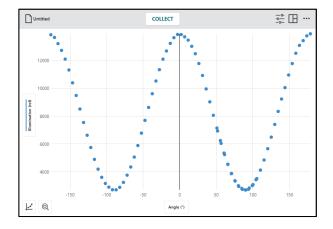
TIP! When displaying multiple graphs, changes to the Graph Options only apply to the graph from which the tool is accessed and are not automatically applied to the other graphs.



## **Points**

Choose Points to show data as unconnected dots.

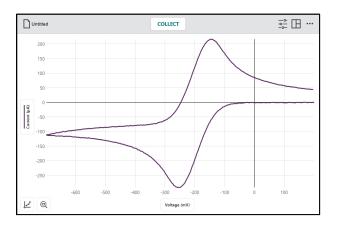
This is the default option for Polarimetry.



#### Lines

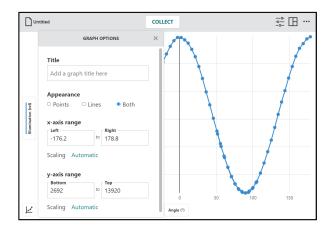
Choose Lines to show linear segments drawn between the data points.

This is the default option for Voltammetry and Gas Chromatography.



### **Both—Points and Lines**

Choose Both to show data as dots connected by linear segments. This option is not displayed by default.



# III. Scaling the Graph

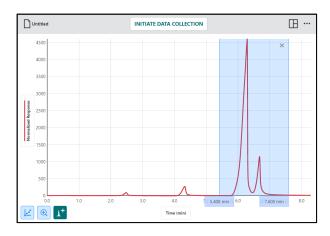
# Zoom to a Selected Region

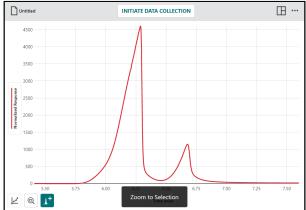
To scale the graph to a specific section of your data, click-and-drag or touch-and-drag across the graph to select the desired region.

TIP! You can click-and-drag or touch-and-drag the boundaries of a selected region to adjust the region as needed.

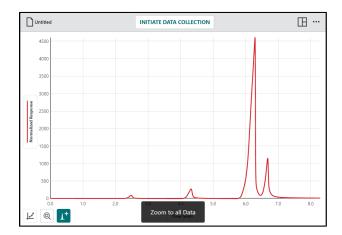
When a region is selected, click or tap to rescale the graph to fit the selection.

The left and right boundaries match the selected region. The top and bottom boundaries automatically adjust to show all data within the region.





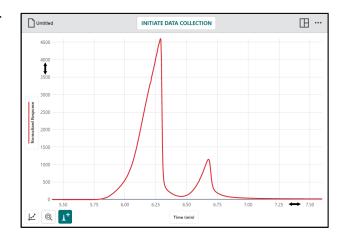
You can click or tap again to rescale the graph to fit all data.



## Panning the Graph

Click-and-drag or touch-and-drag near one of the axes to pan or move the graph without changing the scaling. Starting near the horizontal axis (x-axis) pans the graph horizontally. Starting near the vertical axis (y-axis) pans the graph vertically.

**TIP!** Touch-screen devices can use a twofinger pinch gesture to pan and rescale the graph.



# **Manual Scaling**

Click or tap and choose Edit Graph Options to access the graph configuration tools.

Manually configure the x-axis and y-axis ranges to display the data as desired and adjust the scaling as desired.

#### Scaling—Automatic

This default option allows the graph to scale larger during data collection to ensure all data points are visible.



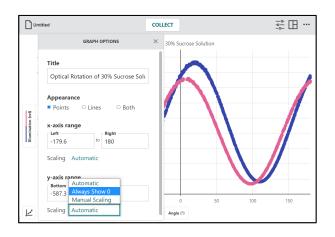
**TIP!** Manually entered range values are not respected when the scaling option is set to Automatic.

#### Scaling—Always Show 0

This option scales the graph to include 0 for that axis. This setting does not change the automatic behavior related to scaling the graph larger but is respected when you manually autoscale the graph.

#### Scaling-Manual

This option disables the automatic behavior related to scaling the graph larger during collection but is not respected when you manually autoscale the graph.

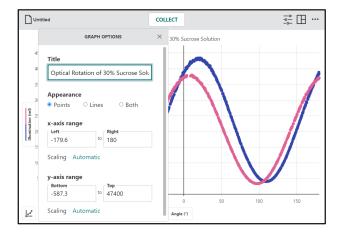


# IV. Labeling the Graph

## Adding a Graph Title

Add or edit the graph title as desired. Click or tap the close button, ×, to dismiss Graph Options.

The title appears centered above the graph.

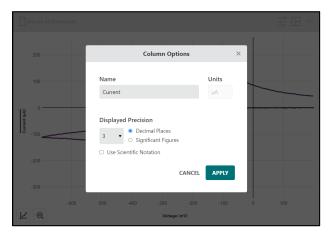


# **Modifying Axes Labels**

The axis labels are populated from the column names. You can change the labels by changing the names of the columns.

Click or tap the y-axis label you want to change. Click or tap  $\cdots$  next to the column you want to change and choose Column Options.

Change the column name as desired. Click or tap APPLY to save the changes.



To change the x-axis label, access the column options for that column from the data table or temporarily plot the column on the y-axis.

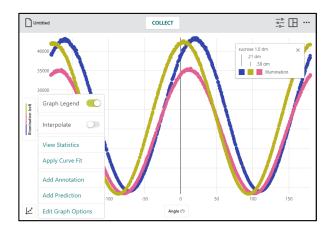
# Adding a Graph Legend

Click or tap 🗾 and select Graph Legend.

When selected, a box showing the color used for each column plotted from each data set is displayed on the graph.

Click-and-drag or touch-and-drag the legend to reposition it on the graph.

To dismiss the legend, click or tap the close button,  $\times$ .



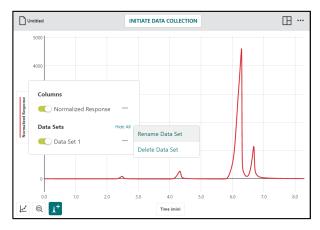
#### **Rename Data Sets**

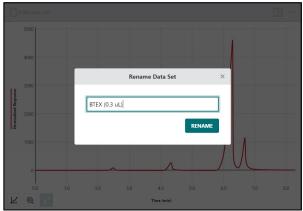
While not shown directly on the graph, data set names are shown in the y-axis graph setup box and in the Graph Legend.

Click or tap the y-axis label, Normalized Response Click or tap ••• next to the data set for which you want to change the name.

Choose Rename Data Set to change the default data set name.

Click or tap RENAME to save the data set name.

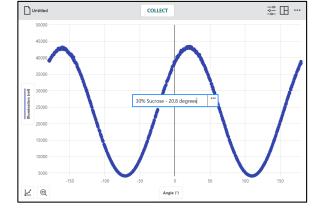




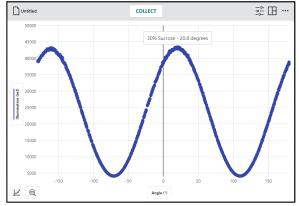
#### **Add Annotations**

You can add text annotations to your graph to label key points or provide information about the data.

Click or tap and choose Add Annotation to add text labels to your graph. Edit the text as desired.

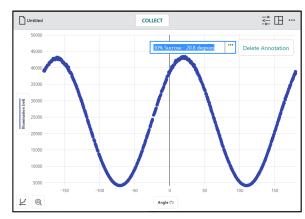


Click-and-drag or touch-and-drag an annotation to reposition it on the graph.



Double-click or double-tap an existing annotation to edit the text.

Click or tap ••• to delete the annotation.



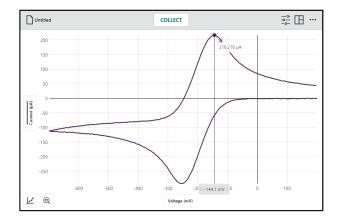
# **CHAPTER 6—ANALYZING YOUR DATA**

# I. Examining Data Points

Click or tap the graph to examine a point of interest. The coordinates of the point are shown.

Click or tap a different point or drag the examine line to further examine your data.

To remove the examine line, click or tap the close button, ×, displayed next to the line.

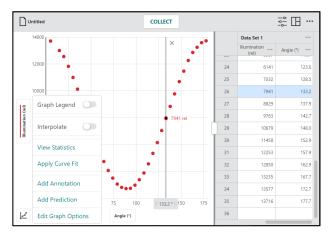


# II. Interpolating and Extrapolating Data

To examine values between and beyond your data points, click or tap and select Interpolate.

The interpolate function affects the behavior of the examine tool.

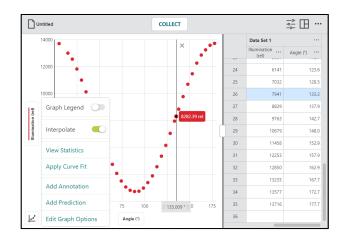
While interpolate is off, the displayed examine values are for plotted data points. As you move the examine line, the value of the nearest data point is displayed.



While interpolate is on, you can estimate values between plotted data points. The values displayed depend on whether you have a curve fit plotted on the graph.

# **Interpolate Without a Curve Fit**

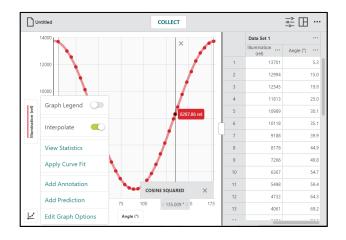
When there is no curve fit, the examine cursor follows the straight-line path between two consecutive points.



#### Interpolate With a Curve Fit

When there is a curve fit, examine follows the curve fit model to determine the examine values.

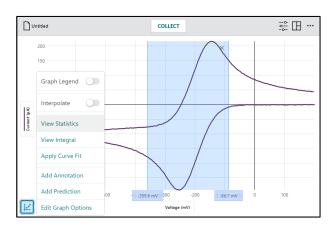
To examine data points beyond your data (extrapolate), you must have a curve fit plotted on the graph and interpolate turned on.



# **III. Viewing Statistics**

Use the Statistics tool to calculate statistical attributes based on your data. Displayed values include number of points, mean, standard deviation, minimum, maximum, and range. Statistics for all plotted columns are calculated.

If desired, select a region of data. If a region of data is not selected, the statistics tool uses all data in the calculation.

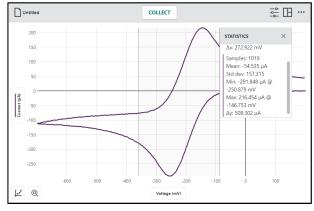


Click or tap and select View Statistics.

Statistics for all plotted columns on the graph are calculated and displayed in the Statistics details box.

To dismiss the Statistics box, click or tap the close button, ×.

TIP! You can slide the Statistics along the right region boundary if needed.

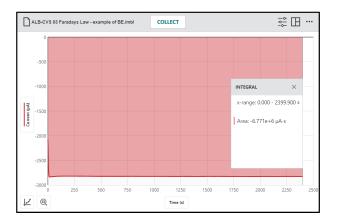


# IV. Viewing Integral

Use the View Integral tool to calculate the numerical integral (area) associated with your data.

Select a region if desired. Click or tap 
and select View Integral to find the integral.

The associated area is shaded, and the value is displayed. Regions above the horizontal axis (x-axis) are positive, while regions below are negative. Areas for all plotted columns are calculated and displayed in the Integral details box.



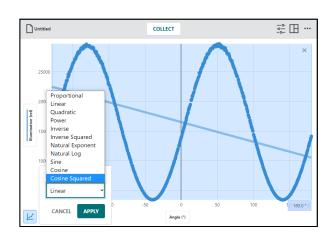
**NOTE:** This feature is not available for Gas Chromatography experiments as the Peak Integration feature is preferred. See Chapter 2 for information on Peak Integration.

# V. Applying a Curve Fit

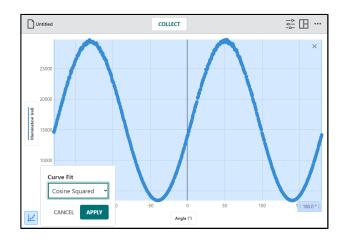
Use the curve fit tool to find a mathematical model that fits your data. Select a region first to fit a section of your data. When you select the tool without first selecting a region, all the data are used to determine the fit model.

Click or tap and select Apply Curve Fit to find the equation of the best-fit curve based on your data.

Curve fit models include Proportional, Linear, Quadratic, Power, Inverse, Inverse Squared, Natural Exponent, Natural Log, Sine, Cosine, and Cosine Squared.

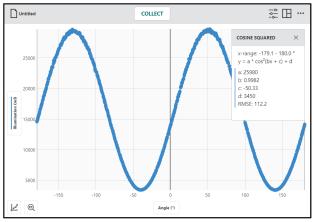


Select a curve fit model to preview the fit to your data.



Click or tap APPLY to display the curve fit equation and coefficients. Curve fits for all plotted columns are calculated.

The curve fit details box includes the RMSE (root mean square error), a measure of how well the fit matches the data. Linear curve fits also show the correlation coefficient (r) associated with the linear fit.



# VI. Adding Additional Columns

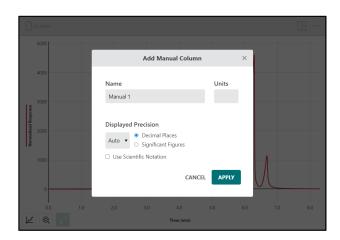
# **Adding a Manual Column**

Add manual columns to bring in data from other files or data found on the internet to compare with your data.

From the data table or y-axis setup box, click or tap ••• next to an existing column. Choose Add Manual Column to create a new manual entry column.

You can modify the column name, add units, and adjust the display precision of the new column as desired.

To add values to the column, display the data table (see Chapter 1 Adjusting the Display) then double-click or double-tap a cell to add or edit the data.



#### **Adding a Calculated Column**

Calculated columns are columns with values that are based on other columns through a mathematical formula. For example, you might define a calculated column to remove a baseline offset of another column, or you might calculate the ratio of voltage and current columns to create a resistance column.

From the data table or y-axis setup box, click or tap ••• next to an existing column. Choose Add New Calculated Column to create a new column.

You can modify the column name, add units, and adjust the display precision of the new column as desired.

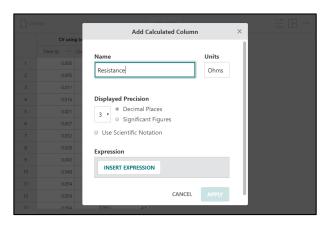
Click or tap INSERT EXPRESSION to view your expression options.

Select the desired expression to use for your calculated column.

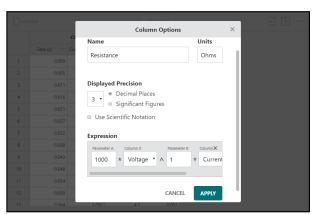
**TIP!** A, B, and C represent constants. X, Y, and Z represent data columns from your data table.

The column from which you accessed the column tools is used in the calculated column expression by default. Adjust the columns and parameters as desired.

TIP! The new calculated column appears to the right of the column used to access the column tools.







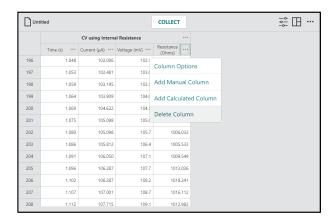
# VII. Managing the Data

#### **Deleting Columns**

From the data table or y-axis setup box, click or tap •••• next to an existing column. Choose Delete Column to remove Manual or Calculated Columns. Sensor and time columns cannot be deleted.

Deleting a column cannot be undone. Click or tap DELETE to confirm the deletion.

TIP! Since data sets are symmetric, deleting a column from one data set removes the corresponding column from all data sets.

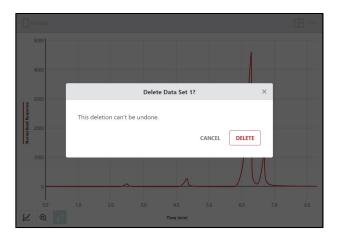


# **Deleting Data Sets**

From the data table or y-axis setup box, click or tap •••• next to an existing data set. Choose Delete Data Set to remove a data set.

Deleting a data set cannot be undone. Click or tap DELETE to confirm the deletion.

**TIP!** The last created data set cannot be deleted; however, any entered or collected data are cleared.



# **CHAPTER 7—MANAGING INSTRUMENTAL ANALYSIS FILES**

# I. Opening Files

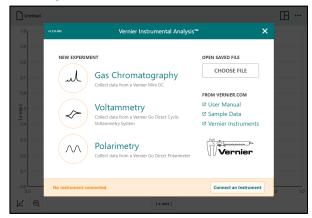
Click or tap untitled and choose Open to display the Open file box. From here, you can access files stored on your device, from an accessible cloud storage location such as Google Drive<sup>TM</sup>, iCloud<sup>®</sup>, or Dropbox, or from a connected storage device such as a USB drive or SD card.

**NOTE:** Not all options are available on every platform. You can choose to open previously saved Instrumental Analysis (.imbl) files or comma separated value (.csv) files.

#### **Accessing Sample Data in Instrumental Analysis**

Click or tap untitled and choose New Experiment. Choose Sample Data to launch the default browser with online access to sample data files for Instrumental Analysis.

See Chapter 1 for a list of Sample Experiments.



# **II. Saving Files**

#### Save

Click or tap untitled and choose Save to save the current file. This action replaces the previously saved file with the current file (in the same file location) without user confirmation. If your file has never been saved, selecting Save is equivalent to selecting Save As.

#### Save As

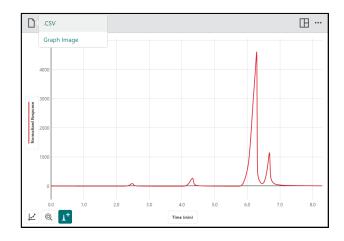
Click or tap untitled and choose Save As to display the Save file box. You can name the file and select where the file is to be stored. You can save the file directly to your device, to an accessible cloud storage location such as Google Drive, iCloud, or Dropbox, or to a connected storage device such as a USB drive or SD card. **NOTE:** Not all options are available on every platform. Save As will not automatically overwrite a previously saved file.

# **III. Exporting Files**

Click or tap Untitled and choose Export. There are two options for exporting a file: Comma-Separated Values (.csv) and Graph Image (.png).

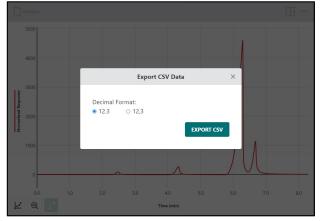
#### **Comma-Separated Values (.csv)**

Choose Export ▶ CSV from the File menu to export your experimental data as a .csv file.



Select the appropriate decimal separator for your data, then click or tap EXPORT CSV to save the file.

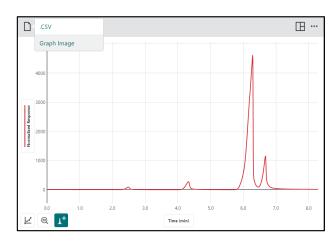
**TIP!** Use this feature to save the data in .csv format for further analysis with a spreadsheet application or to print your data.



# **Graph Image (.png)**

Choose Export • Graph Image from the File menu to export an image file (.png) based on your current view of the app.

**TIP!** Use this feature to create images of your data for inclusion in a lab report or for submission to an instructor via file sharing, emailing, or printing.



# IV. Printing from Instrumental Analysis

You cannot print directly from Instrumental Analysis. To print an Instrumental Analysis file, use File > Export to create the desired file (.csv or .png). Print the resulting file using the print options available on your device.

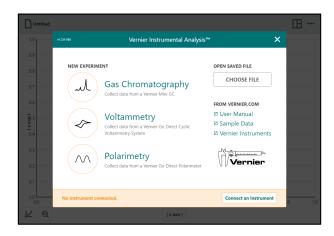
TIP! For more information regarding printing from Instrumental Analysis, see www.vernier.com/til/3789

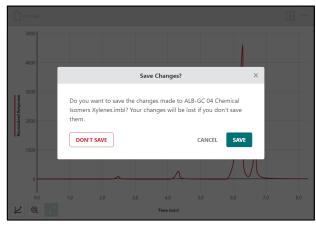
# V. Starting a New Experiment File

Click or tap untitled and choose New Experiment from the File menu to start a new file and reset the data-collection parameters.

**TIP!** Instruments already connected when selecting New Experiment remain connected when the new experiment is created.

If you have unsaved data, you will be prompted to save the existing file before continuing.





# **CHAPTER 8—APPENDIX**

# I. Updating Instrumental Analysis

#### **Determining Your Software Version**

Click or tap ··· from the top toolbar and choose About to see what Instrumental Analysis version you are running.

When using computers, the About box also provides a way to check for updates.



#### **Checking for Updates (Computers Only)**

Click or tap ••• from the top toolbar and choose Check for Updates to ensure you are running the latest version of Instrumental Analysis. You can choose to update if a newer version is available. This option requires your device to have an active internet connection.

**TIP!** This option is displayed for computers only. ChromeOS<sup>TM</sup>, iOS, iPadOS, and Android versions automatically check for and apply updates.



⊞ ...•

About

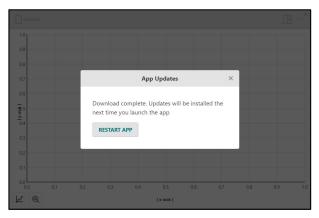
Untitled

Follow these steps to update Instrumental Analysis.

- Click or tap from the top toolbar to access the Other Options menu and select
   Update Available.
- 2. Click or tap **DOWNLOAD UPDATE** to download the update.



3. After the download is complete, click or tap RESTART APP to complete the update.



#### What's New

Click or tap ··· from the top toolbar and choose What's New to view a summary of the new features and fixes available in the most recent version of Instrumental Analysis.

Click or tap show all releases to see changes made in previous versions.



# **II. Getting Additional Help**

#### **Accessing the User Manual**

Click or tap [...] from the top toolbar and choose User Manual to access the user manual as well as online video tutorials for some Instrumental Analysis features. This option requires your device to have a live internet connection.

For access to other user manuals, our Technology Information Library, and chat, visit our website:

www.vernier.com/support

You may also contact Vernier directly by phone or email:

Toll Free: 888.837.6437 Email: support@vernier.com

# **Curriculum Resources from Vernier Software & Technology**

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