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Version 4.12 February 2024

ABOUT THIS GUIDE

The Spectral Analysis User Manual is an extended guide detailing the features of the Spectral Analysis app. This guide can be used with any platform-specific version of the software including the versions for Windows[®] and macOS[®] computers, ChromebookTM notebooks, and iOS and AndroidTM devices.

This document reflects features available in the 4.12 version of the software released in December 2023.

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I. GETTING STARTED WITH SPECTRAL ANALYSIS

Downloading the Software

Windows® and macOS® Computers

Spectral Analysis software for Windows and macOS computers is a free download from the Vernier website.

Chrome™ Computing Devices

Spectral Analysis app for ChromebookTM is a free download from the Chrome Web Store. *Note:* Chromebooks cannot use the Google Play version of this app. They must use the Chrome Web Store version.

iOS Devices

Spectral Analysis app for iPad[®] and iPhone[®] is a free download from the App Store.

Android™ Devices

Spectral Analysis app for Android tablets and phones is a free download from Google Play.

System Requirements

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

Licensing Information

Spectral Analysis computer software is free and can be installed on an unlimited number of computers.

Spectral Analysis apps for Chrome, iOS, and Android are free and distributed through their respective web stores. Terms and licensing are thus determined entirely by these stores.

Privacy Statement

COPPA, SOPIPA, and FERPA Compliance

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

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

II. CONNECTING A SPECTROMETER

Follow these steps to connect a spectrometer to Spectral Analysis. The following devices are supported:

- Go Direct[®] SpectroVis[®] Plus Spectrophotometer
- Go Direct Emissions Spectrometer
- Go Direct Fluorescence/UV-VIS Spectrophotometer
- Go Direct UV-VIS Spectrophotometer
- SpectroVis Spectrophotometer
- SpectroVis Plus Spectrophotometer
- Vernier Emissions Spectrometer
- Vernier Fluorescence/UV-VIS Spectrophotometer
- Vernier UV-VIS Spectrophotometer

Connecting via USB

1. Launch Spectral Analysis app.

 Connect the spectrometer to your computer or ChromebookTM using the USB cable that came with the spectrometer.

You are ready to continue with your experiment.

TIP! Click or tap ① to view information about the connected spectrometer.

TIP! Whenever possible, we recommend using spectrometers connected via USB.





Connecting via Bluetooth® Wireless Technology

TIP! Only Go Direct Spectrometers can be connected via a wireless connection. All other spectrometers must connect directly via USB.

1. Provide power to your Go Direct Spectrometer.

Go Direct[®] SpectroVis[®] Plus has a rechargeable battery. Be sure it is charged or connected to AC power. Press the power button to turn it on. The power LED will glow green and the Bluetooth[®] LED will flash blue.

Other Go Direct Spectrometers must be connected via USB to a power adapter or powered USB hub to power the Bluetooth radio. You cannot plug the USB cable into a computer USB port to power via Bluetooth wireless technology.

2. Launch the Spectral Analysis app.



3. Click or tap Connect a Spectrometer to view a list of available wireless spectrometers. The list can be scrolled if needed.

Click or tap your spectrometer from the list of discovered wireless devices. The app will connect to the sensor. The Bluetooth[®] LED on the sensor will now glow blue (no longer flashing).

TIP! Begin typing part of your sensor's serial number into the filter to more easily find your spectrometer.



4. Click or tap DONE

You are ready to continue with your experiment.

TIP! Click or tap (i) to view information about the connected spectrometer.



III. SELECTING AN EXPERIMENT



When Spectral Analysis is launched the New Experiment dialog displays. This dialog allows you to select experiment setups for the most common spectroscopy experiments. Spectrometer configuration, data-collection settings, and data displays are optimally set based on your selection. You can also use this dialog to open saved experiments, access online tutorials, and view sample data.

TIP! You can access this dialog anytime by clicking or tapping untited and choosing New Experiment.

Absorbance (^



Select this option when you are interested in investigating or utilizing the properties of a substance related to the wavelength(s) of light a substance absorbs. The absorbance values are determined using the percentage of light from a calibrated light source that passes through the substance relative to the unobstructed light. Absorbance is calculated using the following formula:

Absorbance = $2 - \log(\% Transmittance)$



Spectrometer Configuration

Light Source: Internal light source **Calibration:** Required



Linear CCD Array Detector

Data-Collection Settings

• Absorbance *vs*. Wavelength

Independent Variable: Wavelength Data Column: Absorbance Collection Mode: Full Spectrum

 Absorbance vs. Concentration (Beer's Law) Independent Variable: Concentration Data Column: Absorbance Collection Mode: Event Based

You must select a specific wavelength to be used as the basis of the absorbance data.





Absorbance vs. Time (Kinetics)
 Independent Variable: Time
 Data Column: Absorbance
 Collection Mode: Time Based

You must select a specific wavelength to be used as the basis of the absorbance data.



% Transmittance (V

Select this option when you are interested in investigating or utilizing the properties of a substance related to the wavelength(s) of light a substance transmits. The % transmittance values are determined using the percentage of light from a calibrated light source that passes through the substance relative to the unobstructed light.



Spectrometer Configuration

Light Source: Internal light source **Calibration:** Required



Data-Collection Settings

• % Transmittance *vs*. Wavelength (Full Spectrum)

Independent Variable: Wavelength Data Column: Transmittance Collection Mode: Full Spectrum



• % Transmittance *vs*. Concentration (Beer's Law)

Independent Variable: Concentration Data Column: Transmittance Collection Mode: Event Based

You must select a specific wavelength to be used as the basis of the transmittance data.

% Transmittance vs. Time (Kinetics)
 Independent Variable: Time
 Data Column: Transmittance
 Collection Mode: Time Based

You must select a specific wavelength to be used as the basis of the transmittance data.





Fluorescence (A

ce 🔨

Select this option when you are interested in investigating or utilizing the fluorescent properties of a substance relative to an excitation light source. The reported values are based on the electromagnetic radiation (light) emitted as a result of fluorescence.



Spectrometer Configuration

Light Source: Excitation light source

- SpectroVis Plus 405 and 500 nm LEDs built into the unit
- Fluorescence/UV-VIS external LEDs

Calibration: Optional – baseline noise and LED scatter only

Data-Collection Settings

• Fluorescence vs. Wavelength (Full Spectrum)

Independent Variable: Wavelength Data Column: Fluorescence Collection Mode: Full Spectrum



You must select a specific wavelength to be used as the basis of the fluorescence data.

TIP! You are not limited to experiments involving concentration. Select this experiment option for investigations involving fluorescence with other independent variables such as pH or excitation-LED intensity.









To change the name of the Concentration column to match your experiment, click or tap ••• next to the column name in the data table and select Column Options.

• Fluorescence *vs*. Time (Kinetics) Independent Variable: Time Data Column: Fluorescence **Collection Mode:** Time Based

You must select a specific wavelength to be used as the basis of the fluorescence data.



Emissions (

Select this option when you are interested in investigating or utilizing the component wavelengths of a light emitting source.

TIP! While you can use an Emissions Spectrometer without the optional fiber optic cable, we recommend using the cable for data collection. All other supported spectrometers require a fiber optic cable accessory (not included with the spectrometer) in order to collect emissions data.

Spectrometer Configuration

Light Source: External light source Calibration: Optional – baseline noise only





Vernier Spectral Analysis® – User Manual

Data-Collection Settings

Emissions vs. Wavelength
 Independent Variable: Wavelength
 Data Column: Intensity
 Collection Mode: Full Spectrum

Emissions vs. Event
 Independent Variable: Event (user defined)
 Data Column: Intensity
 Collection Mode: Event Based

You must select a specific wavelength to be used as the basis of the intensity data.





Emissions vs. Time
 Independent Variable: Time
 Data Column: Intensity
 Collection Mode: Time Based

You must select a specific wavelength to be used as the basis of the intensity data.



Advanced Full Spectrum

Select this option when comparing multiple experiment types (absorbance, % transmittance, fluorescence, and emission) within the same file. Examples for using this option include investigating the relationship between absorbance and % transmittance, inquiry-based analysis of an unknown sample, and investigating the Stokes shift of a sample using absorbance and fluorescence spectra. This option can also be used to collect the raw output of your lamp.



Light source and calibration options vary based on the Sensor Mode you have selected.

• Absorbance or % Transmittance Light Source: Internal light source Calibration: Required



Absorbance or % Transmittance



• Fluorescence

Light Source: Excitation light source

- SpectroVis Plus 405 and 500 nm LEDs built into the unit
- Fluorescence/UV-VIS external LEDs

Calibration: Optional – baseline noise and LED scatter only

• Emissions

Light Source: External light source **Calibration:** Optional – baseline noise only

TIP! A fiber optic cable, not included with the spectrometer, is required for most spectrometers in order to capture Emissions data.







Data-Collection Settings Independent Variable: Wavelength Data Column: Varies based on Sensor Mode • Absorbance • Transmittance

- Fluorescence
- Intensity
- Raw

Collection Mode: Full Spectrum

TIP! When data from two different sensor modes are collected, a second y-axis control is used to allow independent scaling of data.





The table below shows which experiment types are supported for each spectrometer.

Spectrophometer	Absorbance	% Transmittance	Fluorescence	Emissions	Raw Data
Go Direct [®] SpectroVis [®] Plus	•	•	•	•*	•
SpectroVis	•	•		•*	•
SpectroVis Plus	•	•	•	•*	•
Vernier/Go Direct Emissions Spectrometer				•	•
Vernier/Go Direct Fluorescence/UV-VIS Spectrophotometer	•	•	•	•*	•
Vernier/Go Direct UV-VIS Spectrophotometer	•	•		•*	•

*A fiber optic cable, not included with any spectrometer, is required for measuring emissions spectra from an external light source. For the Vernier/Go Direct Emissions Spectrometer, an optional fiber optic cable is recommended for data collection.

IV. COLLECTING ABSORBANCE DATA (~)

Absorbance vs. Wavelength (Full Spectrum)

In this data-collection mode, absorbance *vs.* wavelength data are plotted. Data for all supported wavelengths are displayed on the graph and in the data table.

1. Select Absorbance vs. Wavelength (Full Spectrum) from the New Experiment dialog.



2. A calibration will automatically begin when you select this experiment type.

It can take 90 seconds or more for the lamp to illuminate fully. It is recommended that you wait for the warm up countdown to complete before proceeding with the calibration.

3. When the lamp warm up is complete, place a blank cuvette in the holder with the clear sides aligned with the arrow on the spectrometer. Click or tap FINISH CALIBRATION to complete the calibration.

TIP! To remove any effects from the solvent used to prepare your samples for testing, use a cuvette containing only the solvent (often just deionized water) for this step in the calibration.





- 4. Place your sample in the cuvette holder making sure the clear sides align with the arrow on the spectrometer.
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- 5. Click or tap <u>COLLECT</u> to start data collection.

TIP! Notice that **COLLECT** changes to **STOP** while you are collecting data.

TIP! You can change samples while collecting data if desired. However, only the data displayed on the graph when you stop data collection will be retained.

6. Click or tap <u>stop</u> to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.





7. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.



To collect another data set, click or tap <u>collect</u> again. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name in the data table for tools to rename or delete a data set.

Recalibrate the Sensor

You can recalibrate your sensor if needed. Click or tap 🔯 to bring up the Collection Settings.

Click or tap **CALIBRATE** to start a new calibration.

TIP! A new calibration will not apply to data that are already collected. The calibration will only apply to data collected after the calibration.

TIP! See Appendix A for a detailed description of the Collection Settings.







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Advanced Full Spectrum

Calibrate

vs. Concentration (Reer's Law)

Absorbance vs. Concentration (Beer's Law)

In this data-collection mode, a specific wavelength is identified as the basis of the collected data. The most common use for this data-collection mode is a Beer's law experiment. Individual data points are collected from samples with known concentrations to create a graph of absorbance data *vs*. concentration at the selected wavelength. Data analysis can determine the concentration of a sample containing an unknown concentration of the solute being studied.

1. Select Absorbance vs. Concentration (Beer's Law) from the New Experiment dialog.

2. A calibration will automatically begin when you select this experiment type.

It can take 90 seconds or more for the lamp to illuminate fully. It is recommended that you wait for the warm up countdown to complete before proceeding with the calibration.

3. When the lamp warm up is complete, place a blank cuvette in the holder with the clear sides aligned with the arrow on the spectrometer. Click or tap FINISH CALIBRATION to complete the calibration.

TIP! To remove any effects from the solvent used to prepare your samples for testing, use a cuvette containing only the solvent (often just deionized water) for this step in the calibration.



4. Once calibration is complete, you will need to select the wavelength you will use for your experiment.

Follow the onscreen instructions for selecting a wavelength to use.

TIP! You can click or tap CALIBRATE SPECTROPHOTOMETER to calibrate the spectrometer again if needed.

5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the graph inset to change the selected wavelength.

TIP! If your independent variable is not Concentration (mol/L), click or tap ••• next to the table column heading and select Column Options to change the column name and units to match your experiment.

6. Place a sample in the cuvette holder making sure the clear sides align with the arrow on the spectrometer.

Click or tap <u>collect</u> to start data collection. This enables the <u>keep</u> button.

TIP! For comparison, the graph inset shows the full spectrum plot of the sample you are testing along with the spectrum used to define the wavelength.

 In this data-collection mode, you will be prompted to enter the solution concentration each time you keep a data point.

Click or tap when the spectrometer reading has stabilized.

TIP! The reading at the time you selected **IVEP** is shown in the dialog. Changes to the value while the Keep Point dialog box is shown are ignored until the dialog box is dismissed.

8. Enter the corresponding concentration value for this data point, then click or tap **KEEP POINT** to record the entry in the data table.

The point is automatically plotted on the graph.

TIP! It may be necessary to move the graph inset to see the collected point. You can drag the graph to a new location or click or tap \times to dismiss it. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

9. Continue collecting data for different samples until you have collected all of your data points.

Click or tap <u>stop</u> to end data collection and continue with data analysis.

TIP! The graph rescales as you each point to ensure all data points are shown on the graph. After data collection is complete, the graph will autoscale to fit the data.

TIP! If you inadvertently stop data collection before all of your data points have been collected, click or tap collect and select APPEND to continue collecting points in the current data set.

TIP! Double-click or double-tap a concentration value in the data table to edit the entry. Note that you can only change the concentration values. Absorbance values cannot be edited.

Collecting Multiple Data Sets

To collect another data set, click or tap collect and select CREATE NEW DATA SET. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set.

TIP! Click or tap ••• next to the data set name in the data table for tools to rename or delete a data set.

SPECTRAL ANALYSIS

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vs. Time (Kinetics)

% Transmittance

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Absorbance vs. Time (Kinetics)

In this data-collection mode, a specific wavelength is identified as the basis of the collected data and data are collected as a function of time. The most common use for this collection mode is a Kinetics experiment where the colorimetric properties of a substance change over time due to a reaction. Analysis of this data can be done to determine the rate, order, affinity, and numerous other properties of the reaction.

1. Select **Absorbance vs. Time (Kinetics)** from the New Experiment dialog.

2. A calibration will automatically begin when you select this experiment type.

It can take 90 seconds or more for the lamp to illuminate fully. It is recommended that you wait for the warm up countdown to complete before proceeding with the calibration.

3. When the lamp warm up is complete, place a blank cuvette in the holder with the clear sides aligned with the arrow on the spectrometer. Click or tap FINISH CALIBRATION to complete the calibration.

TIP! To remove any effects from the solvent used to prepare your samples for testing, use a cuvette containing only the solvent (often just deionized water) for this step in the calibration.

4. Once calibration is complete, you will need to select the wavelength you will use for your experiment.

Follow the onscreen instructions for selecting a wavelength to use.

TIP! You can click or tap CALIBRATE SPECTROPHOTOMETER to calibrate the spectrometer again if needed.

5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the graph inset to change the selected wavelength.

6. Click or tap 🌣 to adjust the Collection Interval.

Adjust the value as needed for your experiment. The Collection Interval can be any whole number from 1 to 3600 seconds. The smallest value is automatically calculated based on your calibration and collection settings.

TIP! To get the fastest data-collection rate, connect directly with USB. Connecting via Bluetooth[®] wireless technology limits the collection interval.

TIP! See Appendix A for a detailed description of the Collection Settings.

7. Prepare your sample for data collection. Place the cuvette in the cuvette holder making sure the clear sides align with the arrow on the spectrometer.

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

8. Click or tap **stop** to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

TIP! You can drag the graph inset anywhere on the graph if needed. Click or $tap \times to$ remove the graph inset. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

9. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.

Collecting Multiple Data Sets

To collect another data set, click or tap collect again. Your original data set is retained and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name in the data table for tools to rename or delete a data set.

V. COLLECTING % TRANSMITTANCE DATA (V

% Transmittance vs. Wavelength (Full Spectrum)

In this data-collection mode, transmittance *vs.* wavelength data are plotted. Data for all supported wavelengths are displayed on the graph and in the data table.

- 1. Select % Transmittance vs. Wavelength (Full Spectrum) from the New Experiment dialog.
- Venere Spectral Address
- 2. A calibration will automatically begin when you select this experiment type.

It can take 90 seconds or more for the lamp to illuminate fully. It is recommended that you wait for the warm up countdown to complete before proceeding with the calibration.

3. When the lamp warm up is complete, place a blank cuvette in the holder with the clear sides aligned with the arrow on the spectrometer. Click or tap FINISH CALIBRATION to complete the calibration.

TIP! To remove any effects from the solvent used to prepare your samples for testing, use a cuvette containing only the solvent (often just deionized water) for this step in the calibration.

4. Place your sample in the cuvette holder making sure the clear sides align with the arrow on the spectrometer.

5. Click or tap <u>collect</u> to start data collection.

TIP! Notice that **COLLECT** changes to **STOP** while you are collecting data.

TIP! You can change samples while collecting data if desired. However, only the data displayed on the graph when you stop data collection will be retained.

6. Click or tap <u>stop</u> to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

7. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.

Collecting Multiple Data Sets

To collect another data set, click or tap <u>collect</u> again. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name in the data table for tools to rename or delete a data set.

Recalibrate the sensor

You can recalibrate your sensor if needed. Click or tap $\textcircled{\basis}$ to bring up the Collection Settings.

Click or tap **CALIBRATE** to start a new calibration.

TIP! A new calibration will not apply to data that are already collected. The calibration will only apply to data collected after the calibration.

TIP! See Appendix A for a detailed description of the Collection Settings.

% Transmittance vs. Concentration (Beer's Law)

In this data-collection mode, a specific wavelength is identified as the basis of the collected data. The most common use for this data-collection mode is a Beer's law experiment. Individual data points are collected from samples with known concentrations to create a graph of transmittance data *vs*. concentration at the selected wavelength. Data analysis can determine the concentration of a sample containing an unknown concentration of the solute being studied.

1. Select % Transmittance vs. Concentration (Beer's Law) from the New Experiment dialog.

2. A calibration will automatically begin when you select this experiment type.

It can take 90 seconds or more for the lamp to illuminate fully. It is recommended that you wait for the warm up countdown to complete before proceeding with the calibration.

3. When the lamp warm up is complete, place a blank cuvette in the holder with the clear sides aligned with the arrow on the spectrometer. Click or tap FINISH CALIBRATION to complete the calibration.

TIP! To remove any effects from the solvent used to prepare your samples for testing, use a cuvette containing only the solvent (often just deionized water) for this step in the calibration.

4. Once calibration is complete, you will need to select the wavelength you will use for your experiment.

Follow the onscreen instructions for selecting a wavelength to use.

TIP! You can click or tap CALIBRATE SPECTROPHOTOMETER to calibrate the spectrometer again if needed.

5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the graph inset to change the selected wavelength.

TIP! If your independent variable is not Concentration (mol/L), click or tap ••• next to the table column heading and select Column Options to change the column name and units to match your experiment.

6. Place a sample in the cuvette holder making sure the clear sides align with the arrow on the spectrometer.

Click or tap <u>collect</u> to start data collection. This enables the <u>keep</u> button.

TIP! For comparison, the graph inset shows the full spectrum plot of the sample you are testing along with the spectrum used to define the wavelength.

 In this data-collection mode, you will be prompted to enter the solution concentration each time you keep a data point.

Click or tap when the spectrometer reading has stabilized.

TIP! The reading at the time you selected **IP** is shown in the dialog box. Changes to the value while the Keep Point dialog box is shown are ignored until the dialog is dismissed.

8. Enter the corresponding concentration value for this data point, then click or tap **KEEP POINT** to record the entry in the data table.

The point is automatically plotted on the graph.

TIP! It may be necessary to move the graph inset to see the collected point. You can drag the graph to a new location or click or tap \times to dismiss it. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

9. Continue collecting data for different samples until you have collected all your data points.

Click or tap <u>stop</u> to end data collection and continue with data analysis.

TIP! The graph rescales as you each point to ensure all data points are shown on the graph. After data collection is complete, the graph autoscales to fit the data.

TIP! If you inadvertently stop data collection before all your data points have been collected, click or tap **COLLECT** and select **APPEND** to continue collecting points in the current data set.

TIP! Double-click or double-tap a concentration value in the data table to edit the entry. Note that you can only change the concentration values. Transmittance values cannot be edited.

Collecting Multiple Data Sets

To collect another data set, click or tap collect and select CREATE NEW DATA SET. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set.

TIP! Click or tap ••• next to the data set name in the data table for tools to rename or delete a data set.

% Transmittance vs. Time (Kinetics)

In this data-collection mode, a specific wavelength is identified as the basis of the collected data and data are collected as a function of time. The most common use for this collection mode is a Kinetics experiment where changes in the colorimetric properties of a substance change over time due to a reaction. Data analysis can determine the rate, order, affinity, and numerous other properties of the reaction.

1. Select % Transmittance vs. Time (Kinetics) from the New Experiment dialog.

2. A calibration will automatically begin when vou select this experiment type.

It can take 90 seconds or more for the lamp to illuminate fully. It is recommended that you wait for the warm up countdown to complete before proceeding with the calibration.

3. When the lamp warm up is complete, place a blank cuvette in the holder with the clear sides aligned with the arrow on the spectrometer. Click or tap **FINISH CALIBRATION** to complete the calibration.

TIP! To remove any effects from the solvent used to prepare your samples for testing, use a cuvette containing only the solvent (often just deionized water) for this step in the calibration.

SPECTRAL ANALYSIS

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PERIMENT

4. Once calibration is complete, you will need to select the wavelength you will use for your experiment.

Follow the onscreen instructions for selecting a wavelength to use.

TIP! You can click or tap CALIBRATE SPECTROPHOTOMETER to calibrate the spectrometer again if needed.

5. Click or tap to use the wavelength you have selected.

TIP! You can click or tap the spectrometer meter (lower right corner of the screen) or graph inset to change the selected wavelength.

6. Click or tap 🌣 to adjust the Collection Interval.

Adjust the value as needed for your experiment. The Collection Interval can be any whole number from 1 to 3600 seconds. The smallest value is automatically calculated based on your calibration and collection settings.

TIP! To get the fastest data-collection rate, connect directly with USB. Connecting via Bluetooth[®] wireless technology limits the collection interval.

TIP! See Appendix A for a detailed description of the Collection Settings.

7. Prepare your sample for data collection. Place the cuvette in the cuvette holder making sure the clear sides align with the arrow on the spectrometer.

Click or tap <u>collect</u> to start data collection.

8. Click or tap <u>stop</u> to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

TIP! You can drag the graph inset anywhere on the graph if needed. Click or $tap \times to$ remove the graph inset. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

9. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.

Collecting Multiple Data Sets

To collect another data set, click or tap <u>collect</u> again. Your original data set is retained, and the new data set is displayed on the graph.







TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.

VI. COLLECTING FLUORESCENCE DATA $(\land$

Fluorescence vs. Wavelength (Full Spectrum)

In this data-collection mode, fluorescence *vs*. wavelength data are plotted. Data for all supported wavelengths are displayed on the graph and in the data table.

1. Select Fluorescence vs. Wavelength (Full Spectrum) from the New Experiment dialog.



2. The Collection Settings will automatically display.

Calibration is not required; however, you may want to calibrate before collecting data to set a baseline reading and to remove excitation-LED light scatter from your data.

TIP! You will need a cuvette filled with the solvent you used to prepare your fluorescence sample. Click or tap calibrate and follow the onscreen instructions.

3. Adjust the Excitation Wavelength to select the wavelength you want to use. The wavelength options shown depend on the spectrometer you are using.

TIP! When using the Vernier Fluorescence UV-VIS Spectrophotometer, the default excitation wavelength is 375 nm. The app cannot automatically detect the wavelength of the LED you are using. Be sure to update this value to match your LED.





4. Click or tap <u>collect</u> to start data collection.

TIP! If you have cuvettes with four clear sides, use them here. If not, be sure the clear sides of your cuvette align with the arrow on the spectrometer.

TIP! Notice that <u>collect</u> changes to <u>stop</u> while you are collecting data.

5. Click or tap 🔅 to bring up the Collection Settings again.

See Appendix A for a detailed description of the collection settings.

TIP! Click or tap off the Collection Settings to dismiss it. When using a computer or ChromebookTM, you can also hit the ESC key to dismiss the dialog.

6. Change the Collection Settings as needed for your experiment.

TIP! Making changes to the settings while you are collecting data will help you understand how these changes affect the collected data.

TIP! Altering Collection Settings may cause your basline or LED scatter to change. You may want to stop data collection and recalibrate before continuing with data collection.







7. Click or tap <u>stop</u> to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

8. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.







To collect another data set, click or tap <u>collect</u> again. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Your data set name will automatically include the excitation wavelength indicated in settings.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.



Fluorescence vs. Concentration

In this data-collection mode, a specific wavelength is identified as the basis of the collected data. Individual data points are collected from samples with known concentrations to create a graph of the fluorescence *vs.* concentration data at the selected wavelength. Data analysis can determine the concentration of a sample containing an unknown concentration of the solute being studied.

You are not limited to experiments involving concentration. This data-collection option can be used for other investigations with independent variables that affect fluorescence such as pH, halide concentration, or excitation-LED intensity.

- 1. Select **Fluorescence vs. Concentration** from the New Experiment dialog.
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- 2. The Choose a Wavelength dialog box will automatically display.

Calibration is not required; however, you may want to calibrate before collecting data to set a baseline reading and to remove excitation-LED light scatter from your data.

TIP! You will need a cuvette filled with the solvent you used to prepare your fluorescence sample. Click or tap CALIBRATE SPECTROPHOTOMETER and follow the onscreen instructions.



3. Select the Excitation Wavelength you are using for your experiment. The wavelength options shown depend on the spectrometer you are using.

TIP! When using a Fluorescence/UV-VIS Spectrophotometer, the default excitation wavelength is 375 nm. The app cannot automatically detect the wavelength of the LED you are using. Be sure to update this value to match your LED.

4. Follow the onscreen instructions for selecting the fluorescence emission wavelength to use for your experiment.

TIP! You may want to start with a Fluorescence vs. Wavelength experiment to find the spectrometer settings that work best for your experiment. The default spectrometer settings may not show a significant spectrum in this dialog box.

5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the spectrometer meter (lower right corner of the screen) or graph inset to change the selected wavelength.

TIP! If your independent variable is not Concentration (mol/L), click or tap ••• next to the table column heading and select Column Options to change the column name and units to match your experiment.







6. If needed, click or tap 🔅 and change the spectrometer settings to optimize the fluorescence data for your sample.

See Appendix A for a detailed description of the Collection Settings.

TIP! This assumes you know the settings that work best. Typically they are predetermined using a Fluorescence vs. Wavelength experiment.

TIP! Click or tap off the Collection Settings to dismiss it. When using a computer or ChromebookTM, you can also hit the ESC key to dismiss the dialog.

 Place your sample in the cuvette holder. Click or tap collection to start data collection. This enables the keep button.

TIP! If you have cuvettes with four clear sides, use them here. If not, be sure the clear sides of your cuvette align with the arrow on the spectrometer.

TIP! For comparison, the graph inset shows the full spectrum plot of the sample you are testing along with the spectrum used to define the wavelength.

8. In this data-collection mode, you will be prompted to enter the solution concentration each time you **KEEP** a data point.

Click or tap when the spectrometer reading has stabilized.

TIP! The reading at the time you selected **KEEP** is shown in the dialog. Changes to the value while the Keep Point dialog is shown are ignored until the dialog is dismissed.







9. Enter the corresponding concentration value for this data point, then click or tap **KEEP POINT** to record the entry in the data table.

The point is automatically plotted on the graph.

TIP! It may be necessary to move the graph inset to see the collected point. You can drag the graph to a new location or click or tap \times to dismiss it. You can click or tap \nvDash and choose Graph Inset to redisplay the graph inset if needed.

10. Continue collecting data for different samples until you have collected all your data points.

Click or tap <u>stop</u> to end data collection and continue with data analysis.

TIP! The graph rescales as you each point to ensure all data points are shown on the graph. After data collection is complete, the graph will autoscale to fit the data.

TIP! If you inadvertently stop data collection before all your data points have been collected, click or tap **COLLECT** and select **APPEND** to continue collecting points in the current data set.







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TIP! Double-click or double-tap a concentration value in the data table to edit the entry. Note that you can only change the concentration values. Fluorescence values cannot be edited.

Collecting Multiple Data Sets

To collect another data set, click or tap <u>collect</u> and select <u>CREATE NEW DATA SET</u>. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.

Fluorescence vs. Time (Kinetics)

In this data-collection mode, a specific wavelength is identified as the basis of the collected data. The most common use for this collection mode is a Kinetics experiment. The fluorescence properties of a substance change over time due to a reaction. Data analysis can determine the rate, order, affinity, and numerous other properties of the reaction.

1. Select Fluorescence vs. Time (Kinetics) from the New Experiment dialog.



Advanced Full Spectrum



2. The Choose a Wavelength dialog will automatically be shown.

Calibration is not required; however, you may want to calibrate before collecting data to set a baseline reading and to remove excitation-LED light scatter from your data.

TIP! You will need a cuvette filled with the solvent you used to prepare your fluorescence sample. Click or tap CALIBRATE SPECTROPHOTOMETER and follow the onscreen instructions.

3. Select the Excitation Wavelength you are using for your experiment. The wavelength options shown depend on the spectrometer you are using.

TIP! When using a Fluorescence/UV-VIS Spectrophotometer, the default excitation wavelength is 375 nm. The app cannot automatically detect the wavelength of the LED you are using. Be sure to update this value to match your LED.

 Follow the onscreen instructions for selecting the fluorescence Emission Wavelength to use for your experiment.

TIP! You may want to start with a Fluorescence vs. Wavelength experiment to find the spectrometer settings that work best for your experiment. The default spectrometer settings may not show a significant spectrum in this dialog.







5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the spectrometer meter (lower right corner of the screen) or graph inset to change the selected wavelength.

6. Click or tap 🌣. If needed, change the spectrometer settings to optimize the fluorescence data for your sample.

See Appendix A for a detailed description of the Collection Settings.

TIP! This assumes you know the settings that work best. Typically, they are predetermined using a Fluorescence vs. Wavelength experiment.

 Adjust the Collection Interval value as needed for your experiment. The Collection Interval can be any whole number from 1 to 3600 seconds. The smallest value is automatically calculated based on your calibration and collection settings.

TIP! To get the fastest data-collection rate, connect directly with USB. Connecting via Bluetooth[®] wireless technology limits the collection interval.

TIP! Click or tap off the Collection Settings to dismiss it. When using a computer or ChromebookTM, you can also hit the ESC key to dismiss the dialog box.







8. Place your sample in the cuvette holder. Click or tap collection to start data collection.

TIP! If you have cuvettes with four clear sides, use them here. If not, be sure the clear sides of your cuvette align with the arrow on the spectrometer.

9. Click or tap **stop** to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

TIP! You can drag the graph inset anywhere on the graph if needed. Click or $tap \times to$ remove the graph inset. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

10. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.

Collecting Multiple Data Sets

To collect another data set, click or tap <u>collect</u> again. Your original data set is retained, and the new data set is displayed on the graph.







TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.

VII. COLLECTING EMISSIONS DATA (

Emissions vs. Wavelength (Full Spectrum)

In this data-collection mode, intensity *vs*. wavelength data are plotted. Data for all supported wavelengths are displayed on the graph and in the data table.

1. Select Emissions vs. Wavelength (Full Spectrum) from the New Experiment dialog.

Insert or connect a fiber optic cable to your spectrometer. The accessory fiber optic cables do not come with the spectrometers.

TIP! When using an Emissions Spectrometer, it is recommended that you use a fiber optic cable even though you can collect data without it.

2. Calibration is not required; however, you may want to take a baseline (dark) measurement before collecting data. Click or tap to bring up the Collection Settings.

TIP! See Appendix A for a detailed description of the Collection Settings.

3. Click or tap **CALIBRATE** and follow the onscreen instructions to calibrate the spectrometer.

TIP! When calibrating the spectrometer, be sure the fiber optic cable is aligned as it would be during data collection and that the emissions light source is off.

TIP! Click or tap off the Collection Settings or hit the ESC key to dismiss the dialog if calibration is not desired.







4. Turn your light source on. Be sure to give it time to fully illuminate before starting data collection.

5. Click or tap <u>COLLECT</u> to start data collection.

TIP! Notice that **COLLECT** changes to **STOP** while you are collecting data.





6. Click or tap **stop** to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.



7. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.



Collecting Multiple Data Sets

To collect another data set, click or tap again. Your original data set is retained and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.

Emissions vs. Event

In this data-collection mode, a specific wavelength is identified as the basis of the collected data. The independent variable "Event" will depend on the experiment you are performing. Individual data points are collected from samples to create a graph of the intensity *vs*. "event" data at the selected wavelength.

1. Select Emissions vs. Event experiment.



2. Calibration is not required; however, you may want to take a baseline (dark) measurement before collecting data.

3. If needed, click or tap CALIBRATE SPECTROPHOTOMETER and follow the onscreen instructions to calibrate the spectrometer.

TIP! When calibrating the spectrometer, be sure the fiber optic cable is aligned as it would be during data collection and that the emissions light source is off.

4. Turn your light source on. Be sure to give it time to fully illuminate. Follow the onscreen instructions for selecting the wavelength to use for your experiment.







5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the spectrometer meter (lower right corner of the screen) or graph inset to change the selected wavelength.

6. Click or tap ••• next to the Event column heading in the data table.

7. Select Column Options and change the column name and units to match your experiment.







8. Click or tap APPLY to use the new column name.

TIP! Notice that the label on the bottomaxis (x-axis) is updated automatically.

9. Click or tap **COLLECT** to start data collection. This enables the **KEEP** button.

TIP! For comparison, the graph inset shows the full spectrum plot of the sample you are testing along with the spectrum used to define the wavelength.





10. In this data-collection mode, you will be prompted to enter the independent-variable value each time you **KEEP** a data point.

Click or tap when the spectrometer reading has stabilized.

TIP! The reading at the time you selected **IVEP** is shown in the dialog box. Changes to the value while the Keep Point dialog is shown are ignored until the dialog box is dismissed.



11. Enter the corresponding independentvariable value for this data point, then click or tap **KEEP POINT** to record the entry in the data table.

The point is automatically plotted on the graph.

TIP! It may be necessary to move the graph inset to see the collected point. You can drag the graph to a new location or click or tap \times to dismiss it. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

12. Continue collecting data for different samples until you have collected all your data points.

Click or tap <u>stop</u> to end data collection and continue with data analysis.

TIP! The graph rescales as you each point to ensure all data points are shown on the graph. After data collection is complete, the graph will autoscale to fit the data.

TIP! If you inadvertently stop data collection before all your data points have been collected, click or tap **COLLECT** and select **APPEND** to continue collecting points in the current data set.







TIP! Double-click or double-tap an independent-variable column value in the data table to edit the entry. Note that you can only change the independent-variable column values. Intensity values cannot be edited.

Collecting Multiple Data Sets

To collect another data set, click or tap **COLLECT** and select **CREATE NEW DATA SET**. Your original data set is retained, and the new data set is displayed on the graph.

TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.

Emissions vs. Time (Kinetics)

In this data-collection mode, a specific wavelength is identified as the basis of the collected data. One use for this collection mode is to investigate changes in the emission properties of an external light source over time. This example experiment is looking at the changes in light intensity (at 723 nm) as a projector bulb warms up.

1. Select Emissions vs. Time (Kinetics) experiment.





2. Calibration is not required; however, you may want to take a baseline (dark) measurement before collecting data.

3. If needed, click or tap CALIBRATE SPECTROPHOTOMETER and follow the onscreen instructions to calibrate the spectrometer.

TIP! When calibrating the spectrometer, be sure the fiber optic cable is aligned as it would be during data collection and that the emissions light source is off.

4. Turn your light source on. Be sure to give it time to illuminate fully. Follow the onscreen instructions for selecting the wavelength to use for your experiment.







5. Click or tap **DONE** to use the wavelength you have selected.

TIP! You can click or tap the spectrometer meter (lower right corner of the screen) or graph inset to change the selected wavelength.

6. Click or tap 🔅. If needed, change the spectrometer settings to optimize the intensity data for your light source.

TIP! This assumes you know the settings that work best. Typically, they are predetermined using an Emissions vs. Wavelength experiment.

TIP! See Appendix A for a detailed description of the Collection Settings.

 Adjust the Collection Interval value as needed for your experiment. The Collection Interval can be any whole number from 1 to 3600 seconds.

TIP! To get the fastest data-collection rate, connect directly with USB. Connecting via Bluetooth[®] wireless technology limits the collection interval.

TIP! Click or tap off the Collection Settings to dismiss it. When using a computer or ChromebookTM, you can also hit the ESC key to dismiss the dialog box.







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

9. Click or tap **stop** to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

TIP! You can drag the graph inset anywhere on the graph if needed. Click or $tap \times to$ remove the graph inset. You can click or tap \bowtie and choose Graph Inset to redisplay the graph inset if needed.

10. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that the point you are examining on the graph is also highlighted in the data table.

Collecting Multiple Data Sets

To collect another data set, click or tap collect again. Your original data set is retained, and the new data set is displayed on the graph.







TIP! To change what is plotted on the graph, click or tap the left-axis (y-axis) label and select the desired data set to plot.

TIP! Click or tap ••• next to the data set name for tools to rename or delete a data set.

VIII. COLLECTING ADVANCED FULL SPECTRUM DATA (

In this data-collection mode, you can collect Absorbance, % Transmittance, Fluorescence, and Emissions data all in the same file. You can also collect Raw data, which can be used to collect the raw signal from your lamp. For this example, we compare the absorbance and fluorescence spectrum of Riboflavin (vitamin B2).

1. Select Advanced Full Spectrum.

2. The Collection Settings will automatically display. The default Sensor Mode is Absorbance.

TIP! The Collection Settings options available depend on the selected Sensor Mode. Corresponding values entered in one mode will persist as you switch between modes.

TIP! See Appendix A for a detailed description of the Collection Settings.

3. For Absorbance and Transmittance modes, calibration is required. Click or tap CALIBRATE and follow the onscreen instructions.

Click or tap **FINISH CALIBRATION** to complete the calibration.

TIP! If you have not calibrated your spectrometer when required, you will be forced to calibrate when you click or tap collect







4. Place your sample in the cuvette holder with the clear sides aligned with the arrow on the spectrometer.

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

TIP! Notice that **COLLECT** changes to **STOP** while you are collecting data.

5. Click or tap **stop** to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.









7. Adjust the Excitation Wavelength to select the wavelength you want to use. The wavelength options shown depend on the spectrometer you are using.

TIP! When using a Fluorescence/UV-VIS Spectrophotometer, the default excitation wavelength is 375 nm. The app cannot automatically detect the wavelength of the LED you are using. Be sure to update this value to match your LED.

8. Change the Collection Settings as needed for your experiment.

See Appendix A for a detailed description of the Collection Settings.

TIP! It may be necessary to make changes to the settings while you are collecting data to see how these changes affect the collected data.

 Calibration is not required in Fluorescence mode; however, you may want to calibrate before collecting Fluorescence data to set a baseline reading and to remove excitation-LED light scatter from your data.

TIP! You will need a cuvette filled with the solvent you used to prepare your fluorescence sample. Click or tap CALIBRATE and follow the onscreen instructions.







10. Click or tap off the Collection Settings or hit the ESC key to dismiss the dialog.

TIP! When data from two different sensor modes are collected, a second (right) y-axis control is used to allow independent scaling of different data types.

TIP! The first collected data type is plotted on the left y-axis. The second data type is plotted on the right y-axis. Subsequent data types are added to the left y-axis.

11. With your sample still in the cuvette holder, click or tap **COLLECT** to start data collection.

TIP! Notice that **COLLECT** changes to **STOP** while you are collecting data.





12. Click or tap stop to end data collection and continue with data analysis.

The graph automatically autoscales to fit the data.

TIP! Data Sets in Spectral Analysis are symmetric. That is why there is an empty Absorbance column in the Fluorescence data set. There will also be an empty Fluorescence column added to the original Absorbance data set.



13. Click or tap the graph to examine a data point. Click or tap another point or drag the examine line to view other data points.

Click or tap \times to dismiss the examine line.

TIP! Notice that you are examining points from both graphs at the same time.



You can continue to collect additional Full Spectrum data using these or other Sensor Modes as needed for your experiment.

TIP! Collecting additional data types (Transmittance, Emissions, or Raw) will have their data plotted on the left-axis. To change what is plotted on the graph, click or tap the left-axis or right-axis label and select the desired columns and data sets to plot.





TIP! When using Go Direct[®] SpectroVis[®] Plus, Vernier SpectroVis Plus, Go Direct Visible Spectrophotometer, or Vernier SpectroVis, collecting Absorbance or Transmittance data after collecting data from one of the other data types (Fluorescence, Emissions) will require calibration of the sensor to maintain data accuracy, even if you had previously calibrated the spectrometer. This is because the spectrophotometer's internal light source must be turned off when using these other sensor modes.

Go Direct UV-VIS, Go Direct Fluorescence/UV-VIS, Vernier UV-VIS, and Vernier Fluorescence/UV-VIS spectrophotometers utilize shutters to block the different light sources, so recalibration is not required.

TIP! Spectral Analysis and Vernier Graphical AnalysisTM can be open at the same time. This is often helpful in Advanced Full Spectrum mode when collecting large sets of data. You can collect your full spectra of absorbance and fluorescence in Spectral Analysis and analyze it at the same time in Graphical Analysis in manual entry mode.

IX. ANALYZING DATA

Applying a Curve Fit

Apply a 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. A curve fit is useful when interpolation and extrapolation are needed to estimate data values using your collected data.

Follow the steps below to apply a curve fit to your data.

1. Click or tap \nvdash to access the graph tools.



TIP! Curve fits are based on all of the data when Apply Curve Fit is selected without first selecting a region. To fit a curve based on a portion of your data, select a region before accessing the curve fit tool.





3. Click or tap the curve fit drop-down to view the available curve fit models.

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





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

The curve fit details dialog includes the RMSE (root mean square error), a measure of how well the fit matches the data.

TIP! You can drag the curve fit details anywhere on the graph if needed.



 To view graph values based on a curve fit model, you will need to use the Interpolate feature. Click or tap ∠ to access the graph tools and select Interpolate.

TIP! When Interpolate is used without a curve fit model, the examine line will follow the straight-line path between two data points and will not move beyond your data points (extrapolate).

7. Click or tap on the graph to examine the curve fit. The data values reported are calculated using the curve model evaluated at the point selected.

TIP! To extrapolate beyond your data points, you will need to rescale the graph.

TIP! Click or tap \times in the curve fit details dialog to remove the curve fit from the graph.





Adding Calculated Columns

Calculated columns are data columns with values calculated from other data columns based on a mathematical formula. A calculated column is useful when you need to transpose data that can be analyzed graphically with a linear or other function.

1. Click or tap ••• next to a column name in the data table to access the column tools.

TIP! The available options depend on the type of column you have. Options include Column Options, Add Manual Column, Add Calculated Column, and Delete Column.

TIP! Since data sets are symmetric, columns added or modified in one data set are likewise added or modified in all data sets.



2. Choose Add New Calculated Column to create a new calculated column.

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

3. Click or tap **INSERT EXPRESSION** to view your expression options.

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

4. Select the desired expression to use for your calculated column.

Modify the constants as needed.







5. Click or tap on the column drop-down and modify the column selection as needed.

TIP! The column from which you accessed the column tools is used in the calculated column expression by default.

6. Click or tap APPLY to create the calculated column.

TIP! The new calculated column will appear in the table to the right of the column used to access the column tools.

TIP! The new calculated column is plotted on the graph replacing the column upon which the calculated column is based. If the original column is not plotted when the calculated column is created, the calculated column will not be plotted automatically.

Click or tap the axis labels to select the columns you want plotted on the second graph.

TIP! You must set up both the left (y-axis) and bottom (x-axis) axes before you will see any plotted data.







TIP! Examining a data point on one graph will automatically examine the corresponding data point on the second graph when the two graphs use the same independent variable.

8. Alternatively, you can use a second, right y-axis to show the data together on a single graph. This feature independently scales the two data columns to fit the graph.

Click or tap \nvdash and select Graph Options.

9. Click or tap Right y-axis range to add a second y-axis control to your graph.





10. Click or tap <u>[y-axis]</u> and select the column(s) you want plotted on the right y-axis.



Deleting a Calculated Column

 To delete a calculated column, click or tap
••• next to the column name in the data table. Choose Delete Column to remove the calculated column.

TIP! Spectrometer data, wavelength, and time columns cannot be deleted.

2. 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 will remove the corresponding column from all data sets.

If the calculated column was plotted when deleted, it is removed from the graph.







Adding Manual Columns

Manual columns are data columns that require manual data entry. Use manual columns when you want to enter hand-calculated data or data from a source outside the app.

1. Click or tap ••• next to a column name in the data table to access the column tools.

TIP! The available options depend on the type of column you have. Options include Column Options, Add Manual Column, Add Calculated Column, and Delete Column.

TIP! Since data sets are symmetric, columns added or modified in one data set are likewise added or modified in all data sets.

2. 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.





3. Click or tap APPLY to create the manual column.

TIP! The new calculated column will appear in the table to the right of the column used to access the column tools.

TIP! A new manual column is not plotted on the graph automatically.


4. Double-click or double-tap in a manual column cell to enter a value.

TIP! You can use Cut, Copy, and Paste tools to add values into manual columns.

TIP! The event-based "Concentration or Event" column is also a manual column that can be edited.

5. Enter data values into the table.



6. Click or tap the left-axis (y-axis) label to change what is plotted on the graph.

TIP! You can also plot the data using a second graph or a second, right y-axis. See Adding Calculated Columns (steps 7–10) for instructions.







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7. Modify the selection to plot the manual column data on the graph.

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

8. Click or tap (a) to autoscale the graph to fit your data.





Modifying a Manual Column Entry

1. Errors in data entry can be corrected.

Double-click or double-tap in a manual column cell in the data table to modify the entry.



2. The graph will automatically update as data values are corrected.



Deleting a Manual Column

 To delete a manual column, click or tap ••• next to a column name in the data table. Choose Delete Column to remove the Manual Column.

TIP! Spectrometer data, wavelength, and time columns cannot be deleted.

2. 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 will remove the corresponding column from all data sets.





If the calculated column was plotted when deleted, it is removed from the graph.



Using Cut, Copy, and Paste Tools

Select Cells

- Click or tap a single cell.
- To select a range of cells, click-and-drag or touch-and-drag.
- To select a single row, click or tap a row number.
- To select a range of rows, click-and-drag or touch-and-drag along the row numbers.
- To select a single column, click or tap a column header.
- To select a range of columns, click-and-drag or touch-and-drag across the column headers.
- To select a single data set, click or tap a data set header.
- To select a range of data sets, click-and-drag or touch-and-drag across the data set headers.

Copy to the Clipboard

- Windows[®]: Right-click and select Copy (or Ctrl-C)
- macOS[®]: Command-C (\mathcal{B}-C)
- ChromebookTM: Alt-click and select Copy (or Ctrl-C)
- iOS and Android[™] (and other touch-screen devices): Long-touch within the selection and select Copy

Cut (and Copy) to the Clipboard

- Windows: Right-click and select Cut (or Ctrl-X)
- macOS: Command-X (\mathbf{H}-X)
- Chromebook: Alt-click and select Cut (or Ctrl-X)
- **iOS** and **Android** (and other touch-screen devices): Long-touch within the selection and select Cut

Paste from the Clipboard

- Windows: Right-click and select Paste (or Ctrl-V)
- macOS: Command-V (\mathcal{K}-V)
- Chromebook: Alt-click and select Paste (or Ctrl-V)
- **iOS** and **Android** (and other touch screen devices): Long-touch within the selection and select Paste

TIP! When using Paste to copy data from multiple columns, you must first add the appropriate number of manual columns to your data table.

Using Other Analysis Tools

Below are some additional data analysis tools available in Spectral Analysis.

Tangent

Click or tap \bowtie and choose Tangent to calculate the rate of change of the data (slope) at the examined point. The tangent value is determined based on the points immediately around the examined point.

TIP! You cannot use Interpolate and Tangent at the same time. Choosing one will de-select the other.

View Statistics

Click or tap \nvDash and choose View Statistics 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.

TIP! The statistics are based on all the data when View Statistics is selected without first selecting a region.

View Integral

Click or tap \nvdash and choose View Integral to calculate the numerical integral (area) associated with your data. The associated area is shaded and the value is displayed. Regions above the bottom-axis (x-axis) are positive, while regions below are negative. Areas for all plotted columns are calculated.

TIP! Integrals are based on all the data when View Integral is selected without first selecting a region.







Scaling the Graph

There are multiple tools within Spectral Analysis to help you adjust the graph to best display your data.

Zoom – 🔍

The Zoom button allows you to quickly rescale the graph.



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 a to rescale the graph to fit the selection.

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





When there are no selected data, click or tap (a) to rescale the graph to fit all data points.

The left and right boundaries will match the left and right extremes of your data. The top and bottom boundaries will automatically adjust to show 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 bottomaxis (x-axis) will pan the graph horizontally. Starting near the left-axis or right-axis (y-axes) will pan the graph vertically.

TIP! In addition to panning, touch-screen devices can use a two-finger pinch gesture to rescale the graph.

Manual Graph Scaling

Click or tap \nvdash and select Graph Options to manually configure the graph range. Adjust the base (x-axis) and left (y-axis) range values as needed.







X. MODIFYING THE APPLICATION DISPLAY

Changing What is Graphed

Left-Axis Label (y-axis)

Click or tap the left-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! Use the Plot All and Hide All options to quickly add or remove all data columns from the graph for a specific data set.

Right-Axis Label (double y-axis)

Click or tap the right-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! The right-axis label provides all the same functionality as the left-axis label.





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Bottom-Axis Label

Click or tap the bottom-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, that column will be removed from the left or right axes.

Changing the Display (Graph, Table, and Meter)

Click or tap 🖽 to change what elements are displayed in Spectral Analysis. Chose to show or hide up to three graphs, a data table, or a large sensor meter.

TIP! When two or more elements are displayed, the split can be adjusted by dragging the resize handle, ______, located on the separating line.



Renaming Data Sets and Columns

Data Set Names

Click or tap ••• next to a data set name in the data table and choose Rename Data Set to change the default data set name.



Column Options (Name and Display Precision)

Click or tap ••• next to a column name in the data table or plot manager and choose Column Options to change the column name and displayed precision.

TIP! For manual and calculated columns, you can also change the units from this dialog.

TIP! For calculated columns, you can also modify the calculation.



Adding Annotations

Adding a Graph Annotation

Click or tap \bowtie and choose Add Annotation to add text labels to your graph.



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

TIP! You can add multiple annotations to a graph.



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

Click or tap ••• to delete the annotation.



Adding a Graph Title

Click or tap \bowtie and choose Graph Options to add a title to your graph. The title will appear centered above the graph.



Adding a Graph Legend

Click or tap Graph Tools, $[\underline{\nu}]$, and select Graph Legend. The legend shows the point symbol, color, and data for each plotted column.

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

Click or tap \times in the legend to remove it from the graph. You can click or tap \bowtie and choose Graph Legend to redisplay the legend if needed.



Point Symbol and Trace Color

Click or tap the y-axis label to access the Plot Manager.

Click or tap the colored point symbol (e.g., \blacktriangle) to choose a different symbol or trace color.

TIP! Changes to Point Colors and Point Symbols apply only to the column that was selected. The change is applied to any graph that is plotting that column's data.

TIP! Point Symbols are only shown if the Graph Appearance is set to show points.





Click or tap **S** for more color options.

TIP! Custom colors can be defined using RGB, HSL, or Hex values. Click or tap the color values (e.g., $\bigcirc B \implies 0$) to change the input option.

TIP! Click or tap *to add a color of an object that is showing on your device screen.*



Click or tap \bowtie and choose Graph Options to manually configure the graph appearance.

• Points

Choose Points to show data as unconnected dots. This is the default option for event-based spectrometer experiments.

TIP! Point symbols can be changed from the y-axis Plot Manager or Column Options.

• Lines

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

This is the default option for full spectrum and time-based spectrometer experiments.







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• Both

Choose Both to show data as dots connected by linear segments.

Overall Presentation

Click or tap \cdots from the top toolbar and choose Presentation to modify the font-size scale factor used in Spectral Analysis. This is particularly useful when presenting the app with a projector or viewing the app on a device with a highresolution screen.

Click or tap \bullet to change the display to dark mode.





XI. MANAGING FILES

Click or tap <u>Untitled</u> to access the File menu. From the File menu, you can open, save, and export files, along with other tasks.



Saving a File

Spectral Analysis files contain data-collection settings, graphs, data tables, and analyses. These files have .smbl extensions and can be opened and modified on any device running Spectral Analysis. The data from these files can also be opened using our Logger $Pro^{\text{(B)}}$ 3 software.

Save

Click or tap \Box untitled to access the File menu. Choose Save to save the current file. If your file has not previously been saved, a Save File dialog will be displayed. Enter the desired file name and storage location to save the file. You can save the file directly to your device, to an accessible cloud storage location, such as Google DriveTM, 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.

If your file has already been saved, choosing Save will overwrite the previously saved file with the current file (in the same file location) without user confirmation.

TIP! The file menu icon will show the name of the file once the file is saved (e.g., D Nickel Sulfate Analysis.smbl).

Save As...

Choose Save As... from the File menu to display the Save file dialog. You can rename the file and save it to a new storage location. Save As will not automatically overwrite a previously saved file.

Opening a File

Click or tap <u>Untitled</u> to access the File menu. Choose Open... to display your device's Open File dialog. You can access files stored on your device, from an accessible cloud storage location, such as Google Drive, iCloud, 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 Spectral Analysis (.smbl) files or comma separated value (.csv) files.

You can also open a file from the New Experiment dialog. Click or tap CHOOSE FILE OPEN SAVED FILE to display your device's Open File dialog. ん Absorbance 🗉 CHOOSE FILE · vs. Wavelength (Full spectrum) FROM VERNIER.COM vs. Concentration (Beer's Law) User Manual • vs. Time (Kinetics) Sample Data Vernier Spect 🖌 % Transmittance 🗉 Vernier ▲ Fluorescence H L) Emissions 🗉 Advanced Full Spectrum

Exporting a File

There are two options for exporting a file: Graph Image and CSV.

Export Graph Image

Click or tap untitled and choose Export to export your Spectral Analysis graph as an image file (.png).

Make any adjustments to line shading, label size, and graph shape, then click or tap **SAVE PNG**.

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.

Export CSV (data file)

Click or tap \Box untitled, choose Export, then click or tap CSV.

Select the appropriate decimal format for your data, then click or tap **SAVE CSV** to save the file.





Printing a File

You cannot print directly from Spectral Analysis. To print a Spectral 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 Spectral Analysis, see www.vernier.com/til/3789

APPENDICIES

APPENDIX A – Spectrometer Settings 🌣

The following information describes the spectrometer setting options available in Spectral Analysis. The available tools depend on the experiment type and the connected spectrometer.



Device Information

Click or tap () to view information about the connected spectrometer.



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Sensor Mode

This option is only shown for an Advanced Full Spectrum experiment.

Select the type of full spectrum data you want to collect. Choices include Absorbance, Transmittance, Fluorescense, Emissions, and Raw Data. Available choices depend on the spectrometer you are using.



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Emissions

) Transmittance

Raw Data

Collection Set

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Collection Settings

The available options depend on the experiment type and the connected spectrometer.

Calibrate

Click or tap **CALIBRATE** to start a new calibration from Collection Settings.

TIP! CALIBRATE is not available while you are actively collecting data.



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• Integration Time

Values are whole numbers between 0 and 500 ms.

The integration time is the time that the individual diodes in the sensor array are exposed to light before the reading is recorded and reset to zero. The diodes respond linearly to light until they approach saturation.

TIP! This is the most commonly manipulated parameter.

TIP! For Absorbance and % Transmittance experiments, the integration time is determined during calibration and is not editable.

Wavelength Smoothing

Values are whole numbers between 1 and 10.

Wavelength smoothing is used to reduce the affects of noise on your spectrometer measurements. The smoothing calculation uses a boxcar average of a specific number of points on either side of the measured wavelength. For example, a value of 5 will average each data point with the five data points on either side of that point, averaging 11 values for each reading.

TIP! The higher the wavelength smoothing value, the higher the signal to noise ratio for your data. However, there is a corresponding loss in spectral resolution. This can result in a peak maxima being shifted and inaccurate.

• Temporal Averaging

Values are whole numbers between 1 and 10.

Use this value to determine the number of internal measurements that are used to determine the reported spectrometer reading. The more readings that are averaged, the better the signal to noise ratio. This directly impacts the time between reported measurements.

TIP! A value of 10 will average ten internal readings before reporting a value. If your Integration Time is set to 500 ms, the spectrometer readings will be updated once every 5 seconds.

TIP! You cannot modify this value when using Go Direct[®] spectrometers connected to your device via Bluetooth[®] wireless technology. In that case, the temporal averaging is done on the spectrometer and not in the software. If adjusting the temporal average is required for your experiment, connect the spectrometer to a computer or ChromebookTM via USB.

• LED Intensity

Values are whole numbers between 0 and 100%.

This value is only available when collecting fluorescence data using a Fluorescence/UV-VIS Spectrophotometer. Use this to control the excitation-LED intensity. Use this feature to explore the affects of excitation intensity on fluorescence.



Collection Interval

The Collection Interval can be any whole number from 1 to 3600 seconds. The smallest value is determined based on the Collection Settings. The software will calculate this value for you. If a smaller value is desired, consider lowering the Integration Time, Wavelength Smoothing, or Temporal Averaging, if possible.

If you are using Go Direct[®] spectrometers connected via Bluetooth[®] wireless technology, the minimum value is 3 seconds.

• Excitation Wavelength

Click or tap the drop-down to select that desired excitation wavelength. The wavelength options shown depend on the spectrometer you are using.

When using SpectroVis[®] Plus or Go Direct SpectroVis Plus, the selection is used to turn on the excitation LED. The default wavelength is 500 nm.

When using a Fluorescence UV-VIS spectrometer, the default excitation wavelength is 375 nm. The app cannot automatically detect the wavelength of the LED you are using.





APPENDIX B – Updating Spectral Analysis on a Computer ····

Spectral Analysis automatically checks for updates when your computer has an internet connection. When an update is available, the Update Available option is shown. Follow the steps below to update Spectral Analysis.

 Click or tap ... to access the Other Options menu and select • Update Available.



2. Click or tap **DOWNLOAD UPDATE** to download the update.

3. The app must restart for the update to install. Click or tap **RESTART APP** to complete the update.

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4. Click or tap ... on the top toolbar to access the Other Options menu. Choose What's New to view a summary of the new features and fixes available in the new version of Spectral Analysis.

TIP! Click or tap **SHOW ALL RELEASES** to see changes made in previous versions.

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Nickel Sulfate Analysis.ambi				\$⊞	
Full S	What's New	×	* 0.24M NISO4 **		
16	Version 4.12 Released 12/7/2023	3.		Absorbance ••	
	NEW 1. 2. or 3 Graph views now available.	2			
.08	NEW Contextual menu for easy access to operations on graph selections.	4			
- 08	NEW Linked X axes in multiple graphs for simultaneous examine lines and orouned scaling.	<u>6</u> 7	366.2 - 267.4		
a	NEW Customize the color of individual graph traces.	E R			
	FIX Subsequent runs after deletion are now plotted properly.	10	390.7		
	CHANGE New OS Minimums: • macOS 11.7 • Windows 10 version 21H2 • Android 10	12	393.0 394.1		
	• chromeus 108 • iOS 15.7.9.	14			
400 500	SHOW ALL RELEASES	116			
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APPENDIX C – Getting Additional Help

Curriculum Resources

The following Vernier lab manuals have experiments that utilize Spectral Analysis:

- Biology with Vernier
- Investigating Biology Through Inquiry
- Chemistry with Vernier

- Advanced Chemistry with Vernier
- Investigating Chemistry Through Inquiry
- Vernier Chemistry Investigations for Use with AP Chemistry

In addition to these resources, Vernier offers a complete set of lab books for elementary through college. For more information, see www.vernier.com/books

Technical Assistance from Vernier Software & Technology

For access to user manuals, forums, and our technical information library, please visit our website at www.vernier.com/support

You can also contact us directly by phone or email:

Toll Free: 888.837.6437 Email: support@vernier.com



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