Spectrometer User's Guide

(Order Codes: V-SPEC, SPRT-VIS, SP-VIS, SP-UV-VIS, ESRT-VIS)

The spectrometer is a portable light spectrophotometer, combining a spectrometer and a light source/cuvette holder. The light source/cuvette holder may be detached and an optical fiber assembly attached to the spectrometer for emission spectrum experiments.

What is included with the Vernier Spectrometer?

- One spectrometer with light source/cuvette holder (Vernier Spectrometer, Ocean Optics™ Red Tide Spectrometer, Ocean Optics Red Tide Emissions Spectrometer, Ocean Optics VIS-NIR Spectrometer, Ocean Optics UV-VIS Spectrometer)
- Reference Guide (this document)
- One package of 15 plastic cuvettes and lids
- One USB cable

Important Note

Logger *Pro* 3.4.5 (or newer) software is required. If you own a previous version of Logger *Pro* 3, you may upgrade to 3.4.5 (or newer) free of charge.

Get Started

Install Logger *Pro* 3.4.5 Software on Your Computer

1. Place the Logger *Pro* 3.4.5 CD into the CD-ROM drive of your computer.
2. Follow the onscreen instructions to install the software.
   a. Windows computers (Windows 98, 2000, ME, or XP). In many cases the installation will launch automatically. Otherwise, choose Settings → Control Panel from the Start menu. Double-click on Add/Remove Programs. Click the Install button in the dialog box.
   b. Double-click on the Install Logger *Pro* icon on the CD.
3. The first time you connect a Vernier Spectrometer, or an Ocean Optics Spectrometer, to a computer it will need to be recognized as a USB hardware device.
   a. Windows computers (Windows 98, 2000, ME, or XP) Follow the New Hardware Wizard instructions.
   b. Macintosh computers (Mac OS 10.3 or newer) Follow the New Device instructions.

Tutorial

This tutorial will guide you through the process of setting up the Spectrometer and conducting three types of data collection: a full spectrum analysis, Beer's law, and the kinetics of a chemical reaction. The tutorial is written to test a crystal violet solution. If you do not have crystal violet, other indicators may be substituted (bromcresol green, for example, works well).

If you decide not to complete the tutorial in its entirety, complete Part I and any of the other parts of the tutorial. The Spectrometer needs to be calibrated before use, except when you are measuring emission spectra.

Materials Needed for the Tutorial

- 2.0×10^{-5} M crystal violet solution (Prepare the solution by adding 0.16 g of solid crystal violet to ~500 mL of distilled water and dilute to 2 liters. Measure out 100.0 mL of this solution and dilute to 1 liter.)
- 0.10 M sodium hydroxide solution
- 4–5 dilute crystal violet solutions (1.75×10^{-5} M, 1.5×10^{-5} M, 1.25×10^{-5} M, etc.)
- unknown crystal violet solution (dilute from the stock 2.0×10^{-5} M solution)
- 50 mL or 100 mL beakers for mixing solutions
- plastic Beral pipets or eyedroppers to transfer solutions to cuvettes
- two 10 mL graduated cylinders

Part I Set Up the Spectrometer

1. Use a USB cable to connect the Vernier Spectrometer to the computer. The cuvette holder/light source should be attached to the Spectrometer. The Spectrometer is powered by your computer through the USB cable.
2. Start the Logger *Pro* 3.4.5 software.
3. Select Connect Interface → Spectrometer → Scan for Spectrometers from the Experiment menu.
4. To calibrate the Spectrometer, choose Calibrate → Spectrometer from the Experiment menu. The calibration dialog box will display the message: "Waiting …seconds for lamp to warm up." (see Figure 1) The minimum warm up time is one minute. **NOTE: For best results, allow the spectrometer to warm up for at least three minutes.** Follow the instructions in the dialog box to complete the calibration. Click OK.

Figure 1

Part II Measure the Absorbance Spectrum of an Aqueous Sample (Absorbance *vs*. Wavelength)

1. Fill a cuvette about ¾ full of 2.0×10^{-5} M crystal violet solution. Place the sample in the cuvette holder of the Spectrometer and click Collect. Click Stop to end the data collection. Examine the graph and note the wavelength region of maximum absorbance.

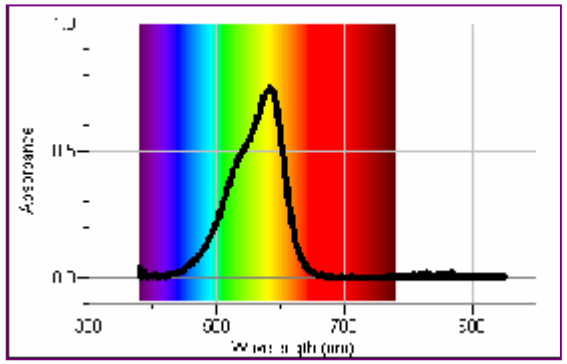


Figure 2: Absorbance spectrum of a 1×10^{-5} M crystal violet solution

2. To store the spectrum data, choose Store Latest Run from the Experiment menu.

Part III Conduct a Beer's Law Experiment (Absorbance *vs*. Concentration)

1. Place a cuvette of 2.0×10^{-5} M crystal violet solution in the Spectrometer. Click on the Configure Spectrometer Data Collection icon, , located on the right hand side of the toolbar to open the Configure Spectrometer Data Collection display.
2. Click Abs *vs.* Concentration (under Set Collection Mode). The wavelength of the maximum absorbance will be automatically selected (see Figure 3). Click OK to close the display.

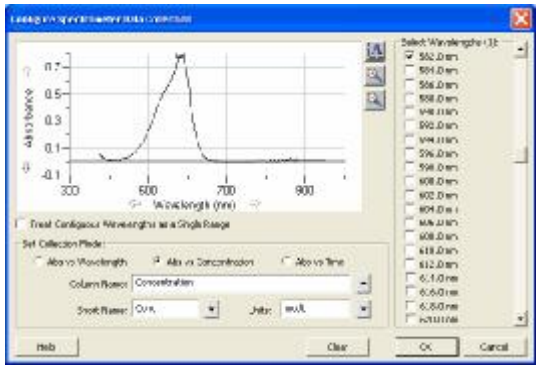


Figure 3: The Configure Spectrometer Data Collection dialog box

3. Place your first Beer's law standard solution in the cuvette slot. Click Collect and then click Keep. Enter the concentration of the sample and click OK. Repeat this step for the remaining standard samples. After you have tested the final standard, click Stop to end the data collection.
4. Click linear fit, , to see the function for the standard solutions.
5. Place an unknown sample of crystal violet solution in the cuvette holder. Choose Interpolation Calculator (**not** Interpolate!) from the Analyze menu. A helper box will appear, displaying the absorbance and concentration of the unknown. Click OK (see Figure 4).
6. To store the data, select Store Latest Run from the Experiment menu.

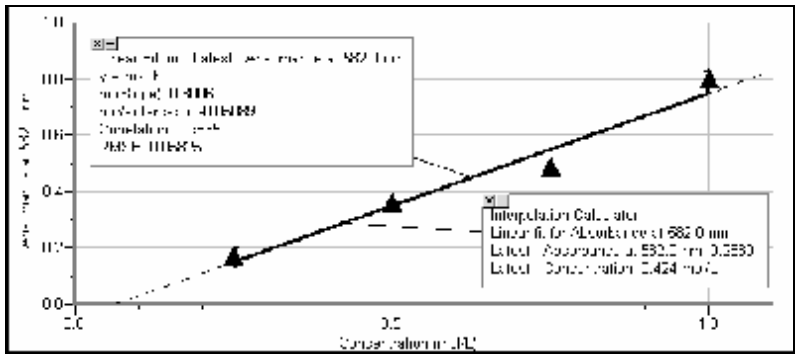


Figure 4: Typical Beer's law analysis of an unknown sample of crystal violet

Part IV Conduct a Kinetics Experiment (Absorbance *vs*. Time)

1. Click on the Configure Spectrometer Data Collection icon, .
2. Click Abs *vs.* Time (under the Set Collection Mode). The wavelength of maximum absorbance will be selected as before. Click OK.
3. Select Data Collection from the Experiment menu. The default settings are 1 sample per second for 200 seconds, which works well for this experiment. Click Done.
4. Use graduated cylinders to measure out 10 mL each of 2×10^{-5} M crystal violet solution and 0.10 M NaOH solution. Mix the solutions together in a small beaker. Transfer ~2 mL of the reaction mixture to a cuvette and place the cuvette in the Spectrometer. Click Collect. You may click Stop to end the data collection early.
5. Analyze the graph. Note the gradually decreasing absorbance as the reaction proceeds (see Figure 5).

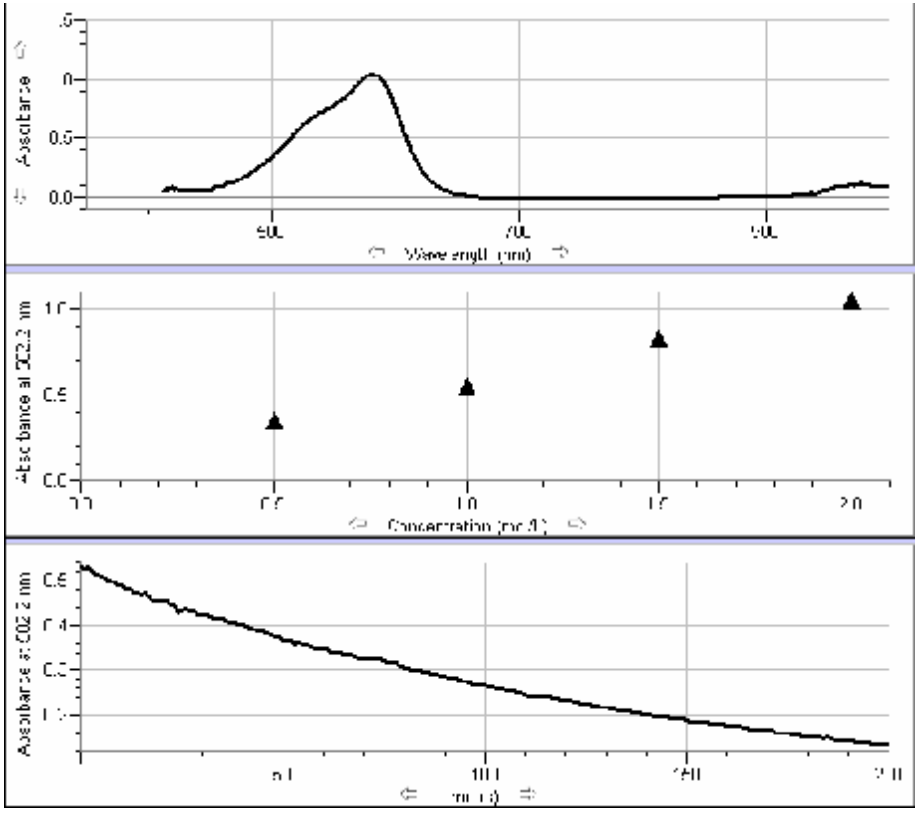


Figure 5

6. Click curve fit, , to calculate a function for your data (see Figure 6). Try an exponential function to fit the data.

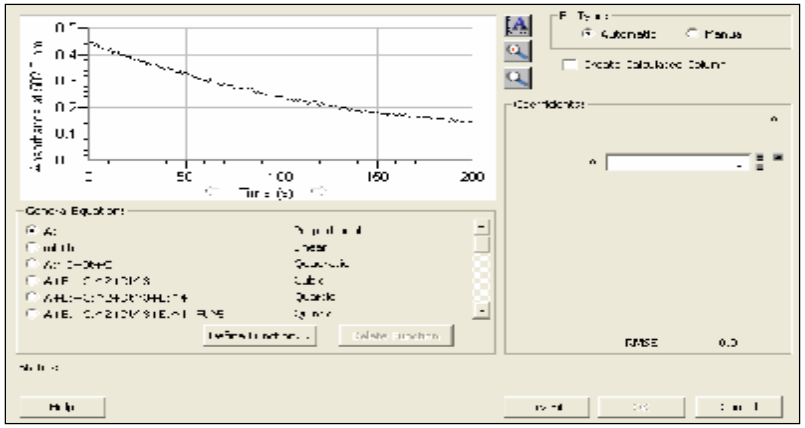


Figure 6

Using the Spectrometer to Measure Emission Spectra

You may use your spectrometer to measure the emission spectrum of a light source such as an LED or a discharge tube. To do so, you may want to purchase an optical fiber assembly (order codes: VIS-NIR or UV-VIS). You may also purchase an optical fiber assembly directly from Ocean Optics.

Part I Set Up the Spectrometer for Emission Spectrum

1. Use a small screwdriver to loosen the two bolts that connect the cuvette holder to the Spectrometer (see Figure 7). Remove the cuvette holder and connect an optical fiber assembly to the Spectrometer.

Figure 7

2. Use a USB cable to connect the Spectrometer to your computer.
3. Start Logger *Pro* 3.4.5. Choose Connect Interface → Spectrometer → Scan for Spectrometers from the Experiment menu.

Part II Measure an Emission Spectrum

1. Choose Change Units → Spectrometer → Intensity from the Experiment menu. Intensity is a relative measure.
2. Aim the tip of the optical fiber cable at a light source. Click Collect. Observe the graph of intensity *vs.* wavelength. Click Stop to end data collection. **Note**: If the spectrum maxes out with flat tops to peaks, reduce the integration time.

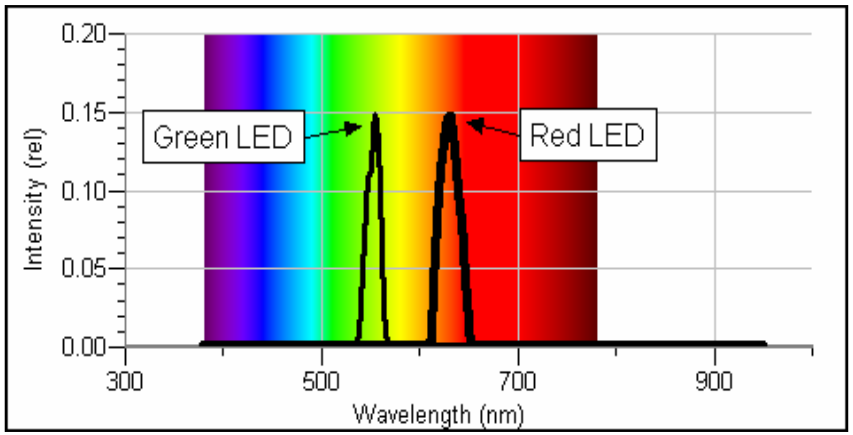


Figure 8: Emission spectra of green and red LEDs

3. You can use the optical fiber assembly to conduct an interesting analysis of the visible spectrum display on your computer screen. Aim the top of the optical fiber assembly at your computer screen and click Collect. Move the assembly slowly across the screen. Observe the changes on the graph of emission as you move the optical fiber.

The Logger *Pro* 3.4.5 Dialog Boxes for the Spectrometer

Spectrometer Dialog Box

The Spectrometer dialog box lists all of the settings for the device (see Figure 9). You can display this box by choosing Set Up Sensors → Show All Interfaces from the Experiment menu.

Note: For most experiments, the default settings work well. If you change any of the settings, we recommend recalibrating the Spectrometer for the best results.

Figure 9

There are four parameters listed in the dialog box.

- Integration Time: think shutter speed of a camera. Logger Pro automatically selects the proper integration time during calibration. **Note:** For emission studies, you may need to change Integration time manually.
- Wavelength Smoothing: the number of adjacent readings on either side of a given value that is used to calculate an average value.
- Samples to Average: the number of readings taken at a given wavelength to calculate an average reading.
- Wavelength Range: the range is determined by the type of spectrometer in use.

By clicking on the picture of the Spectrometer in this dialog box, you can gain access to three options: calibrate, configure data collection, and units of measure (see Figure 10). Click on an item to select it.

Figure 10

Configure Spectrometer Data Collection Dialog Box

To display this box, click on its icon, , located on the right hand side of the toolbar (see Figure 11).

Figure 11

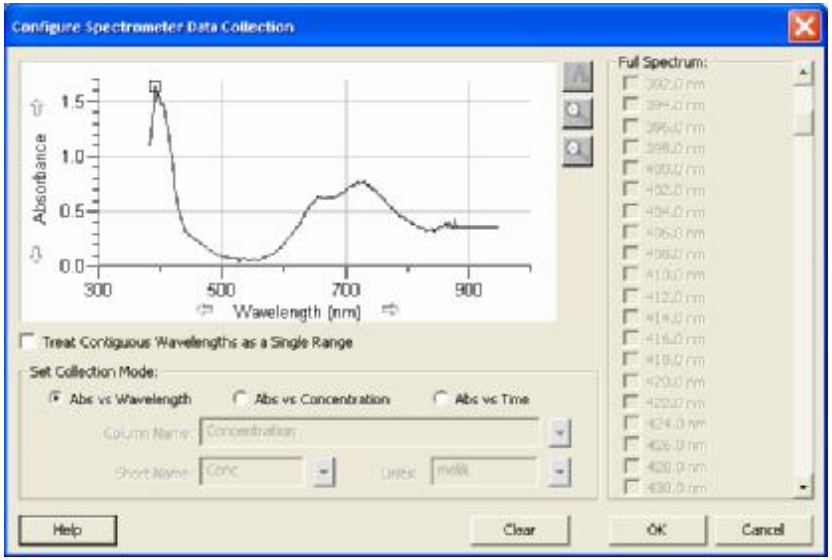
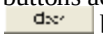


Figure 12

There are three regions in this box and four buttons at the bottom (see Figure 12).

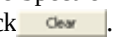
- Graph: The graph displays a full spectrum analysis of the sample in the cuvette holder. By default, the wavelength of greatest absorbance (peak) will be

marked with a box. You may select other wavelengths by clicking on the plot at the desired wavelength. A checkbox beneath the graph allows you select a portion of the graph and analyze it as a single range of wavelengths.

- Set Collection Mode: Three options for data collection are offered. A full spectrum analysis (Abs *vs.* Wavelength) is the default.
- Full Spectrum/Select Wavelength: This column lists all the available wavelengths. It becomes active when you select Abs *vs.* Concentration or Abs *vs.* Time. Check the box for each wavelength you wish to use in an experiment. When you select a wavelength from the list, a box appears on the graph.
- For the most part, the four buttons across the bottom of this dialog box are self-explanatory. However, the  button's job may not be obvious—use it to remove all of the wavelengths selected on the graph.

Determining the Wavelength(s) to Use in an Experiment

When you conduct a Beer's law lab or a kinetics lab, it is common to select one wavelength at which to follow the experiment. However, in Logger Pro 3.4.5 you may select as many wavelengths as you wish. There are three ways to select the wavelength or wavelengths.

1. **Perform a Full Spectrum Analysis of the Solution to Be Tested**
   This method is best when you wish to keep a copy of a full spectrum graph. Conduct the full spectrum of a sample of solution and examine the graph. Go to the Configure Spectrum Data Collection dialog box and select Abs *vs.* Time. The wavelength of maximum absorbance will be automatically selected.
2. **Use a Sample of Solution to Determine the Peak Absorbance**
   This is a variation of the previous method, in cases where you don't wish to keep a copy of the full spectrum analysis. After calibrating the Spectrometer, place a sample of solution in the Spectrometer and go to the Configure Spectrum Data Collection dialog box. Select Abs *vs.* Time for a kinetics experiment, or select Abs *vs.* Concentration for a Beer's law experiment. The wavelength of maximum absorbance will be automatically selected.
3. **Select the Wavelength of Maximum Absorbance Manually**
   This method can be used when you already know the precise wavelength to be used in an experiment. After calibrating the Spectrometer, go to the Configure Spectrum Data Collection dialog box. Click  . Select a wavelength on the graph or in the list of wavelengths.

Selecting a Range of Wavelengths to Use in an Experiment

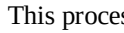
In many experiments you may wish to measure the absorbance or %T of a sample over a group of wavelengths rather than a single wavelength. There are two ways to select a group of wavelengths from the Configure Spectrum Data Collection dialog box. You may select the wavelengths one at a time by checking the boxes in the Full Spectrum column, or place the cursor on the graph in the dialog box. Left click and drag across the region of wavelengths that you wish to analyze. Make sure to check the "Treat Contiguous Wavelengths as a Single Range" box.

Choosing a Unit of Measure

You may use absorbance or % transmittance when you are conducting spectrophotometric studies. To select a unit of measure, choose Change Units → Spectrometer from the Experiment menu. Click on the unit of choice from the list.

Using the Interpolation Calculator

In a typical Beer's law experiment you will measure the absorbance of a set of standard solutions, after which you will calculate a best-fit line equation. Later, you will measure the absorbance of an unknown solution and use the best-fit line equation to determine the concentration of the unknown. Logger *Pro* 3.4.5 contains an option called the Interpolation Calculator that helps you test unknowns more efficiently. Follow the steps below.

1. Measure the absorbance of the standard solutions.
2. Click linear fit,  , to calculate the best-fit line equation for the standard solutions.
3. Place an unknown sample in the cuvette holder. Select Interpolation Calculator from the Analyze menu. A helper box will appear, displaying the absorbance and concentration of the unknown.
4. Click  . This process can be repeated with multiple unknowns.

   The Interpolation Calculator can also be used with imported or sample data as part of a pre-lab activity, or as a method of predicting the concentration of selected samples before measuring their actual absorbances.

Specifications

Vernier Spectrometer (order code: V-SPEC)

Dimensions: 10 cm × 8.7 cm × 3 cm (includes cuvette holder/light source)

Power: from computer via USB cable

Wavelength Range: 380 nm–950 nm

Resolution: 2 nm

Red Tide Spectrometer (order code: SPRT-VIS)

Dimensions: 10 cm × 8.7 cm × 3 cm (includes cuvette holder/light source)

Power: from computer via USB cable

Wavelength Range: 380 nm–950 nm

Resolution: 1 nm

Red Tide Emission Spectrometer (order code: ESRT-VIS)

Dimensions: 6.3 cm × 8.7 cm × 3 cm (no cuvette holder/light source)

Power: from computer via USB cable

Wavelength Range: 380 nm–950 nm

Resolution: 1 nm

Ocean Optics VIS-NIR Spectrometer (order code: SP-VIS)

Dimensions: 10 cm × 8.7 cm × 3 cm (includes cuvette holder/light source)

Power: from computer via USB cable
Wavelength Range: 380 nm–950 nm
Resolution: 0.2 nm

Ocean Optics UV-VIS Spectrometer (order code: SP-UV-VIS)
Dimensions: 14.2 cm × 8.7 cm × 3 cm (includes cuvette holder/light source)
Power: AC adapter (included)
Wavelength Range: 200 nm–850 nm
Resolution: 0.2 nm

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