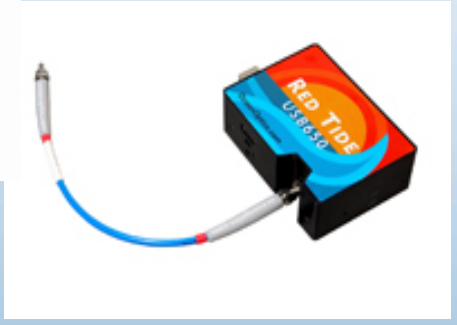
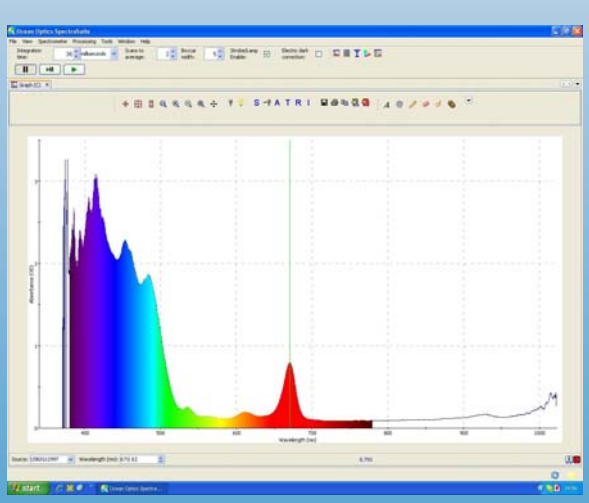
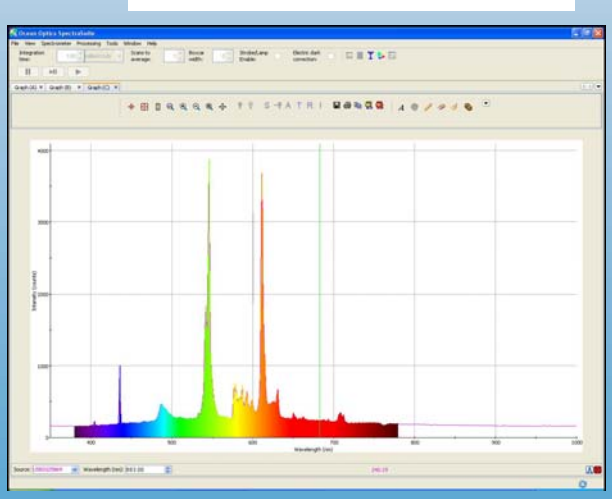
Ocean Optics Educational Spectrometers

Getting Started Manual







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PACKAGE CHECKLIST

Verify that your package contains the following:

- **Ocean Optics spectrometer**
- **USB cable (USB-CBL-1):** Connects your spectrometer to a PC's USB port.
- **Packing List:** Attached to the outside of the shipment box (the invoice arrives separately).
- **Wavelength Calibration Data Sheet:** SpectraSuite Operating Software reads this calibration data from your spectrometer when it interfaces to a computer via the USB port.
- **Software and Technical Resources CD:** Contains software, operating instructions, and product information for all Ocean Optics software, spectrometers, and spectroscopic accessories. You need Adobe Acrobat Reader version 6.0 or higher to view these files (version 7.0 is included on the CD).
- **Passwords:** For any password-protected software that you have purchased. SpectraSuite software requires a password. Passwords are located on the back of the *Software and Technical Resources* CD jacket.

Spectrometers requiring a power supply have one included in the package.

INSTALLING SPECTRASUITE SOFTWARE

Caution! : Install the software BEFORE connecting the spectrometer to your PC. The SpectraSuite software installs the drivers required for spectrometer installation. If you do not install SpectraSuite first, the system will not properly recognize the spectrometer.

1. Close all other applications running on the computer.
2. Load the *Software & Technical Resources CD*.
3. Start installing SpectraSuite.

To install on a Windows PC: The CD automatically launches. Navigate to **Install Ocean Optics Software | SpectraSuite | Windows OS**. The installation process begins.

To install on a Mac: Double-click on the CD icon and open the OceanOptics.html file to launch the CD. Then, navigate to **Install Ocean Optics Software | SpectraSuite | Mac OS.** Double-click on the newly selected .dmg file, and copy the SpectraSuite icon to Desktop or Applications.

4. Follow the prompts on the Installation Wizard.
5. Click the **OK** to restart your computer. You have now installed the SpectraSuite software.

CONNECTING THE SAMPLING SYSTEM

If using the ISS-VIS sampling unit for chemistry experiments using cuvettes, simply connect to Red Tide using the two captive bolt connectors. Use a small screwdriver and do not over tighten.

INSTALLING YOUR SPECTROMETER

To connect the USB cable that came with the spectrometer to your computer via the USB port.

1. Locate the USB cable (USB-CBL-1) provided with the spectrometer.
2. Insert the square end of the cable into the side of the spectrometer (USB port).
3. Insert the rectangular end of the cable into the USB port of the computer (the USB port can be on either the front or the rear of the computer). The computer installs the spectrometer's drivers.

START UP

1. Check that Red Tide is connected.
2. Run the SpectraSuite software by double-clicking on the SpectraSuite icon or navigating to the folder where you stored SpectraSuite when you installed it.

The SpectraSuite screen appears (in Scope mode) with your spectrometer shown in the **Data Sources** pane on the left. Scope mode is the normal start up mode. It displays a live spectrum with the y-axis calibrated in Intensity (counts) In this case the spectrometer is detecting light from a fluorescent lamp showing mercury emission lines. See Fig.1

Note: If the Red Tide image does not appear, select **Spectrometer>Rescan Devices** (F5). When it appears, go to **File>New>Spectrum Graph** (Ctrl+G).

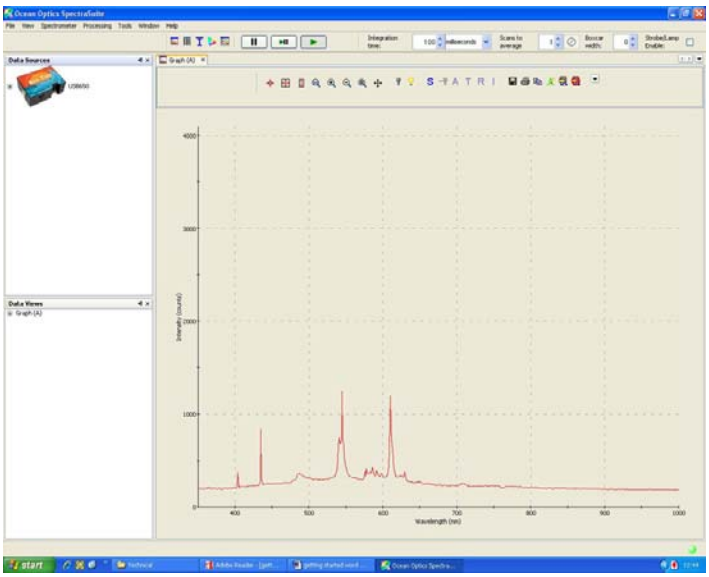


Fig. 1

If you click on the + sign to the left of the spectrometer image shown on your screen, the following information appears:
Acquisition parameters that you set (integration time, scans-to-average, boxcar smoothing).

Whether dark and/or reference spectra have been stored, the graph (A, B, C, etc.) associated with this spectrometer that appears in the right pane (important if you have installed more than one spectrometer)

Spectrometer's properties (serial number, firmware level, number of pixels, and wavelengths).

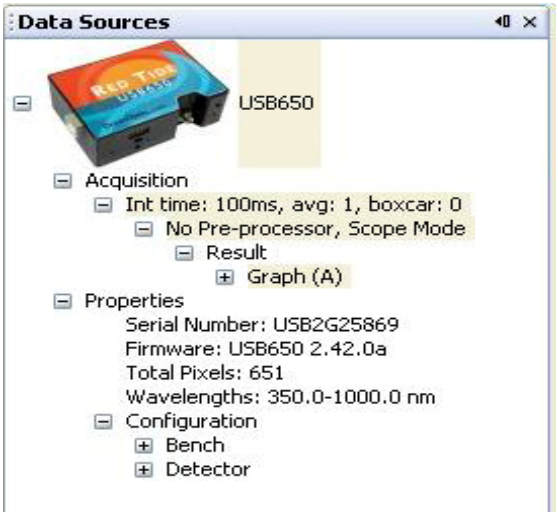


Fig. 2

INTEGRATION TIME

Integration time is the "exposure time" for the CCD array. The default value is 100ms. If the integration time is too high the trendline will "saturate" by exceeding the maximum count of 4095. (See Fig.3) No harm is done, but to see the full trace the integration time must be reduced, or the light source attenuated.

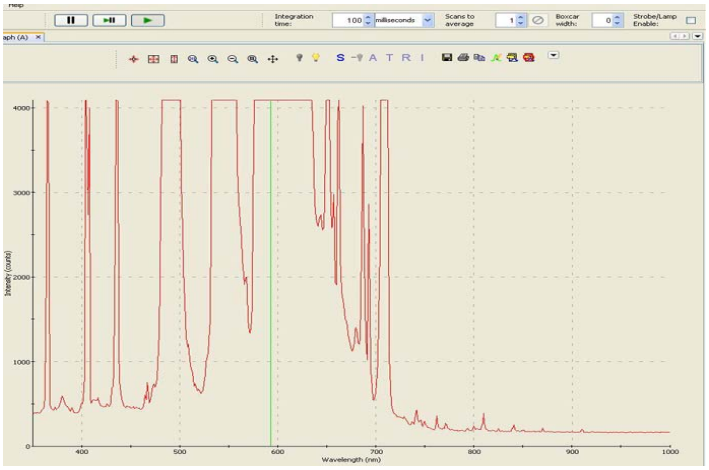


Fig. 3

SCANS TO AVERAGE

SpectraSuite can average consecutive scans to smooth out noise. This is normally not required but can be useful for low intensity sources.

BOXCAR WIDTH

Boxcar is the averaging of the counts from adjacent groups of pixels. The effect of increasing the boxcar width is to reduce the wavelength resolution. For Red Tide it is not normally required.

EXPERIMENT DATA

The start mode is called Scope mode. This shows raw data in photon counts and is fine for most physics applications. Note that only the **S** is live. The other experiment modes are grayed out.
Before experiment data can be collected, dark and reference readings must be taken.

DARK READING

The trendline in Scope mode does not drop to zero. The dark reading is about 160.

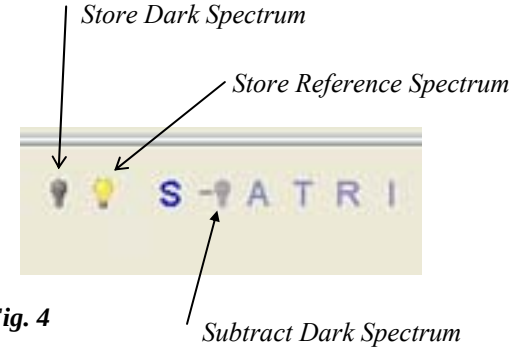


Fig. 4

To perform quantitative experiments the dark reading must be recorded and subtracted from the Scope mode values. To do this, block any light entering the spectrometer and then click on the Store Dark Spectrum icon. The Subtract Dark Spectrum icon will go live. Clicking on it will subtract the dark value and the trendline will drop to the x-axis. Zero is now zero and the math will work.

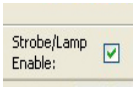
REFERENCE READING

A reference reading is a spectrum that is stored for mathematical comparison with sample readings to be taken.

Reference readings are normally taken with the ISS-VIS lamp with cuvette holder attachment as shown, using an empty cuvette or one containing the solvent in use.

Fig. 5

Reference readings can be taken using the fiber optic probe. However the probe and source must be clamped in position for this to work. The slightest movement in the probe will change the readings.
Switch on the lamp by checking the Strobe/Lamp Enable box.



Adjust the integration time to give a reference reading that has a maximum count of about 3500.

Click on the Store Reference Spectrum icon (See Fig.4).

When both dark and reference readings have been taken, all the experiment modes go live. See Fig 6.

A - Absorbance
T - Transmission
R - Reflectance (Advanced users)
I - Irradiance (Advanced users)

Fig. 6

Note:
Reference and dark readings must be taken with the same integration time. All samples must stick to this integration time or the results will be meaningless.

TRANSMISSION

T

Transmission is the sample intensity as a percentage of the reference intensity. When you select Transmission mode, the y-axis units change to percentage.

$$\textbf{Transmission \%} = \left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \right) \times 100$$

A

ABSORBANCE

Absorbance is the inverse of transmission, but on a log scale. When you select Absorbance mode the y-axis changes to a log scale of Absorbance number.

$$\textbf{Absorbance} = -\log_{10} \left(\frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \right)$$

Where:
S_λ = Sample intensity at wavelength λ
D_λ = Dark intensity at wavelength λ
R_λ = Reference intensity at wavelength λ

Reference and dark spectra must be stored before collecting experiment data. If you pass the cursor over the **No-preprocessor** line in either the Data Sources or Data Views pane, a tool tip box informs you whether reference and/or dark spectra have been stored.

For Reflectance and Irradiance, please refer to the main SpectraSuite manual. This is in the Help menu.

GRAPH CONTROLS

Fig. 7

These icons all have tool tips. Hold the cursor over each to see its function.

1. Zoom to maximum. Useful “home” control if you get lost.
2. Scale graph to fill window.
3. Scale graph height to fill window. Useful for magnifying small y-axis detail.
4. Set axes ranges manually. Useful if you just want to study a limited waveband.
5. Zoom in.
6. Zoom out.
7. Zoom to a selected region. Useful for looking at fine detail.
8. Graph panning.

ACQUISITION CONTROLS

Use the Spectrum Graph icon to create a new graph in Scope mode. Until you do this all the tools are grayed out. Spectrum Table launches a live numeric data table for export to spreadsheet applications.

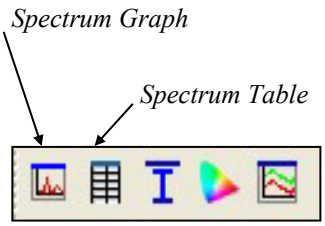


Fig. 8

Note:
If Spectrum Graph is clicked when an active graph is already running, you will have a choice of running two active graphs simultaneously. This should not be done with one spectrometer; it causes pulsing of the strobe-lamp and data will be corrupted.

SPECTRUM I/O

Overlays
An overlay is a spectrum trendline that is not active, but placed in the active graph for comparison. You can create instant overlays using the *Convert Active Spectrum* to overlay icon (see Fig. 9). You can also add saved spectra as overlays and selectively delete overlays.

As overlays are not active spectra, they cannot be saved to file. To save a screen with overlays, use the **File>Screen Capture** command.

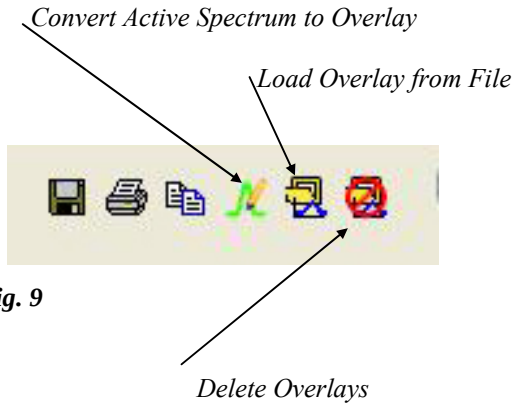


Fig. 9

LAYER TOOLBAR

The Layer toolbar allows annotations and drawing to be made over a graph. These are not spectral data and can only be saved by using the **File>Screen Capture** command.

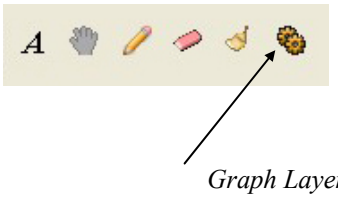


Fig. 10

The Graph Layer Options icon opens the Graph Layer Options window (Fig. 11) for the active graph. You can also reach this by right clicking anywhere on the graph.

GRAPH LAYER OPTIONS WINDOW

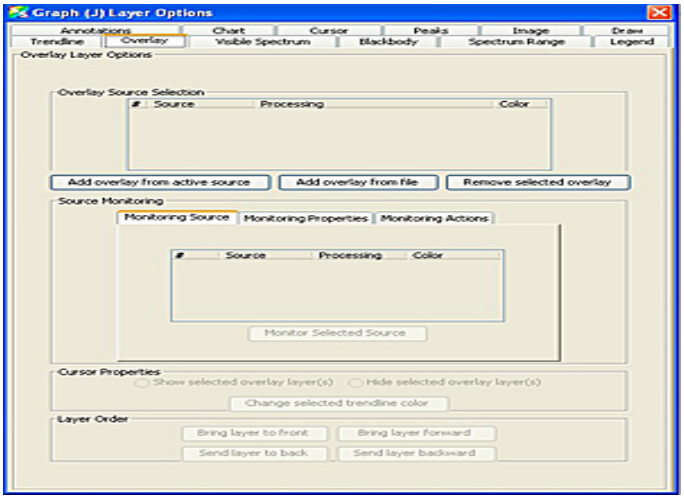


Fig. 11

Visible Spectrum
This adds the visible spectrum to the graph. The spectrum color is filled between 380 and 780nm.

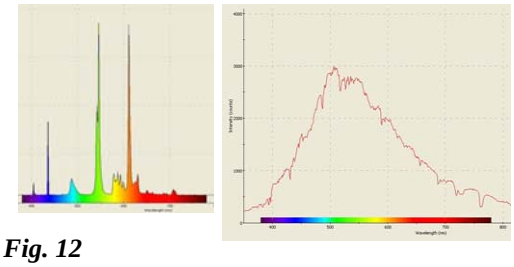


Fig. 12

The visible spectrum color can be attached to the trendline, shown as a bar, or full screen.

CURSOR LAYER

In Graph Layer Options, the Cursor tab allows you to switch the cursor layer on or off and change the color of the cursor line.

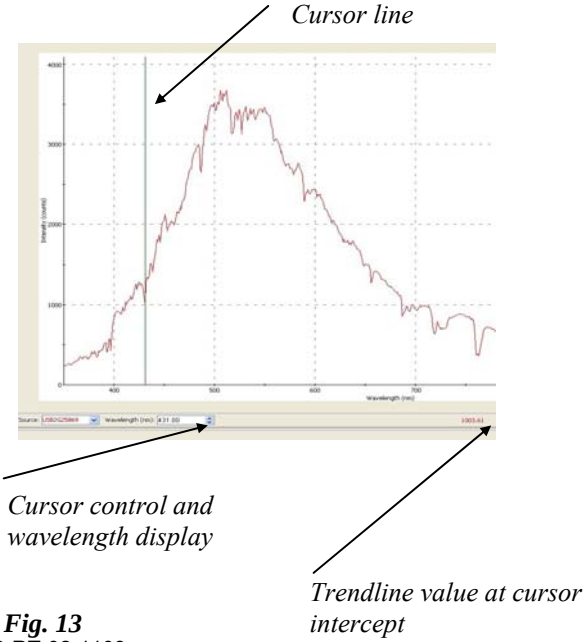


Fig. 13

To move the cursor line, click anywhere in the chart. For fine control, use the cursor control.
Note: A shortcut is: click on the chart to open the cursor layer. Click in the cursor bar to close it.

CHART LAYER

The chart area color and line color and format and be changed.

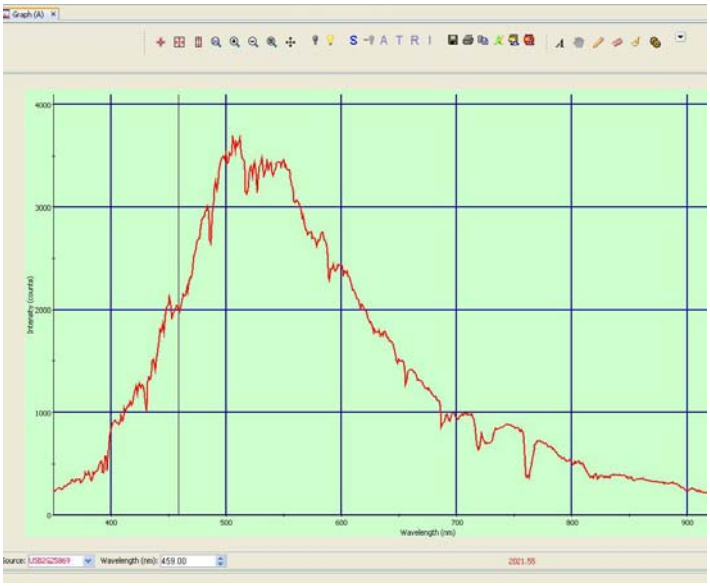


Fig. 14

TRENDLINE LAYER

The color and thickness of the trendline can be changed.

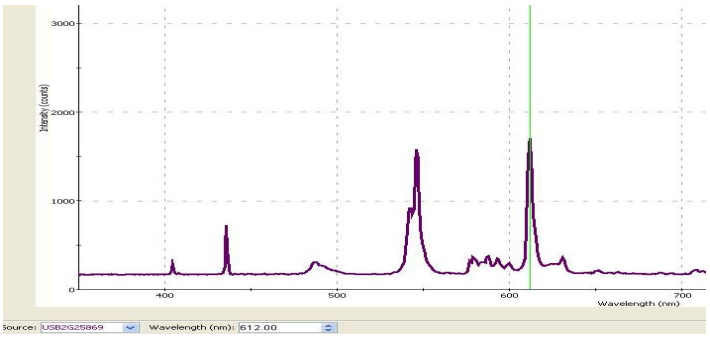


Fig. 15

USING WIZARDS

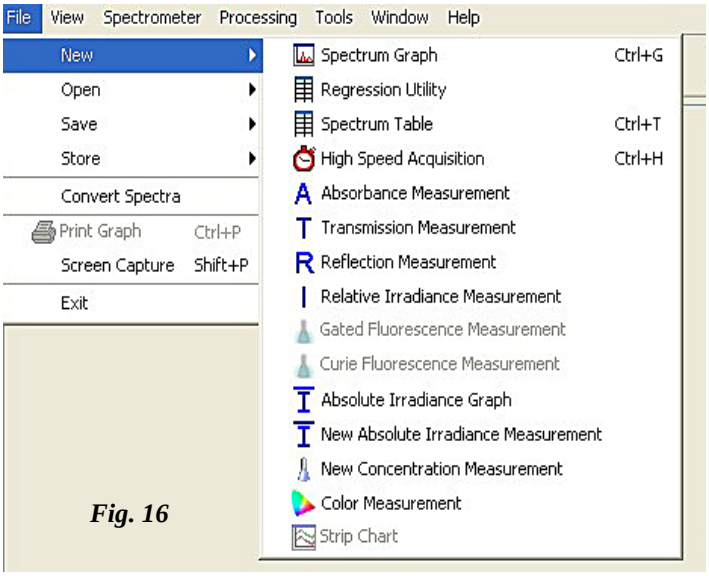


Fig. 16

The **File>New** command opens wizards for Absorbance, Transmission, Reflection and Relative Irradiance. The wizards guide you through the process of taking reference and dark readings. This can also be done in the main chart window by using the toolbar icons.

NEW CONCENTRATION MEASUREMENT

First check that no graph is active. Then select ***File>New>New Concentration Measurement***
In the dialogue box select *New absorbance processing* and click the *Accept* button.

Note:
You can select *Active processing* only if an absorbance graph is already running. Always use Active processing once you have completed the wizard to avoid repeating the process.

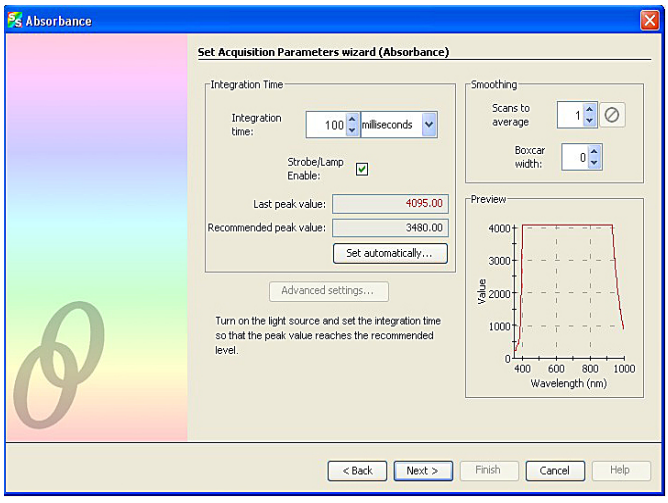


Fig. 17

Switch on the lamp in the Strobe Lamp Enable checkbox. A saturated spectrum will appear in the preview box. Reduce the integration time or use the *Set automatically* button (you must click it twice). The trendline will drop to a maximum of about 3500. (See Fig 18)

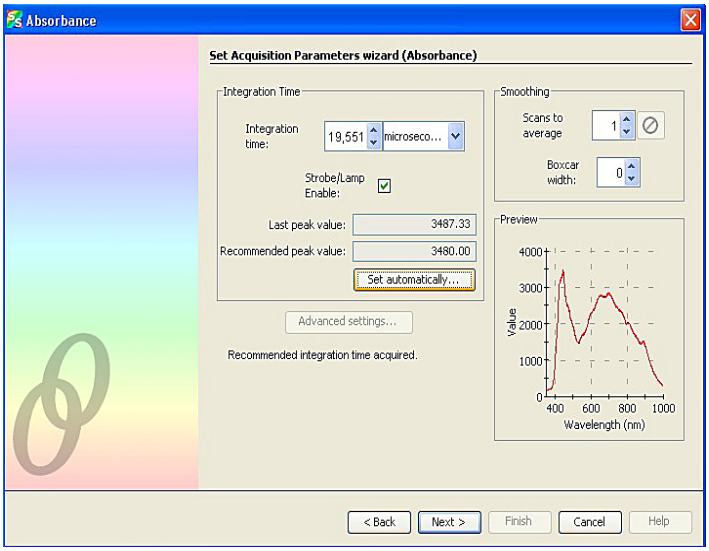


Fig. 18

Next store this spectrum as a reference spectrum by clicking on the Store Reference button.
See Fig. 19

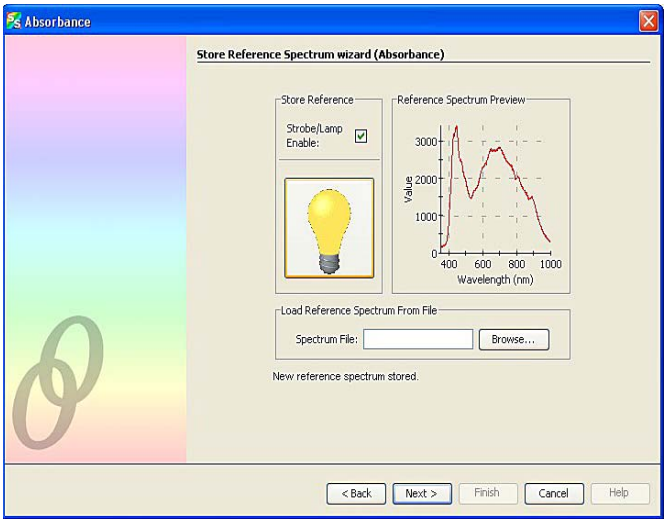


Fig. 19

Next, store a dark spectrum. Either switch off the lamp, or place an opaque object in the cuvette holder to block the light path. Then click the Store Dark button.

Note:
The lamp must be **ON** before you click the Finish button.

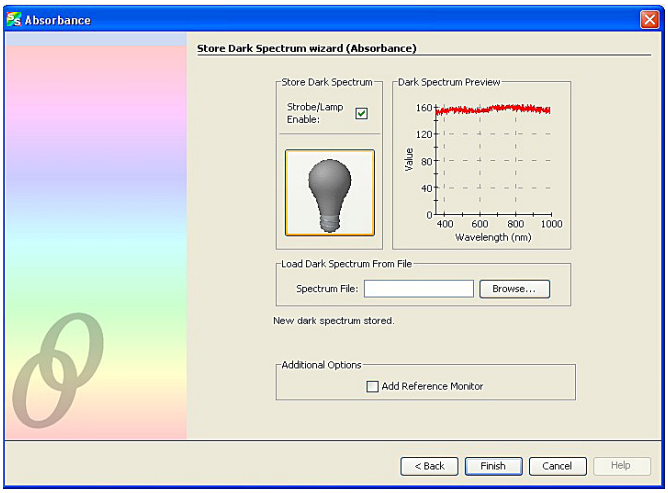


Fig. 20

Click *Finish.*
A dialog box appears giving you three choices. See Fig. 21.

- Beer-Lambert Law
- Calibrate from solutions of known concentration
- Load calibration from file

Notice that an Absorbance graph is running in the chart window. See Fig.21.

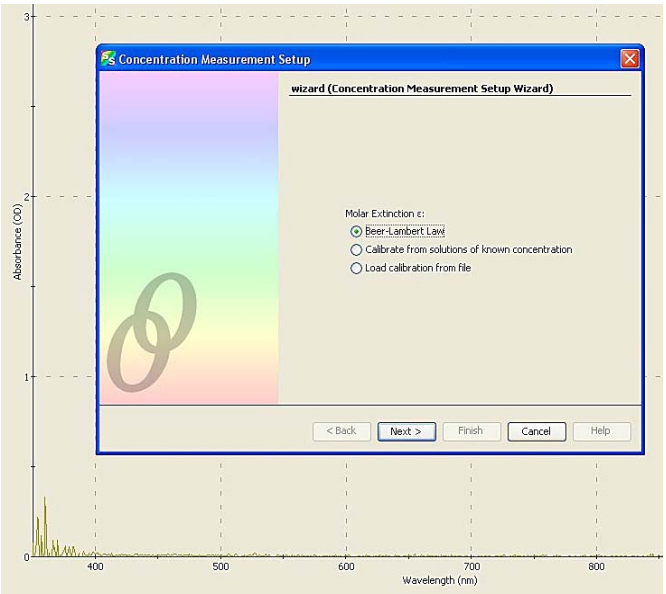


Fig.21

BEER-LAMBERT LAW

Click the radio button for Beer-Lambert Law.

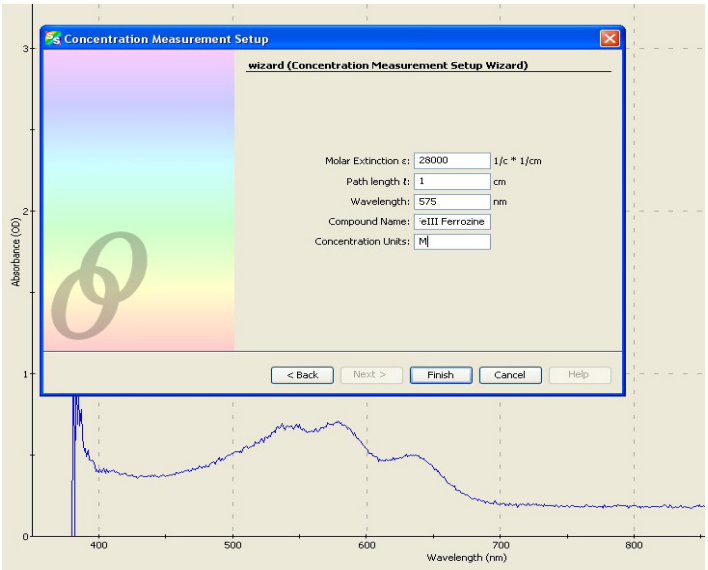


Fig. 22

Enter the data. The value of ε will either come from a reference text or from the experiments with known concentrations described in the next section.
Click *Finish* to see the concentration reading. Now you can use any concentration in a cuvette and get an instant concentration reading by clicking *Single Update* or *Continuous Update.*

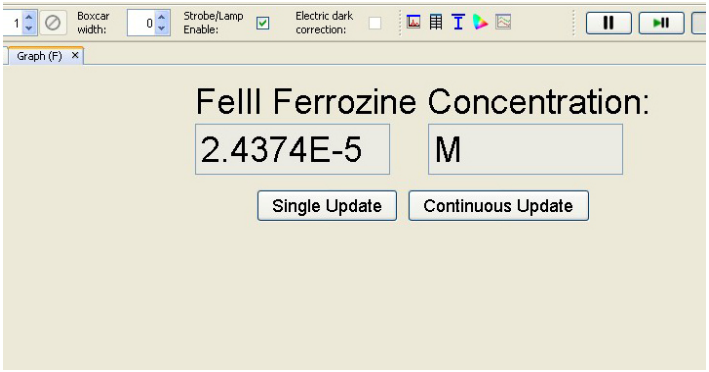


Fig. 23

To run another concentration measurement use ***File>New>New Concentration Measurement***, but use *Active Processing* because you have an active absorbance graph already running.

CALIBRATE FROM SOLUTIONS OF KNOWN CONCENTRATION

(Also see the SpectraSuite manual for more information.)
Go to ***File>New>New Concentration Measurement***

This time click the radio button
Calibrate from solutions of known concentration.
See Fig.21.

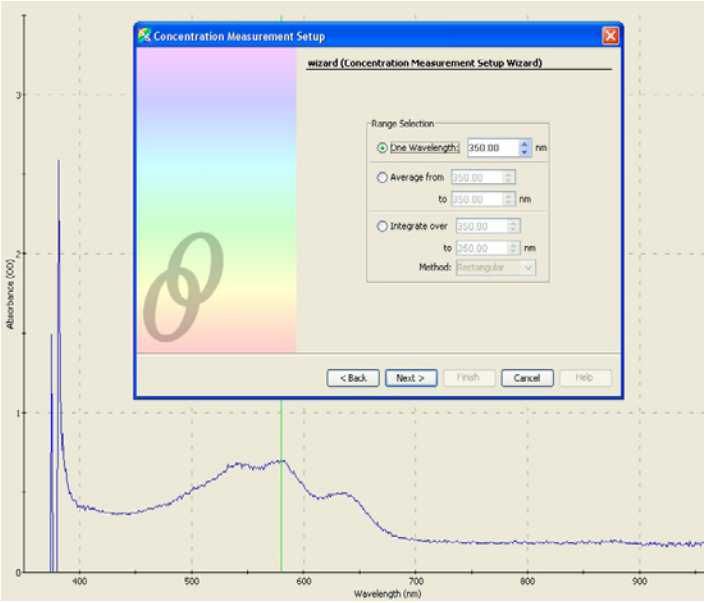


Fig.24

Select a single wavelength, average, or integral over a range. A single wavelength would normally be the maximum absorbance wavelength for the solution,$\lambda_{max,}$ but a range of wavelengths can give a more reliable result. See Fig. 24.

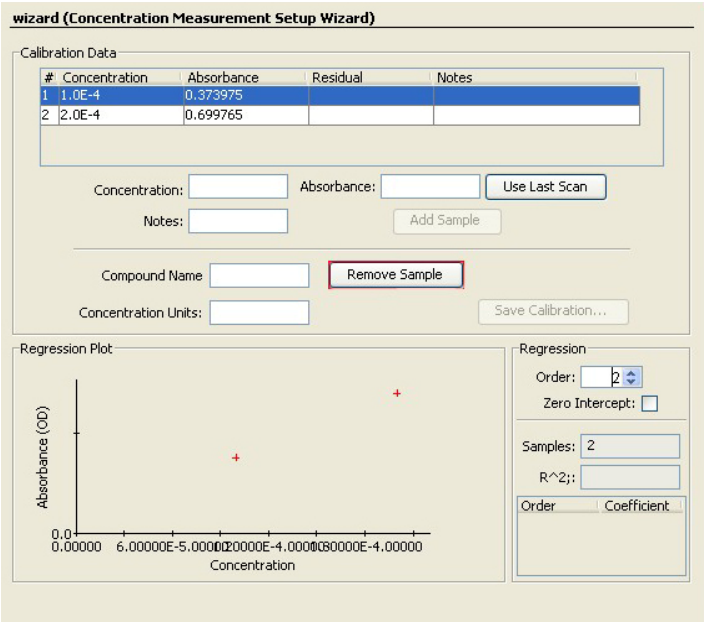


Fig. 25

Click *Next.*
Put your known concentration sample in the cuvette holder. Enter the concentration, using mathematical notation E–4 ,for example, to indicate x 10 $^{-4}$
Click *Use Last Scan* to enter the Absorbance for that sample automatically, or key in the value.
Click *Add Sample* to add the plot point to the *Regression Plot.* Click *Remove Sample* to remove an unwanted sample.

When you have two or more plot points (the more the better), select the regression order and check *zero intercept (zero concentration = zero absorbance)* as required to plot a regression line.

The slope of the line is ε (be careful with units and magnitudes).

The R ^{2} (R^2) value is a measure of how well the regression line fits to your points. The closer it is to 1.0, the better the fit.

SpectraSuite also caculates the Residual, which is the difference between the line and the plot point and should be very small if the fit is good.

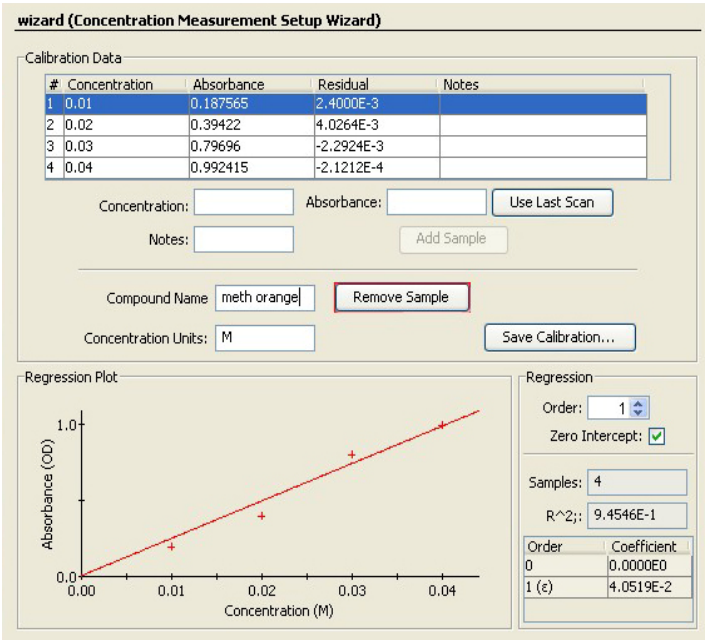
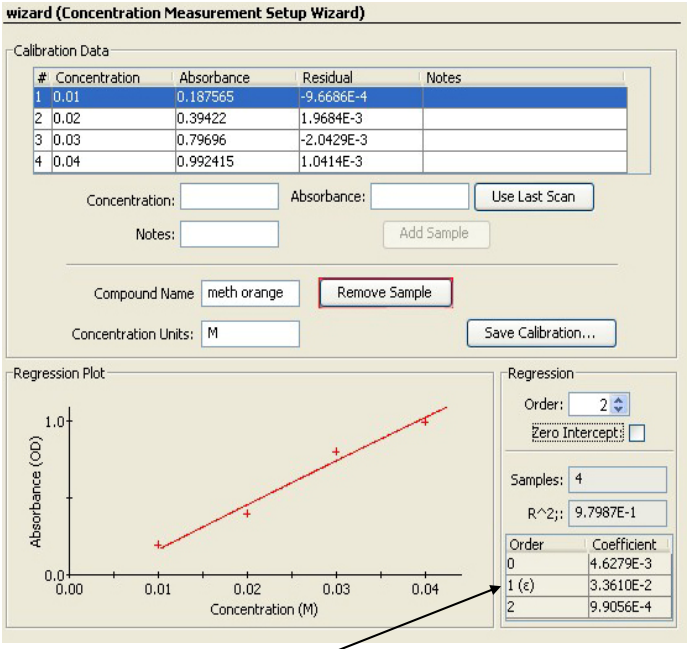


Fig.26

Fig.27 shows a second order regression line without zero intercept.



1st order straight line gives a value for ε.
2nd order line gives a more accurate calibration for concentration.

Fig.27

IMPORTANT
Always save your calibration before clicking *Finish*.

Click *Finish* to run the concentration page. See Fig 23.

SAVING CALIBRATIONS

Running a calibration may take hours of lab work making up solutions. It is a good idea to save your calibration plots.
Click *Save Calibration.*

To run a saved calibration:
1. Go to ***File>New>New Concentration Measurement***
2. Select *Active processing* if you have an absorbance graph running or *New absorbance processing* if not.
3. Click the radio button *Load calibration from file (*see Fig. 21). Find the file and click *Next.* The regression plot you worked so hard to create will appear.
4. Click *Finish* to run the concentration page (Fig.23).

REACTION KINETICS –STRIP CHARTS

Strip charts plot the Y-axis value of a graph at a set wavelength against time. For reaction kinetics the most useful of these is Absorbance against time, which is directly proportional to concentration against time.

See the SpectraSuite manual for more information.

CHANGING X-AXIS UNITS

The default X-axis unit is nanometres.
Go to ***Processing >X-axis units*** to change the units.

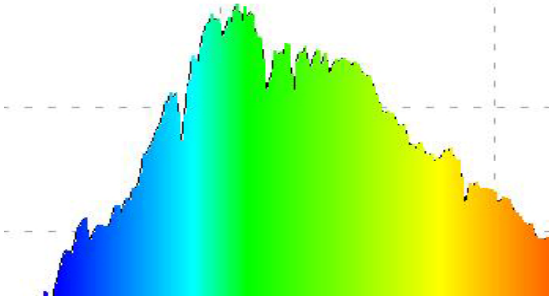
Note:
The trace usually disappears when you change units. To recover it, click the zoom to maximum icon. See Fig.7

Note that the trendline is reversed when the X-axis unit is an inverse of wavelength (GHz and wave number).

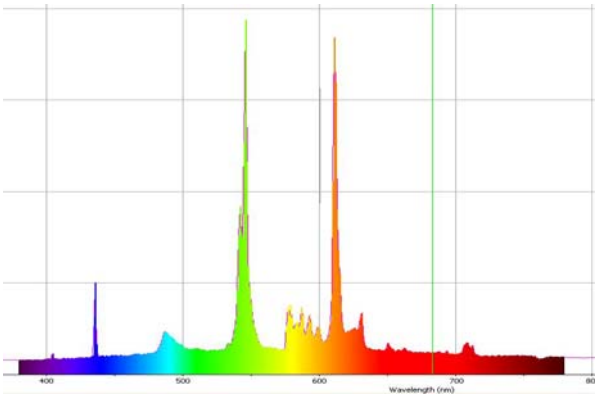
SOFTWARE UPDATES

SpectraSuite is updated frequently. You can download the latest version from the Ocean Optics website **www.oceanoptics.com** or use the update center in SpectraSuite.

INTERESTING SPECTRA

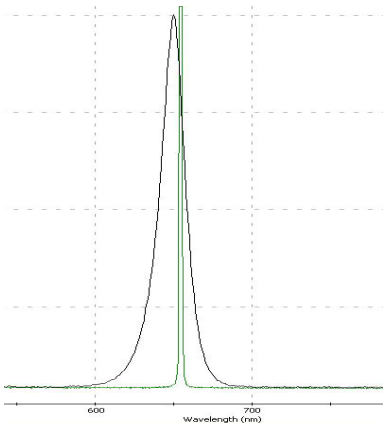


Daylight - Fraunhofer absorption lines can be seen as sharp dips. Compare with reference values. Where do these lines come from? Below a compact fluorescent "daylight" bulb.

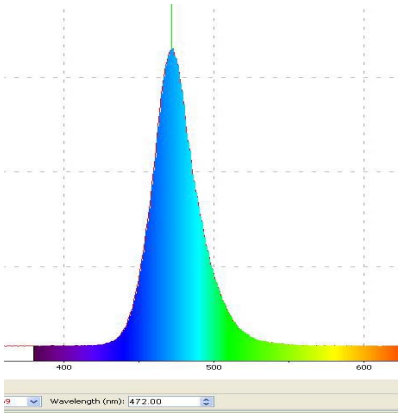


LEDs - compare red and infrared. The spectrometer can see infrared but you can't. How do white LEDs work? What is the peak wavelength of a blue LED?

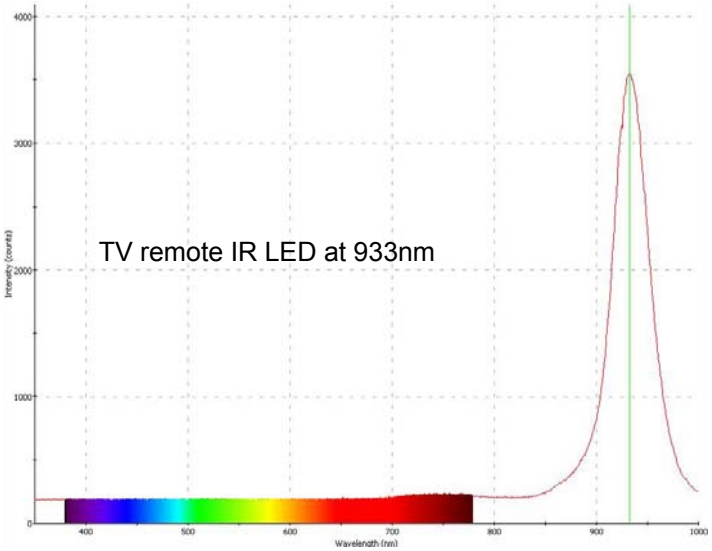
Diode and HeNe Lasers—how much more monochromatic are lasers? (Hint: shine the laser onto white card and point the fiber optic probe to the laser dot on the card). **Observe laser precautions.**



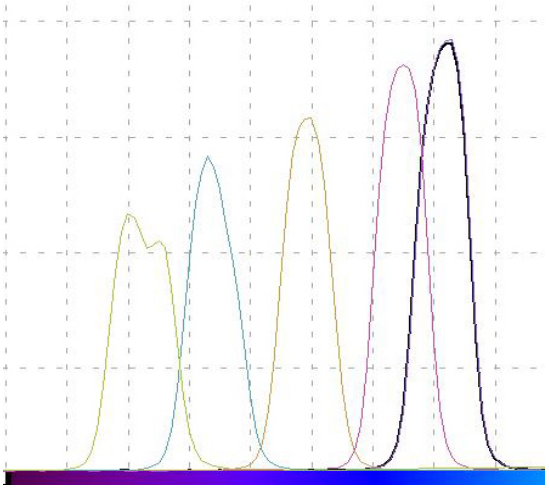
Red LED vs Laser



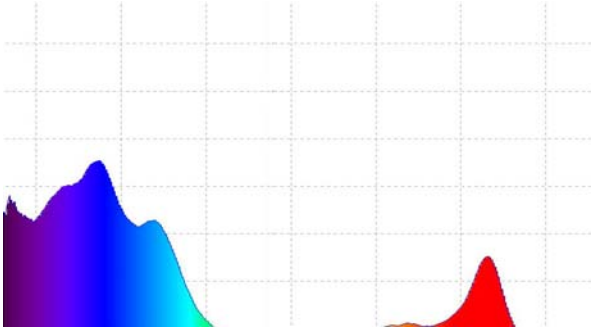
Blue LED



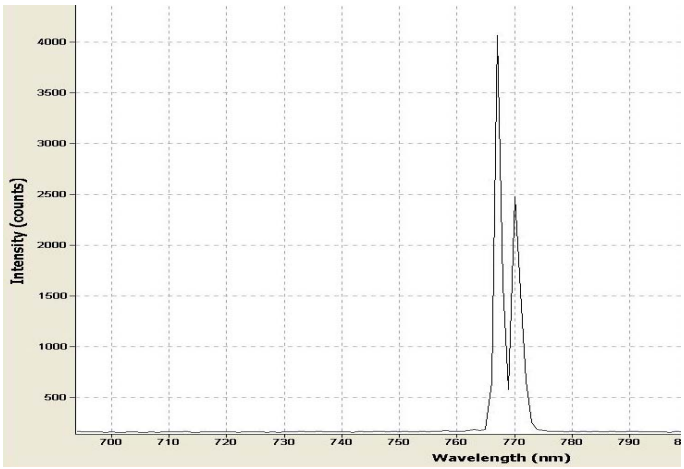
TV remote IR LED at 933nm



Wavelength shift with angle for an interference filter



Absorbance peak of chlorophyll from beech leaves



Potassium K doublet from burning a banana chip in a Bunsen flame

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