

# **Spectrometry User's Guide**

Computer/Tablet

1.0





# **Teacher and Technical Support**

For help with Spectrometry and other PASCO products, you can contact PASCO Teacher and Technical Support staff by phone, email, or on the Web.

1-800-772-8700 (in the U.S.)

Phone: +1 916 786 3800 (worldwide)

Email: support@pasco.com

Web: www.pasco.com/support/

Tech Notes: www.pasco.com/support/technical-support/technote/





# **Spectrometry Resources**



More 21st century science lab resources available online!

http://pasco.com/spectrometer/

- Software Download
- Video Tutorials & User Guide
- Replacement Parts
- Accessories
- Sample Labs



# Contents

Te	eacher and Technical Support	
	pectrometry Resources	
	ontents	
1	About PASCO Spectrometry	. 1
	Application Tools	
	Analyze Light	
	Analyze Solution	
	Analyze Concentration	
	Analyze Time	



# 1 About PASCO Spectrometry

The PASCO Spectrometry software works with the <u>PASCO wireless Spectrometer</u> as well as Ocean Optics Red Tide Spectrometers\*.

Version 1.0 is freely available to download for Macs & PCs. The free app for iPads is available in the App Store $^{\text{\tiny B}}$ .





# 2 Application Tools



#### **Tool Icon States**

Icons indicate state as follows:

Example Sta
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Yellow: Selected (currently in use)



White: Active (available for use)



Grey: Disabled (not available for use)

# **Application Tool Descriptions**

**Application Toolbar Functions:** 

## Icon Description



## **Experiment Options**

Opens the file structure of the software to Open, Create and Save the .sp files



## Analyze a graph of Intensity vs. Wavelength

Analyze a Solution in terms of Intensity vs Wavelength.



## Analyze a graph of Absorbance vs. Wavelength

Analyze a Solution in terms of Absorbance, Transmittance and/or Fluorescence vs wavelength.



#### Icon Description



#### Analyze a solution's concentration

Analyze a Solution in terms of Absorbance, Transmittance and/or Fluorescence vs solution concentration.



## Analyze a solution's reaction over time

Analyze a Solution in terms of Absorbance, Transmittance, Fluorescence and/or concentration vs reaction time.



#### **Connection Status**

**OR** 

Error

OR



Connected



## **Take Journal Snapshot**



## **Show Journal Snapshots**



#### Info and Settings

Software information and settings

## **Export Snapshots To HTML**



Sharing Options (Tablet only)

Open in Another App: Save the .sp file into Google Drive, DropBox, Evernote ... that are installed on the device.

Open in iTunes: Save the .sp file into iTunes.



#### Import Document From iTunes

Import from iTunes (Tablet only)

Import a .sp file from the iTunes account associated with the device.



# 3 Analyze Light

# **Procedure**

- 1. Attached a Fiber Optics Cable to your Spectrometer.
- 2. Point the Fiber Optics Cable at the Light Source.
- 3. Start Data Recording
- 4. Autoset the Integration Time in the Left-Hand Tools panel
- 5. Stop Data Recording
- 6. Select the Source to either Rename or Delete
- 7. Analyze the Graph with the Options Below

# **Graph Tools**

Analyze Light Graphing Functions:

Icon	Description
	Record
OR	Start recording data.  OR
	Stop recording data.
	Scale to Fit Scale to Fit the Graph.
	Add Coordinate Tool
- <b>့</b> -	Add Coordinates tool to select points on the graph.  Note: For additional Solution Analysis with Concentration and Time experiments, an Analysis wavelength MUST be selected.
A	Add Annotation Tool Add Text Annotation.
Ì≊	Show Comparison Mode  Compare spectra of multiple light sources.





**Show Color Spectrum Background** 

Show Color Spectrum Background.



## Reference Spectra

Add Reference Lines. Lines include: Hydrogen, Helium, Argon, Xenon, Mercury Sodium, Neon from NIST (National Institute of Standards and Technology) Atomic Spectra Database.



Previous reference



**Next reference** 

# **Light Analysis Tools**

Left-Hand Tools Slider can be Revealed or Hidden:

Icon	Description
	Pick the best integration time
	Integration Time is analogous to the shutter speed of a Camera. With a Higher Integ-
Integration Time	ration time, the spectrometer is more sensitive to less intense light.
	The "Auto Set" Button will automatically adjust the Integration time to maximize the current sample spectrum.
	Number of Scans to Average
Number of Scans to Average	This property specifies the number of discrete acquisitions that are collected and averaged before displaying and recording a spectrum or data point.
	A higher the value results in a better the signal-to-noise ratio.
Smoothing	Smoothing
Smoothing	Average groups of adjacent data points.



# 4 Analyze Solution

**Note:** You MUST select an Analysis Wavelength with the Coordinates Tool to perform subsequent Concentration and Time based Experiments for the solution you are studying.

#### **Procedure**

- Insert a cuvette containing the blank (solvent)
- 2. Perform a Dark Calibration
- 3. Allow the Light source to warm up (~1-2 minutes)
- 4. Perform a Light Calibration
- 5. Start Data Recording
- 6. Insert the cuvette containing the sample
  - a. Adjust the concentration of the solution if the spectrum is too low or too high
- 7. Stop Data Recording
- 8. Select the Solution to either Rename or Delete
- 9. Analyze the Graph with the Options Below

#### **Details**

Analyze Solution Absorbance / Transmittance Details

- Select "Absorbance" on the Graph to Switch from Absorbance to Transmittance
   Analyze Solution Fluorescence Details
- A Calibration is not required for this Measurement
- After Data Collection is Started, Auto Set the Integration time to obtain the best spectrum.



# **Solution Types**

Solution Analysis types in "Analyze Solution", "Concentration" and "Time" Experiments.

Solution Type	Description
Absorbance/Transmittance	Absorbance/Transmittance  Analysis of the Absorbance / Transmittance of a white light source through the sample.
Fluorescence (405 nm)	Fluorescence (405 nm)  Analysis of the Fluorescence of the sample with 405 nm excitation.
Fluorescence (500 nm)	Fluorescence (500 nm)  Analysis of the Fluorescence of the sample with 500 nm excitation.

# **Graph Tools**

Analyze Solutions Graphing Functions::

Icon	Description
	Record
OR	Start recording data.  OR
	Stop recording data.
	Calibrate Dark
<b>₹</b>	Calibrate Reference
	Scale to Fit Scale to Fit the Graph.



## Icon Description

#### **Add Coordinate Tool**



Add Coordinates tool to select points on the graph.

**Note:** For additional Solution Analysis with Concentration and Time experiments, an Analysis wavelength MUST be selected.



#### **Add Annotation Tool**

Add Text Annotation.



## **Show Comparison Mode**

Compare spectra of multiple light sources.



## **Show Color Spectrum Background**

Show Color Spectrum Background.



#### **Show Dual Y-Axes**

Show Dual Y axes of Absorbance and Transmittance data only.



# **Solution Analysis Tools**

Left-Hand Tools Slider can be Revealed or Hidden:

Icon	Description
	Pick the best integration time
	Note: For Fluorescence Only.
Integration Time	Integration Time is analogous to the shutter speed of a Camera. With a Higher Integration time, the spectrometer is more sensitive to less intense light.
	The "Auto Set" Button will automatically adjust the Integration time to maximize the current sample spectrum.
	Number of Scans to Average
Number of Scans to Average	This property specifies the number of discrete acquisitions that are collected and averaged before displaying and recording a spectrum or data point.
	A higher the value results in a better the signal-to-noise ratio.
Smoothing	Smoothing
	Average groups of adjacent pixels.



# 5 Analyze Concentration

#### **Procedure**

- 1. Select the Concentration Units in the Table Header to modify (if necessary)
- 2. Select the Concentration Values in the Table to modify (if necessary)
- 3. Select the empty Absorbance cell next to the appropriate Concentration value
- 4. Start Data Recording
- 5. Press "Check" to Keep the Spectrometer Data
- 6. Continue for each of the known standard concentration values
- 7. Stop Data Recording
- Analyze the Graph with the Options Below

**Note:** You can always edit the concentration value in a cell. If you suspect the Absorbance value is incorrect, simply select the cell again while the data is being recorded and press "check" with the new Absorbance value.

# **Unknown Concentration Analysis Details**

After multiple known concentration samples have been recorded, an unknown can be analyzed

- 1. Select the empty Absorbance cell in the Determine Unknown Concentration Table
- 2. Start Data Collection
- 3. Press "Check" to Keep the Spectrometer Data
- 4. Enter a value for the concentration of the Unknown based on the Absorbance Data and a graphical analysis of the known samples.
- 5. Verify a correct determination of the unknown based on the Graph
- 6. Reassess if necessary.



# **Solution Types**

Solution Analysis types in "Analyze Solution", "Concentration" and "Time" Experiments.

Solution Type	Description
	Absorbance/Transmittance
Absorbance/Transmittance	Analysis of the Absorbance / Transmittance of a white light source through the sample.
	Fluorescence (405 nm)
Fluorescence (405 nm)	Analysis of the Fluorescence of the sample with 405 nm excitation.
	Fluorescence (500 nm)
Fluorescence (500 nm)	Analysis of the Fluorescence of the sample with 500 nm excitation.

# **Graph Tools**

Analyze Concentration Graphing Functions:

Scale to Fit the Graph.

Icon	Description
	Record
OR	Start recording data. OR
	Stop recording data.
	Active Solution
Active Solution	Pick the Active Solution for Analysis.
Blue dye	<b>Note:</b> Active solutions MUST have a wavelength selected to perform Concentration Experiments.
<b>7</b>	Scale to Fit





Icon

Description

**Add Coordinate Tool** 



Add Coordinates tool to select points on the graph.

**Note:** For additional Solution Analysis with Concentration and Time experiments, an Analysis wavelength MUST be selected.



**Add Annotation Tool** 

Add Text Annotation.



**Show Linear Fit** 



**Show Live Scan Display** 



# 6 Analyze Time

## **Procedure**

- 1. Start Data Recording
- 2. Allow the desired amount of time to pass
- 3. Stop Recording
- 4. Analyze the Graph with the Options Below.

# **Analyze Time Details**

- Select "Absorbance" on the Graph to Switch from Absorbance to Transmittance or Concentration (Concentration data will only be meaningful if the Absorbance and Concentration relationship is established in a Concentration experiment or by manually adding the slope and intercept.)
- Select the "Calculator" button on the Graph to switch through QiuckCalcs of Y, Y<sup>-1</sup> or InY.

# **Solution Types**

Solution Analysis types in "Analyze Solution", "Concentration" and "Time" Experiments.

Solution Type	Description
Absorbance/Transmittance	Absorbance/Transmittance  Analysis of the Absorbance / Transmittance of a white light source through the sample.
Fluorescence (405 nm)	Fluorescence (405 nm)  Analysis of the Fluorescence of the sample with 405 nm excitation.
Fluorescence (500 nm)	Fluorescence (500 nm)  Analysis of the Fluorescence of the sample with 500 nm excitation.



# **Graph Tools**

Analyze Time Graphing Functions:

## Icon D

## Description



#### Record

OR

OR

Start recording data.

• •



Stop recording data.

## Reference Spectra



Pick the Active Solution for Analysis.

**Note:** Active solutions MUST have a wavelength selected to perform Concentration Experiments.



#### Scale to Fit

Scale to Fit the Graph.

#### Add Coordinate Tool



Add Coordinates tool to select points on the graph.

**Note:** For additional Solution Analysis with Concentration and Time experiments, an Analysis wavelength MUST be selected.



#### Add Annotation Tool

Add Text Annotation.



#### **Show Linear Fit**

Apply a Linear Fit to the Data.



#### **Show Selection Tool**

Selection tool to highlight a range of data.



Icon	Description
<b>Ì</b> ≈	Show Comparison Mode  Compare multiple runs of kinetics data.
	Show Live Scan Display

# **Time Analysis Tools**

Left-Hand Tools Slider can be Revealed or Hidden:

Icon	Description
Sample Rate	Sample Rate The number of measurements taken per unit of time.
	Bandwidth  Bandwidth specifies the range of wavelength that will be measured in time acquisition mode.
Bandwidth	The Bandwidth value is equal to the number of pixels on either side of the pixel specified by the Wavelength parameter.  Therefore, the total number of pixels that will contribute to a measurement equals "Bandwidth" × 2 + 1.
Absorbancevs. Concentration	Absorbance vs. Concentration  The slope and intercept values that relate the Absorbance to concentration of the sample.
	These constants are determined by the software on through a "Concentration" experiment, or they can be manually entered.