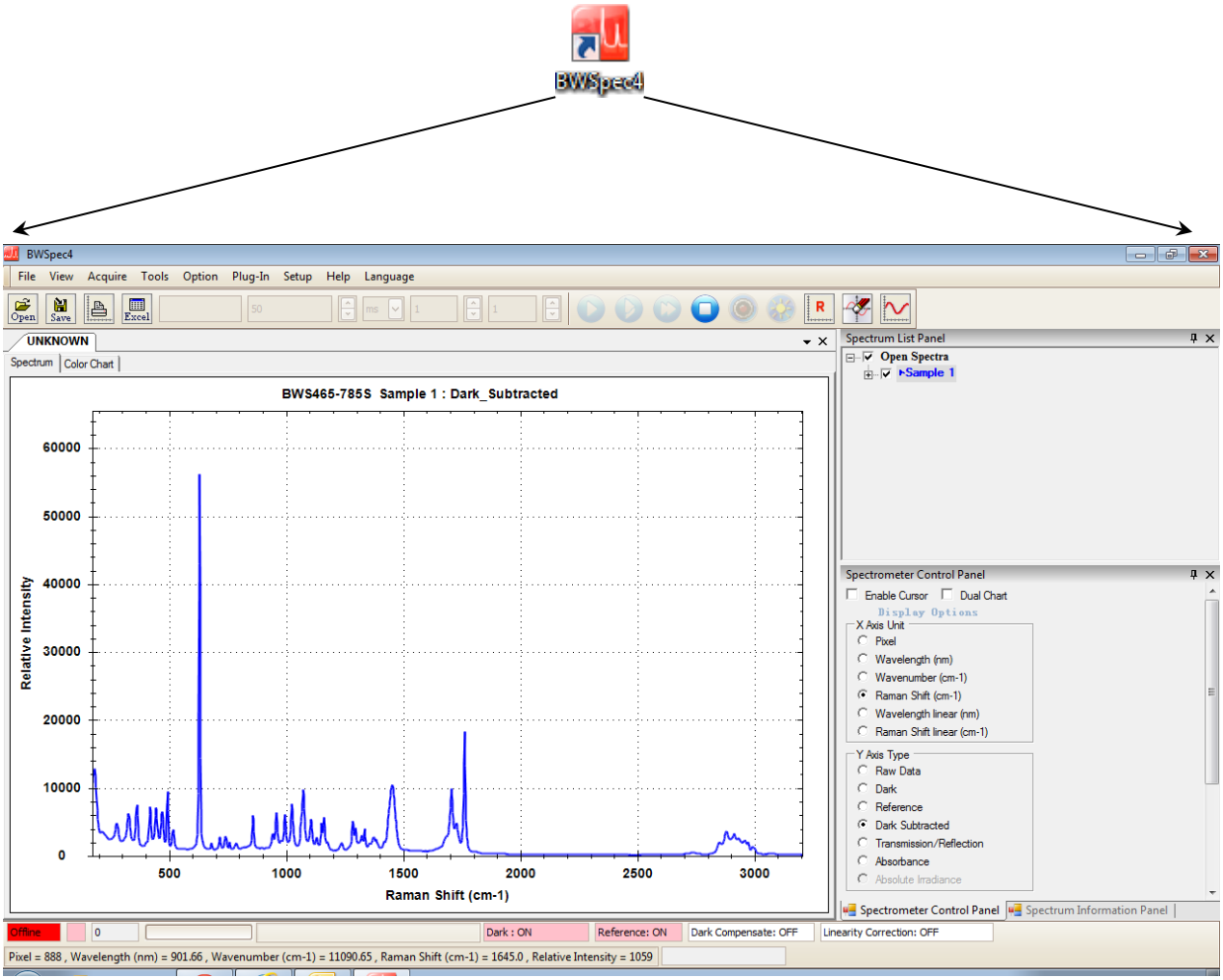

BWSpec™ 4 Software User Manual

19 Shea Way, Newark, DE 19713 Tel: (302) 368-7824 Fax: (302) 368-7830 Web: www.bwtek.com

290020235-G (09/16/2015)

Table of Contents

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1 INTRODUCTION

BWSpec™ 4 is a Spectrometer Data Acquisition Software Program. It supports two types of B&W Tek, Inc. spectrometer interface: USB2.0 and USB 3.0.

2 INSTALLATION

2.1 Supported Operating Systems

Windows XP (32 bit)
Windows Vista (32 bit & 64 bit)
Windows 7 (32 bit & 64 bit)
Windows 8 / 8.1 (32 bit & 64 bit)

*Note although the above operating systems are supported, Windows 7 and 8 / 8.1 are preferred.

2.2 Minimum System Requirements

Meets or exceeds the System Requirements for your PC's Operating System respectively
Processor: 1.5GHz or faster
RAM: 1GB or more
Hard disk space: 250MB available or more*

* Excluding additional hard disk space required to store generated data by the application.

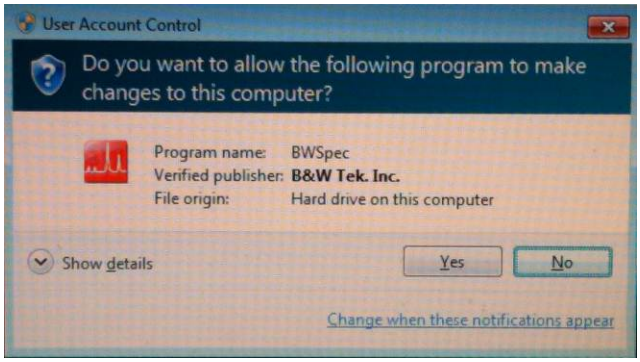
2.3 Software & Hardware Installation

- Insert the BWSpec 4 CD into the computer's CD/DVD Drive; if it's in a USB flash drive, copy the installation file to local computer.
- Refer to **"BWSpec Software and Hardware Installation Guide":**
    - **General Installation Guidelines**
        - Install the software;
        - After software installation, **do not** run/open the BWSpec program;
        - Connect the spectrometer to the PC via an USB Cable;
        - Install the Hardware Driver(s) for the spectrometer;
        - After hardware driver installation, open/run the BWSpec program.

3 RUN BWSPEC

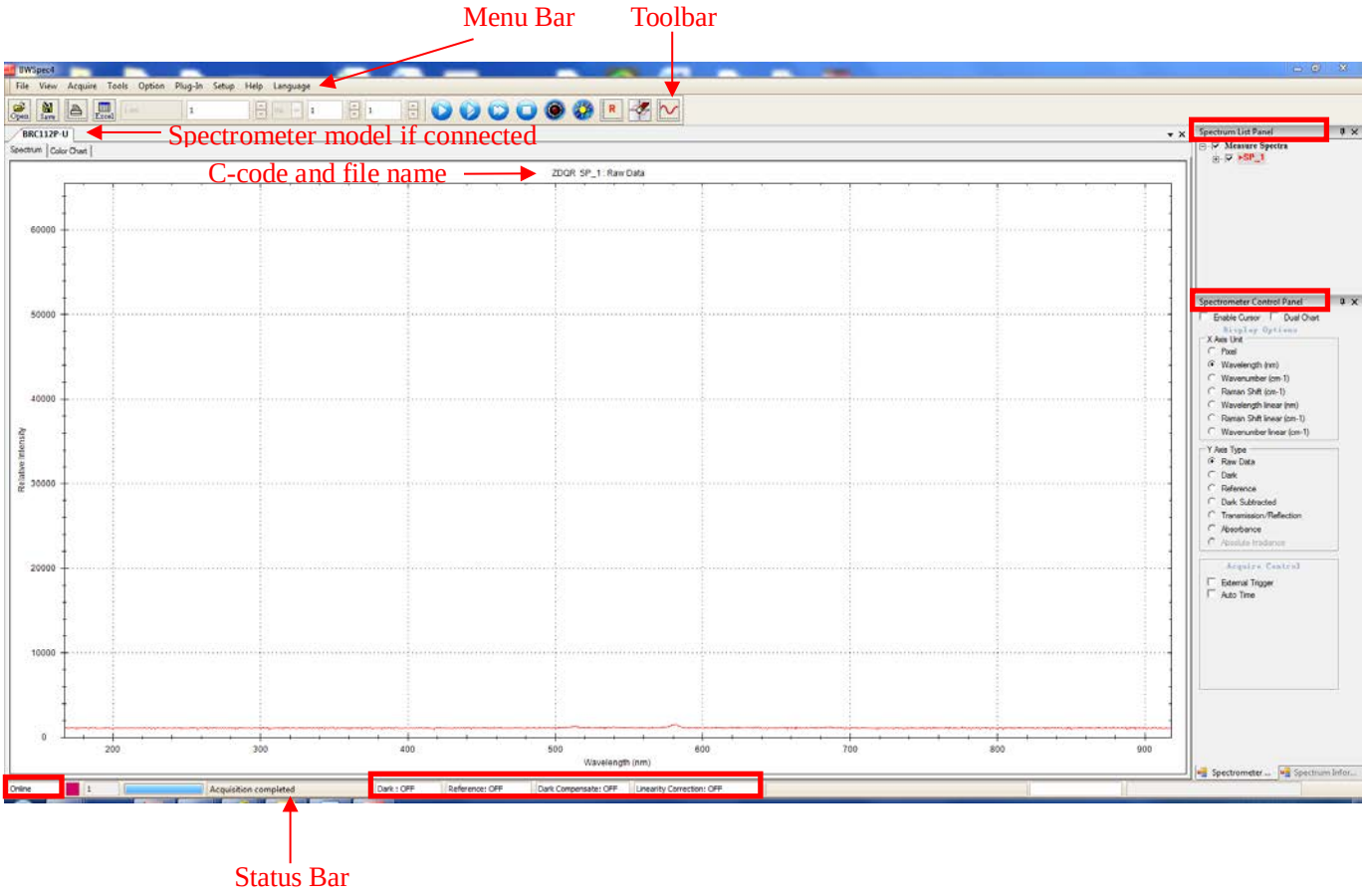
Double click the BWSpec icon on the desktop: 

If the User Account Control is active, the following message will appear:



Click **Yes** to continue.

4 MAIN WINDOW

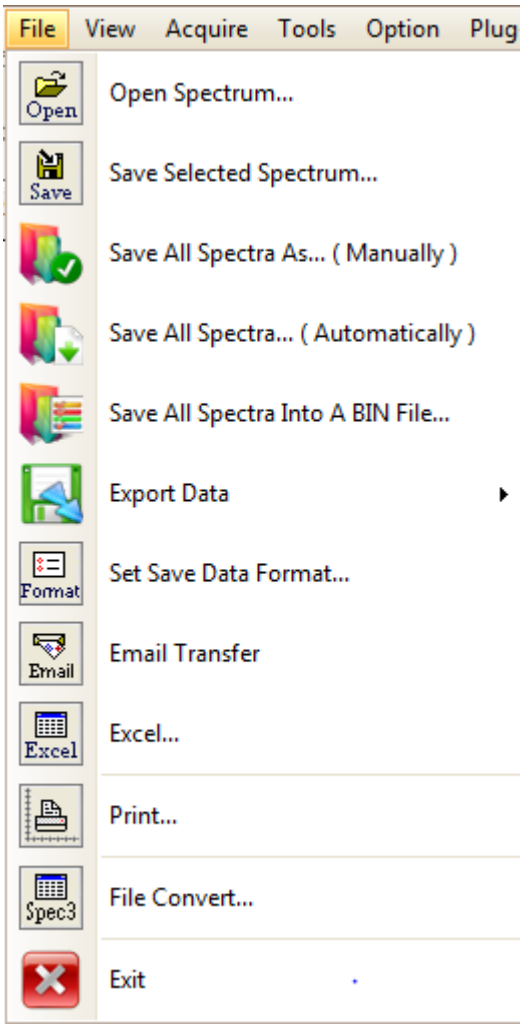


5 MENU BAR

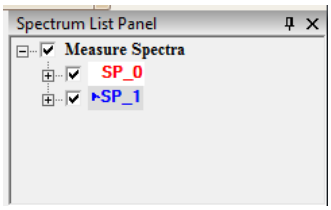
File View Acquire Tools Option Plug-in Setup Help Language

The following sections are detailed descriptions of the dropdown menus provided for each menu option in the BWSpec 4 Menu Bar.

5.1 File

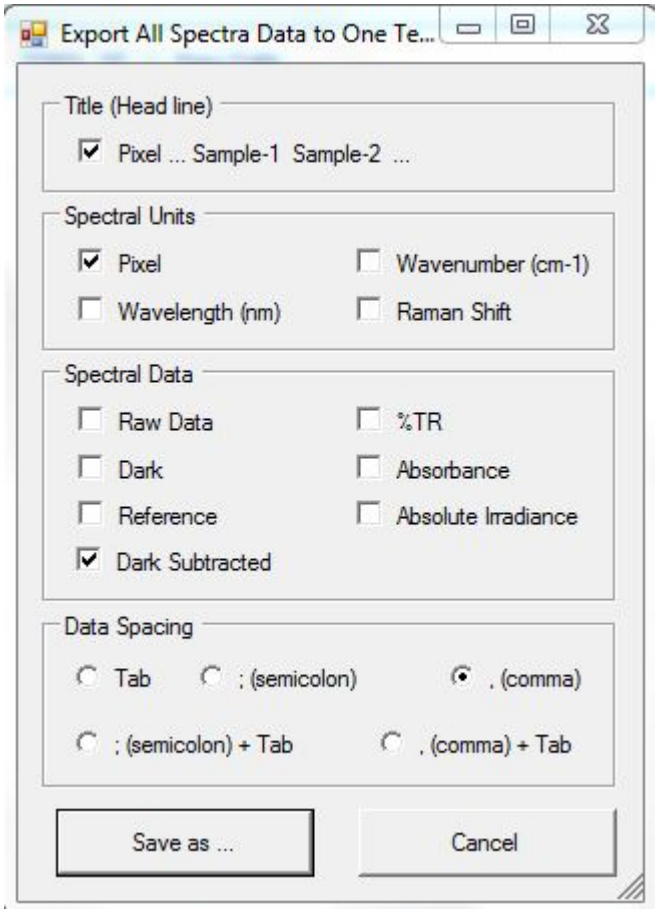


- Open Spectrum…
  - Open a window to load a spectrum file.
- Save Selected Spectrum…
  - Open a window to save the spectrum selected in the **Spectrum List Panel**.

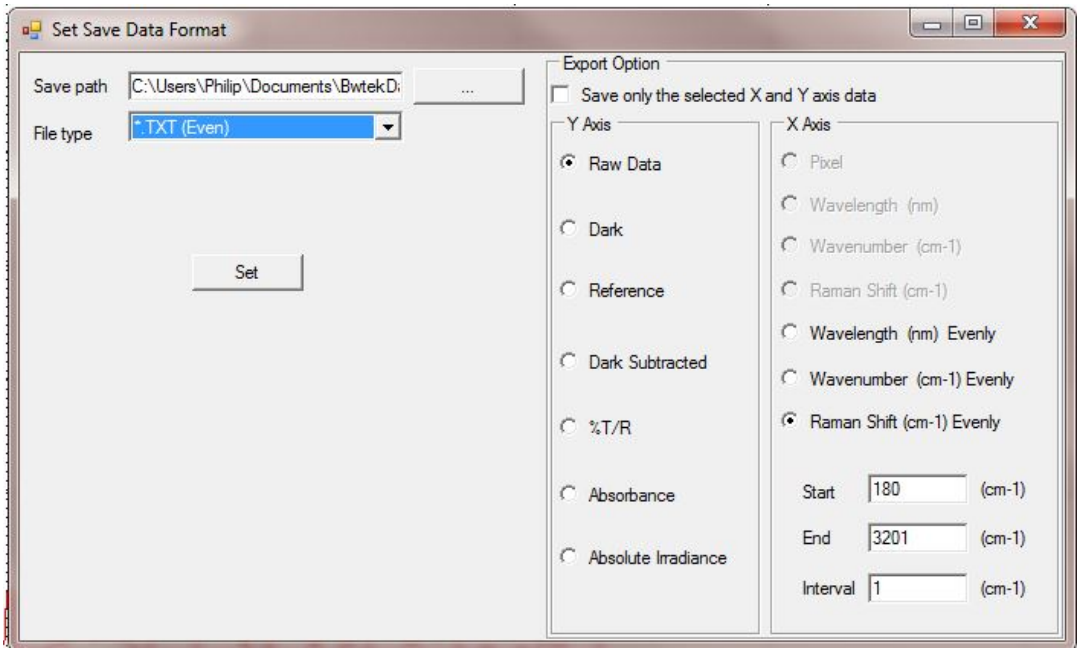


- Save All Spectra As…(Manually)
  - Open a window to save one after another, all the spectra listed in the **Spectrum List Panel**.

- Save All Spectra…(Automatically)
  - Open a window to save all the spectra in the **Spectrum List Panel** all at once.
- Save All Spectra into a BIN File…
  - Open a window to save all the spectra in the **Spectrum List Panel** all at once with .BwRams file extensions, which can then be loaded in BWSpec.
- Export Data
  - Export selected data into one text file, setting the type of data to be exported for each spectrum. This function needs to be enabled through **Plug-in Manager**.



- Set Save Data Format…
  - Open a window to configure the preferred preset setting when saving spectra, i.e. for file type ***.TXT (Even)*** and ***.SPC***:



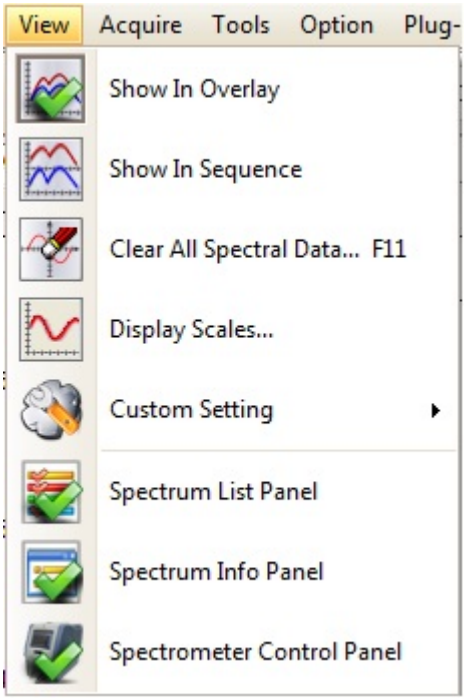
- Email Transfer
  - For importing and exporting spectral signatures. This feature is only for use with handheld Raman units such as TacticID Client.
- Excel
  - Export the active/selected single spectrum from the **Spectrum List Panel** to Excel. The file will open in Excel when the export is complete.
    - **Do NOT click on the Excel File during export. This will interrupt the exporting process.**

- Print…
  - Open a **Print Preview** window from which the user can then select to save or export the plot as an image file or select a printer to print a hard copy.

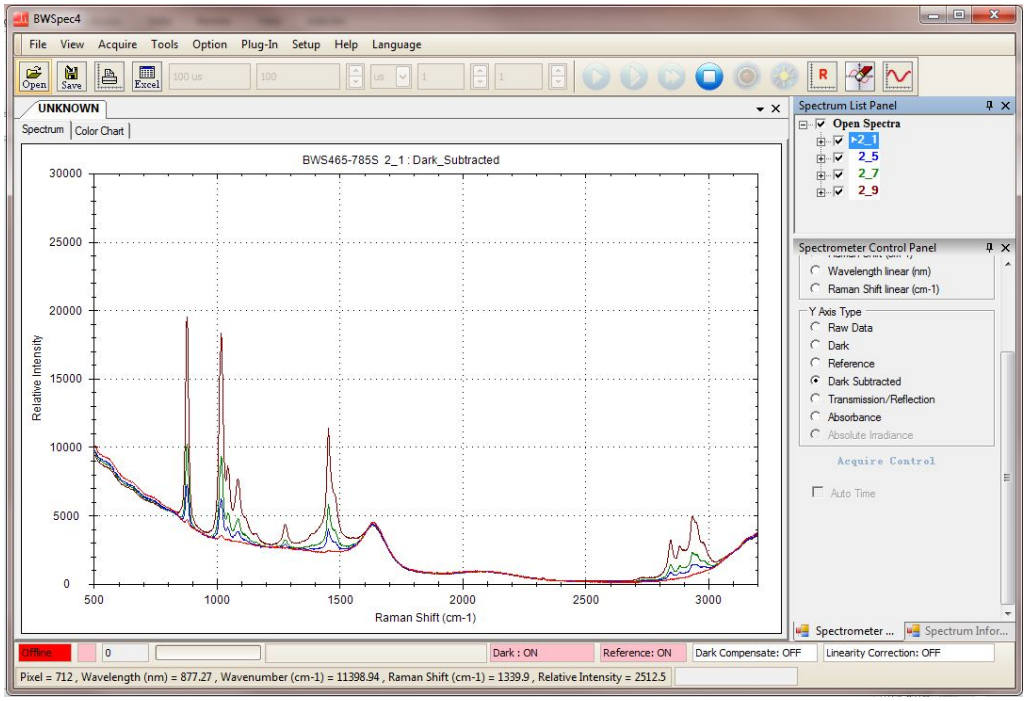
- File Convert…
  - Convert BWSpec 3 saved data file which contains multiple spectra (up to 3) into individual BWSpec 4 compatible files.

- Exit
  - Close BWSpec

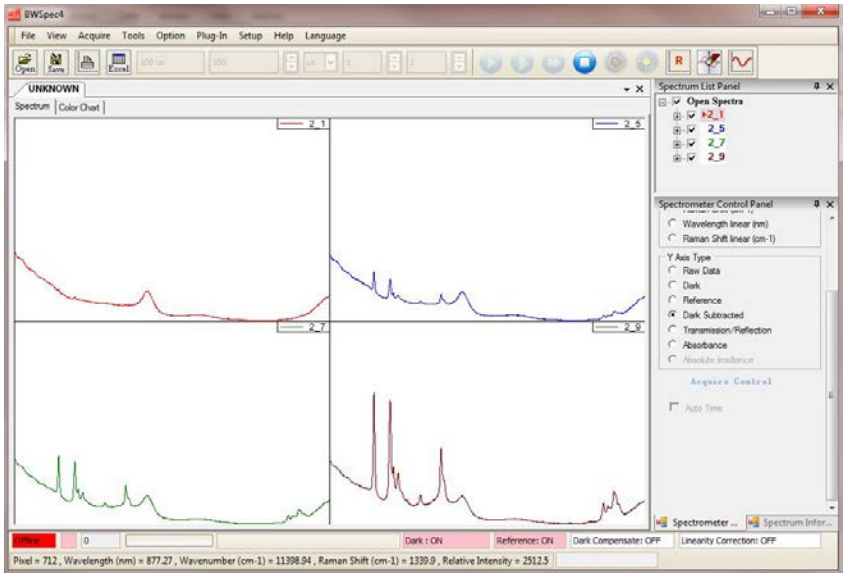
5.2 View



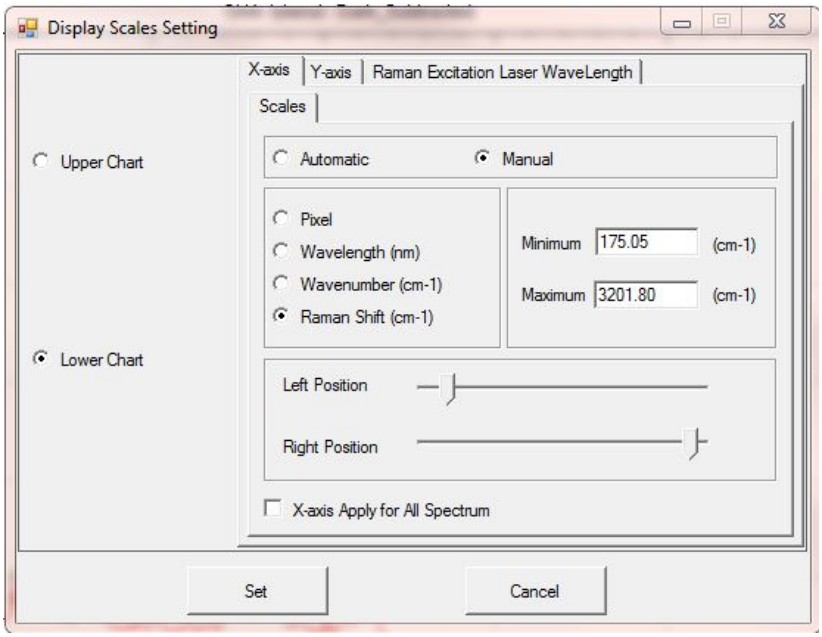
- Show In Overlay
  - When viewing more than one spectrum, an overlay of spectra will be displayed on the graph.

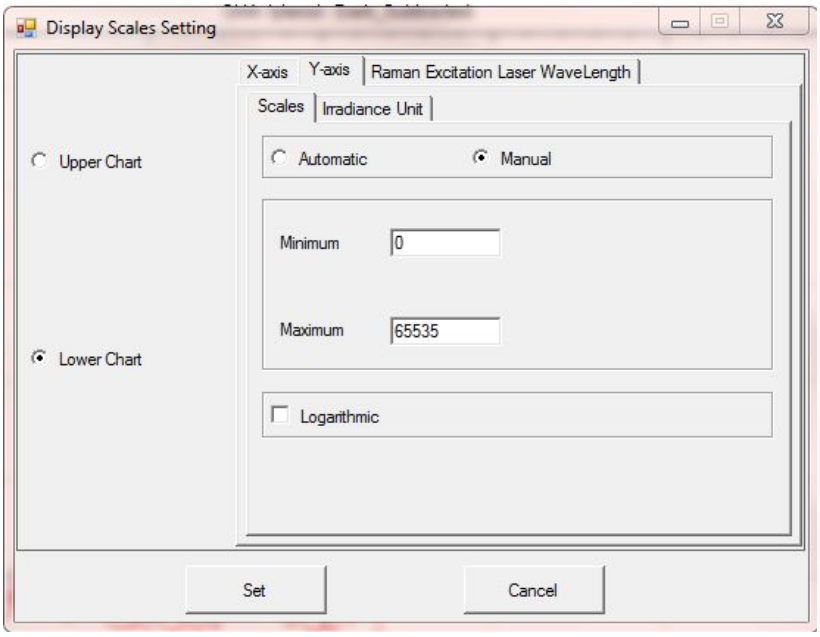


- Show In Sequence
    - When viewing more than one spectrum, individual boxes will appear in the order in which they are listed in the Spectrum List panel.



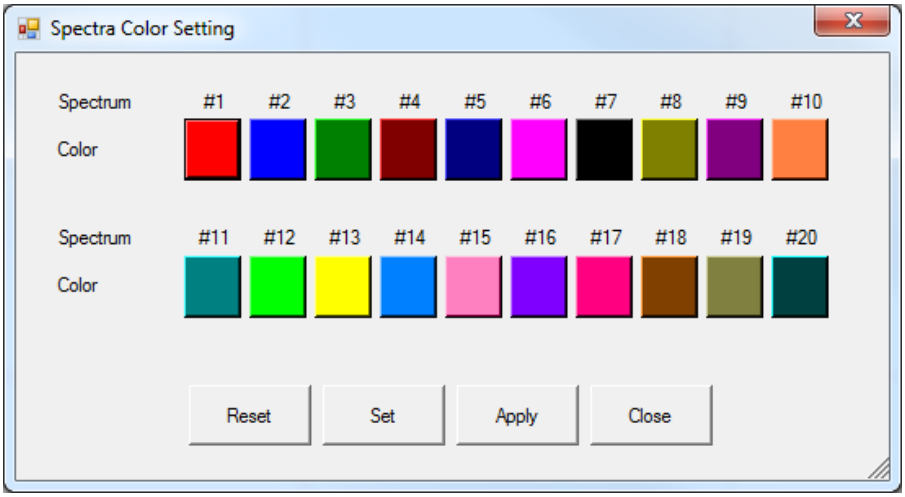
- Clear All Spectral Data…
    - Clear all spectra shown in the screen from the display.
- Display Scales……
    - A **Display Scales Setting** window will appear:



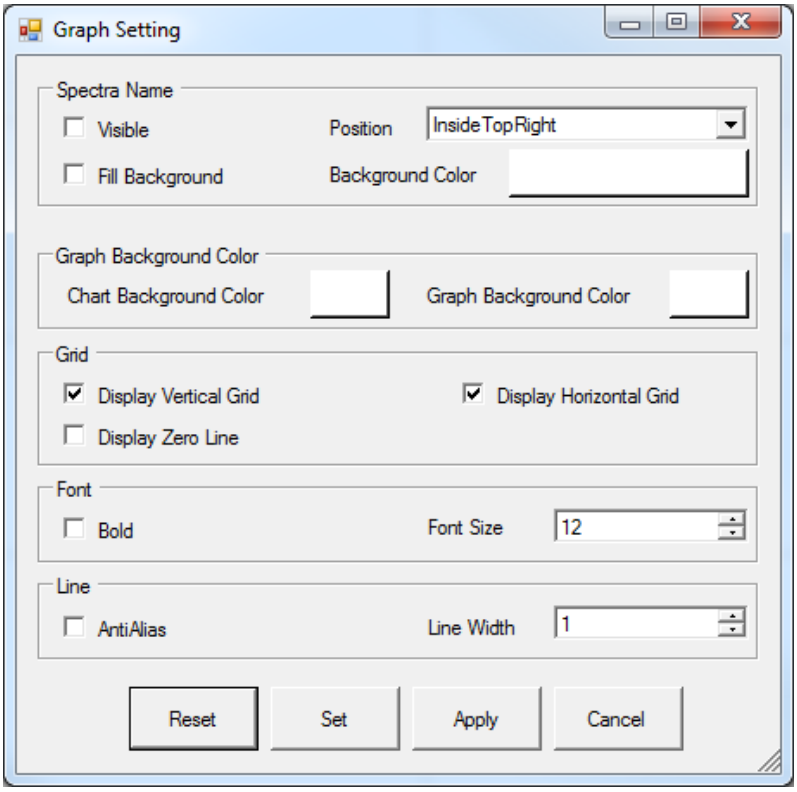


- This window will show the X-axis and Y-axis settings for the software for the spectrometer.
  - X-axis scale settings are based on the calibration settings for the spectrometer.

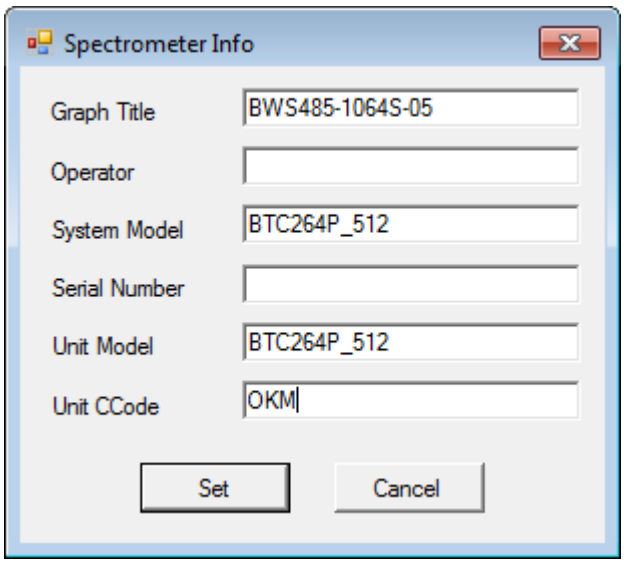
- Custom Setting
  - Spectra Color Setting…
    - Opens a **Spectra Color Settings** window where the spectrum color order for overlays can be set / adjusted. The sequence is based on spectrums listed in the spectrum list panel.



- Spectra Graph Setting…
  - Opens a **Graph Setting** window where the variables relating to the graph window display can be set / adjusted to create a customized graph.

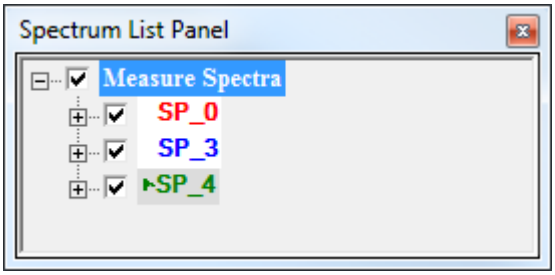


- Spectrometer Info…
  - Opens a **Spectrometer Info** window which displays details of the spectrometer for the selected spectrum:

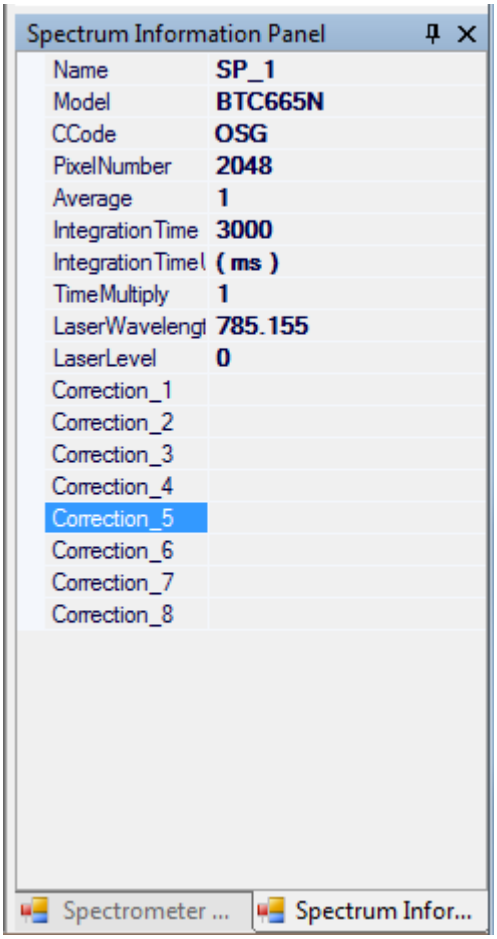


  - Additional information can be input by the user for tracking purposes when printing/saving data.

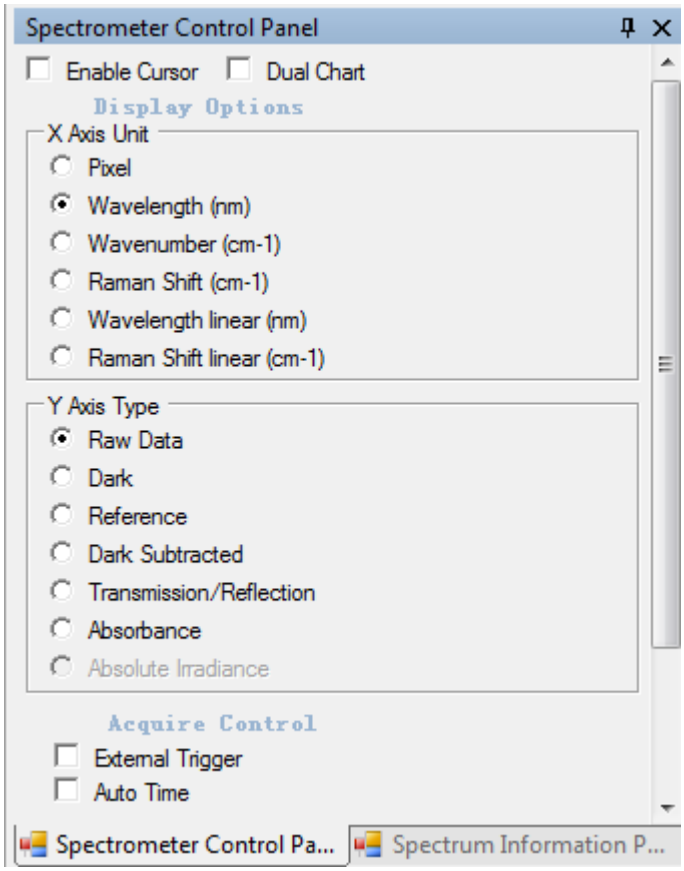
- Spectrum List Panel
  - Toggle On/Off viewing of the **Spectrum List Panel** on the right side of the display.



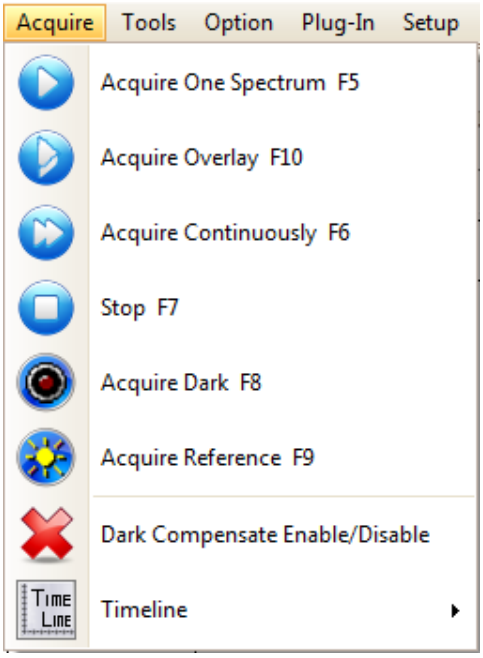
- Spectrum Info Panel
  - Toggle On/Off viewing of the **Spectrum Information Panel**.



- Spectrometer Control Panel
  - Toggle On/Off viewing of the **Spectrometer Control Panel**.



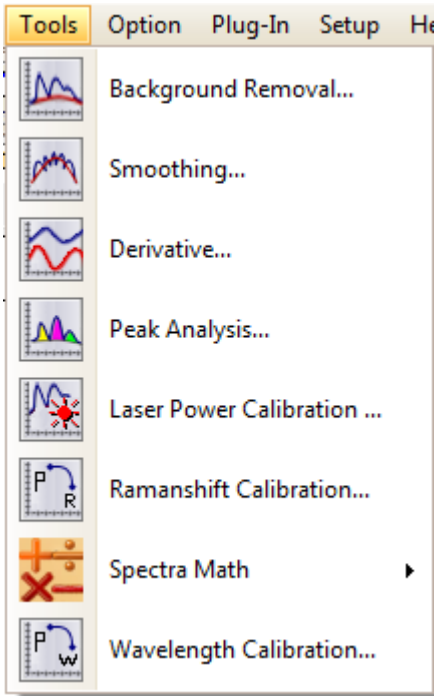
5.3 Acquire



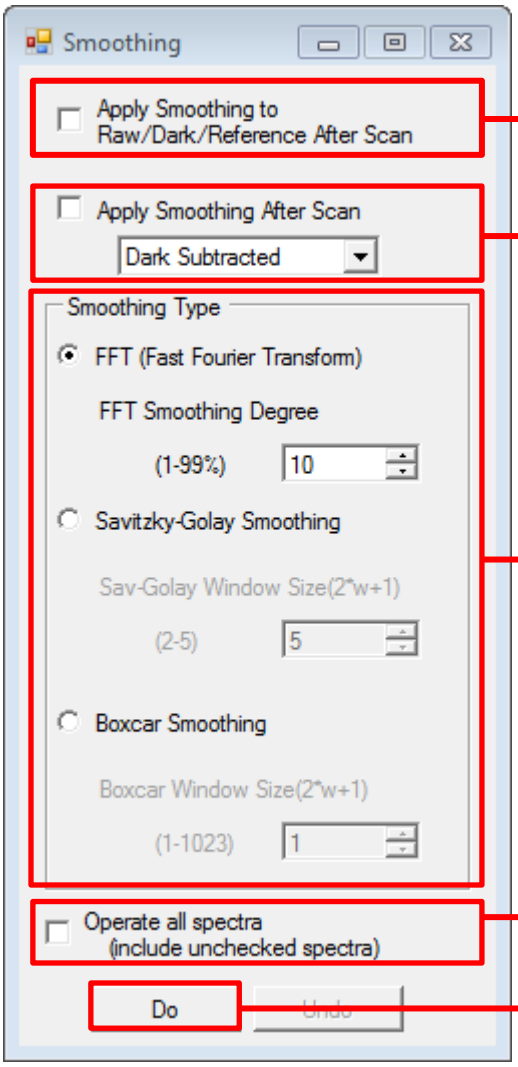
- Acquire One Spectrum
  - Acquires a single spectrum from the spectrometer and displays it on the graph.
- Acquire Overlay
  - Acquires a single spectrum from the spectrometer and displays it as an overlay on top of the previously displayed spectra on the graph.
- Acquire Continuously
  - Acquires continuous data from the spectrometer while continuously updating the active spectrum displayed on the graph.
- Stop
  - Stops acquisition while using **Acquire Continuously**.
- Acquire Dark
  - Acquires a single spectrum which is stored as the Dark Array.
- Acquire Reference
  - Acquires a single spectrum which is stored as the Reference Array.
- Dark Compensate Enable/Disable
  - Enable/Disable the **Dark Compensate** feature.
  - Provides an electronic dark reference that is available with some spectrometers which automatically subtracts out this dark reference array from acquired spectra.
- Timeline
  See section 11.9

5.4 Tools

The default items in the Tools menu are Smoothing, Derivative and Peak Analysis. Additional tools will become visible in the menu after being selected as Plug-ins.



- Background Removal…
  - See section 11.1
- Smoothing…
  - Open a **Smoothing** window:



Apply smoothing to Raw, Dark, and Reference spectrum after each scan

Apply smoothing to selected spectrum from the drop-down menu after each scan.

Configure desired Smoothing method.

Check to apply smoothing to all spectra in Spectrum List Panel

Apply manual smoothing to currently displayed spectrum

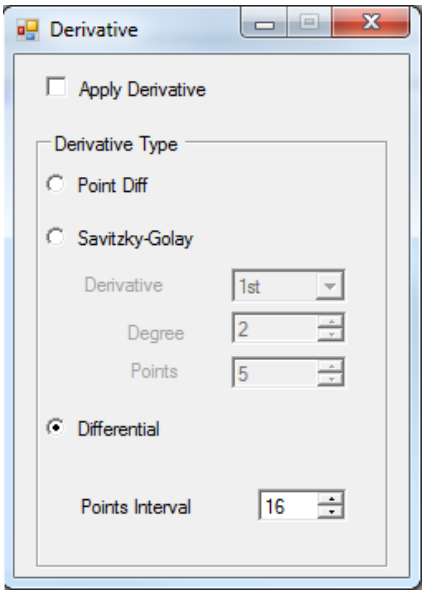
- FFT (Fast Fourier Transform)
  - Smoothing can be applied to the original spectrum using a smoothing factor of 1-99%. The smoothing factor needs to be carefully selected so as not to cause a distorted spectrum.

- Savitzky-Golay Smoothing
  - Savitzky-Golay (Savitzky-Golay Filters): smoothing can be applied to the original spectrum with a "window size" setting from 2-5. This is a very commonly used smoothing method with less chance to cause distortion and degradation to the spectral resolution.

- Boxcar Smoothing
  - Boxcar: smoothing can be applied to the original spectrum using a "window size" setting from 1-1023. The smoothing function will apply the forward moving smoothing by taking the average of the specified number of pixels plus one pixel to the left of the group and one pixel to the right of the group. This is an effective smoothing operation that comes at the expense of degraded spectral resolution; hence, do not use a larger than necessary "window size" setting in order to preserve the needed spectral information.

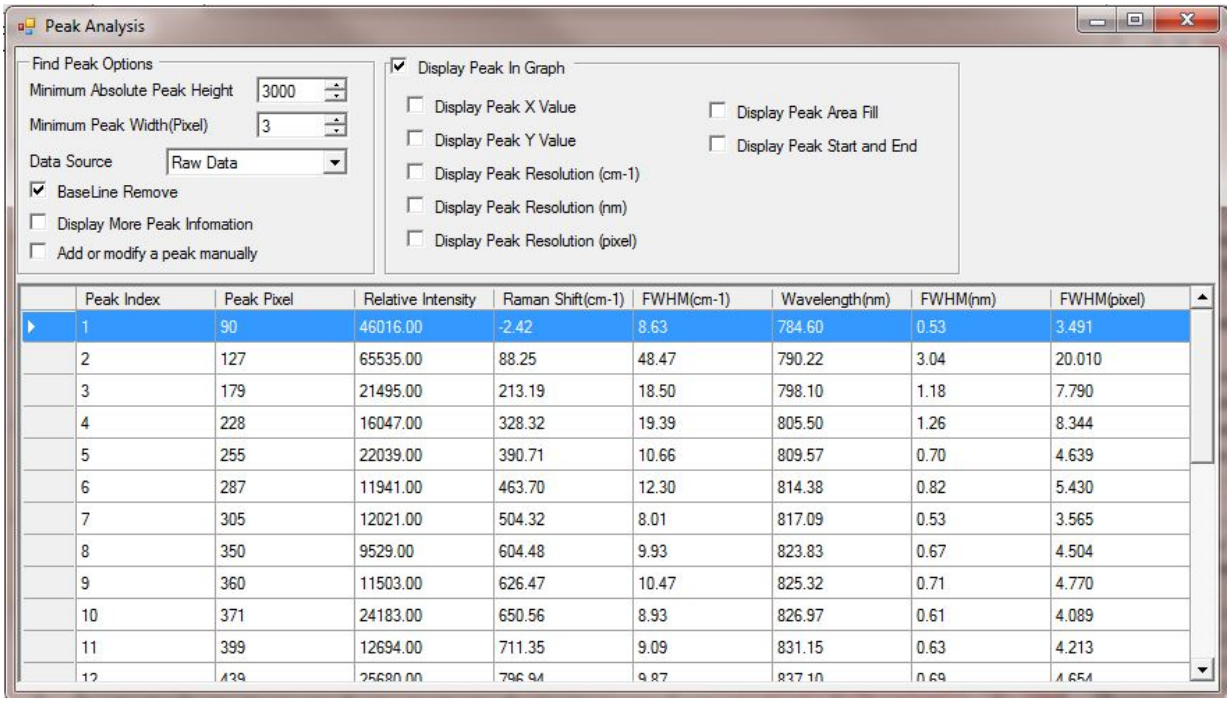
- Operate all spectra (include unchecked spectra)
  - This will apply smoothing to all the currently open spectra, including all unchecked spectra.

- Derivative…
  - Opens a **Derivative** window for applying derivatives to the active spectrum.



  - Three derivatives are provided for data analysis:
    • Point Diff;
    • Savitzky-Golay: With this option, a user can choose the derivative order, the degree (of the polynomial fit), and the number of points over which to compute the derivative;
    • Differential: With the differential derivative, the user can set the point interval to use from 5 to 20.
  - Select the desired derivative method and check the **Apply Derivative** box to apply the derivative calculation to the currently active spectrum.

- Peak Analysis…
  - Information on peaks in the spectrum can be shown live in the software's display window.



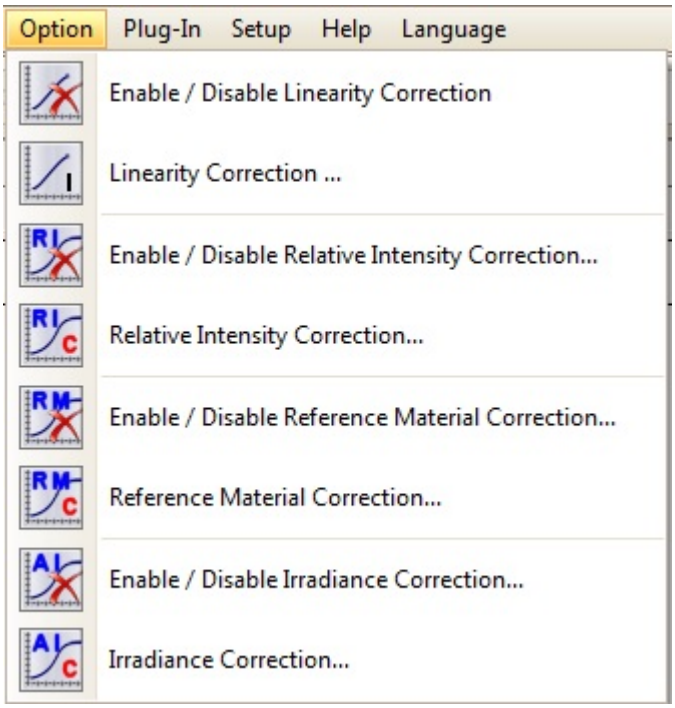
Peak Index	Peak Pixel	Relative Intensity	Raman Shift(cm-1)	FWHM(cm-1)	Wavelength(nm)	FWHM(nm)	FWHM(pixel)
1	90	46016.00	-2.42	8.63	784.60	0.53	3.491
2	127	65535.00	88.25	48.47	790.22	3.04	20.010
3	179	21495.00	213.19	18.50	798.10	1.18	7.790
4	228	16047.00	328.32	19.39	805.50	1.26	8.344
5	255	22039.00	390.71	10.66	809.57	0.70	4.639
6	287	11941.00	463.70	12.30	814.38	0.82	5.430
7	305	12021.00	504.32	8.01	817.09	0.53	3.565
8	350	9529.00	604.48	9.93	823.83	0.67	4.504
9	360	11503.00	626.47	10.47	825.32	0.71	4.770
10	371	24183.00	650.56	8.93	826.97	0.61	4.089
11	399	12694.00	711.35	9.09	831.15	0.63	4.213
12	439	25680.00	796.94	9.87	837.10	0.69	4.654

  - Automatic Peak Identification
    In the top left hand corner of the menu, input the value at **Minimum Absolute Peak Height** (threshold). All identified peaks are listed in a table in the window. This table provides detailed information on the identified peaks. Check the box for **Display Peak In Graph** and the identified peaks will be marked on the spectrum. Select the information to display by checking the desired items.

Note: *Peak Analysis Tool currently does not support Y-axis Mode in Absorbance or Absolute Irradiance.*

- Spectra Math
  - See section 11.8
- Wavelength Calibration…
  - See section 11.10
- Raman Shift Calibration
  - See section 11.11
- System Response Standardization
  - See section 11.13

5.5 Option



- Enable/Disable Linearity Correction
  - Enable/Disable linearity correction in ***Dark Subtracted*** spectrum for spectrometers with linearity correction coefficients available.
    - **Linearity correction coefficients can be created using the **Linearity Correction Plug-in** found under **Plug-in** on the Menu Bar.
      See section 11.5

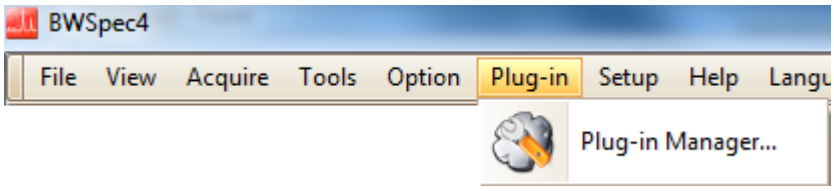
- Enable/Disable Relative Intensity Correction…
  - Enable/Disable relative intensity correction. Corrects the unit's spectral response against a known reference. A unique intensity correction file must be used for the correction to be accurate.
    - **A **Relative Intensity Correction File** can be created using the **Relative Intensity Correction Plug-in** found under **Plug-in** on the Menu Bar.
      See section 11.7

- Enable/Disable Reference Material Correction…
  - Enable/Disable the reference material correction function. This function is useful for accurate measurements in applications such as percent reflectance. A unique reference material correction file must be used for the correction to be accurate.

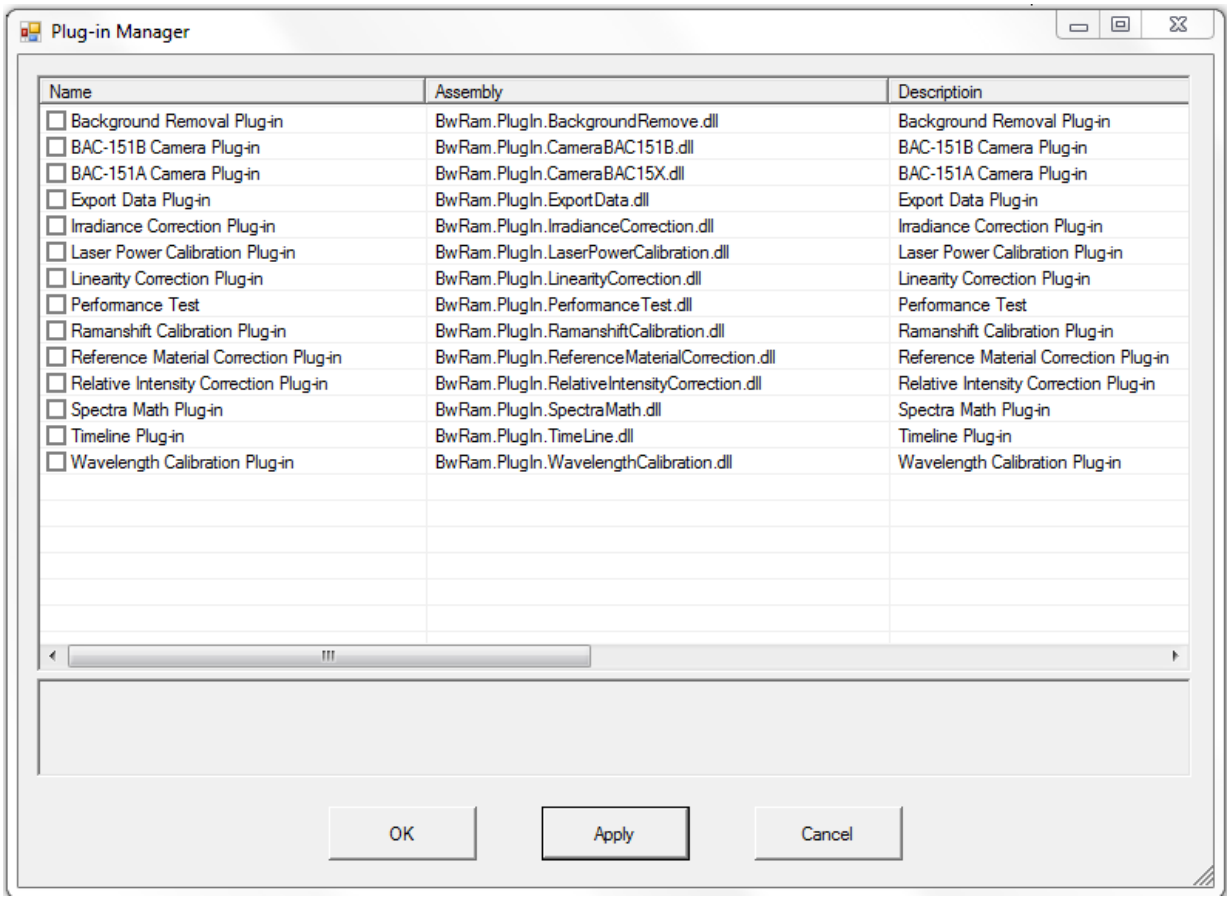
- **A **Reference Material Correction File** can be created using the **Reference Material Correction Plug-in** found under **Plug-in** on the Menu Bar.
  See section 11.6

- Enable/Disable Irradiance Correction…
  - Enable/Disable irradiance correction. A unique irradiance correction file must be used for the correction to be accurate.
    - **An **Irradiance Correction File** can be created using the **Irradiance Correction Plug-in** found under **Plug-in** on the Menu Bar.
      See section11.4

5.6 Plug-in

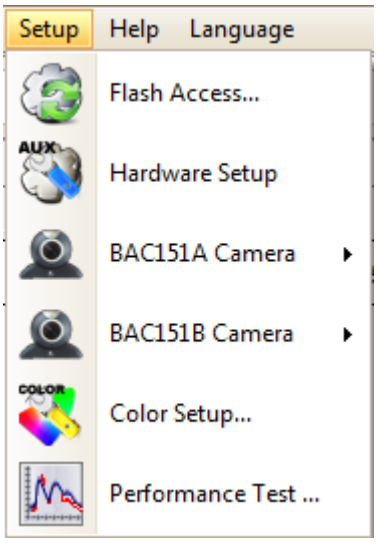


- Plug-in Manager…
  - Opens a **Plug-in Manager** window which lists all the available Plug-ins to the software.

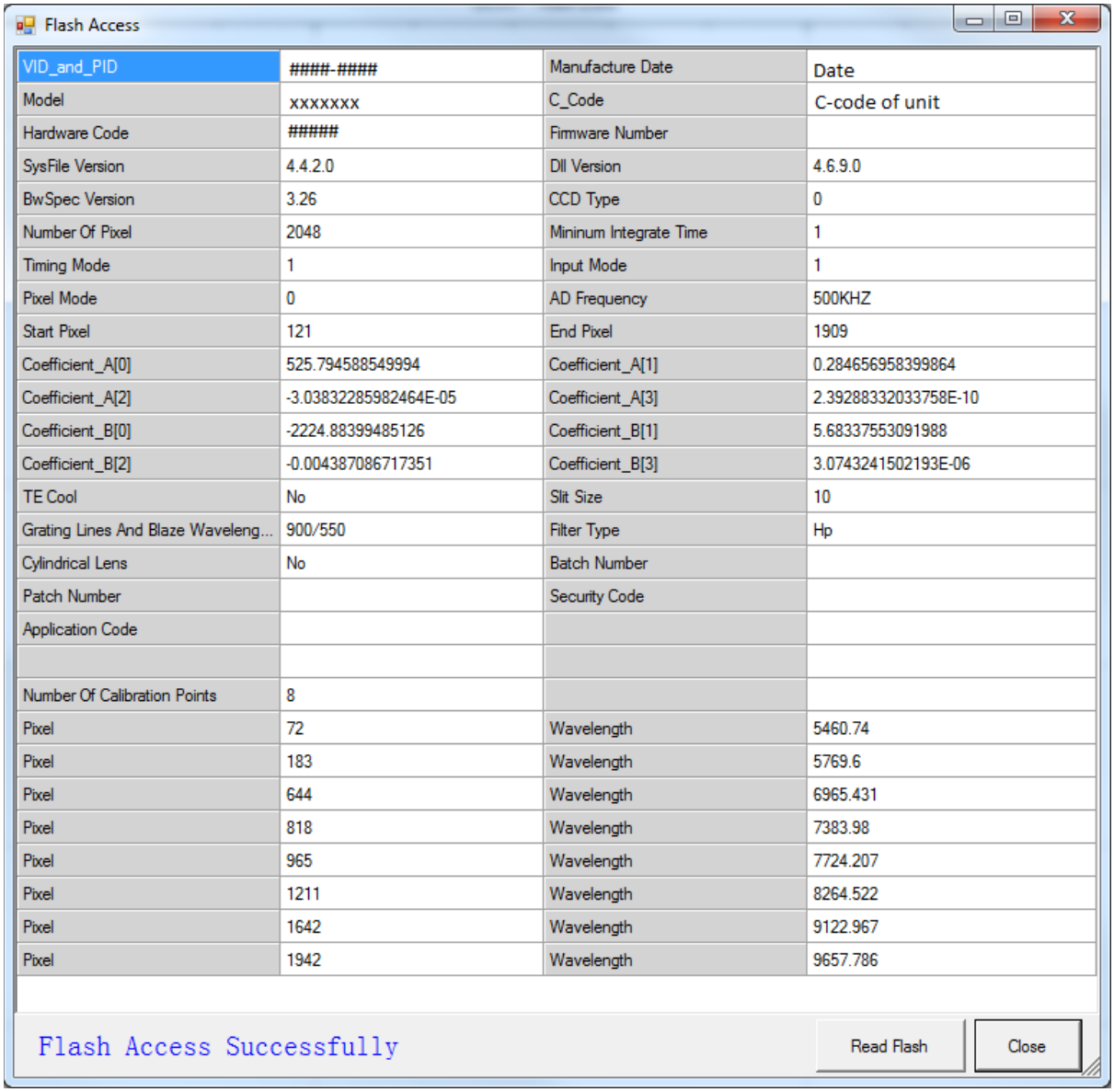


  - Check the box next to a given plug-in to activate it. Click **Apply** and then **OK** to activate the plug-in in the BWSpec Menu Bar. The Plug-Ins will be added to the appropriate menu on the BWSpec Menu Bar.
    - See section 11: ***Plug-In Manager*** for additional information about these Plug-ins.

5.7 Setup

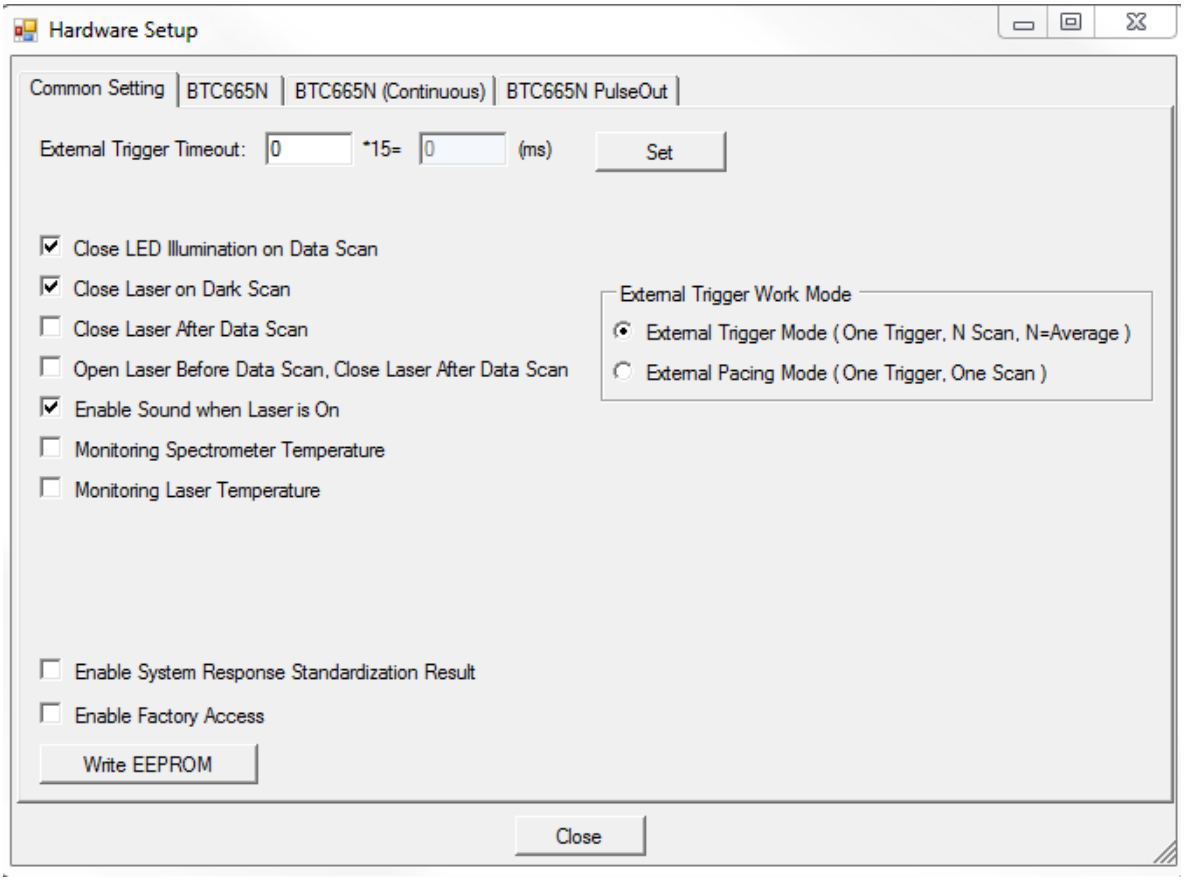


- Flash Access…
  - Opens a Flash Access window.
  - Unique information pertaining to the defaults of the spectrometer will be displayed in this window.
  - Clicking the **Read Flash** button will read the EEPROM of the spectrometer and reset the BWSpec variables back to their default values.

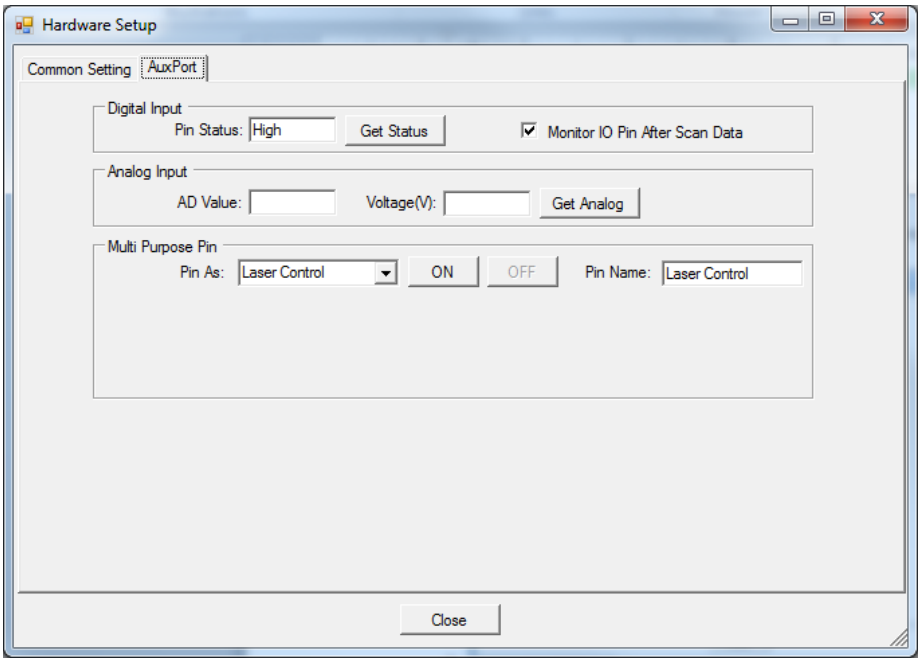


VID_and_PID	####-####	Manufacture Date	Date
Model	xxxxxxx	C_Code	C-code of unit
Hardware Code	#####	Firmware Number	
SysFile Version	4.4.2.0	Dll Version	4.6.9.0
BwSpec Version	3.26	CCD Type	0
Number Of Pixel	2048	Mininum Integrate Time	1
Timing Mode	1	Input Mode	1
Pixel Mode	0	AD Frequency	500KHZ
Start Pixel	121	End Pixel	1909
Coefficient_A[0]	525.794588549994	Coefficient_A[1]	0.284656958399864
Coefficient_A[2]	-3.03832285982464E-05	Coefficient_A[3]	2.39288332033758E-10
Coefficient_B[0]	-2224.88399485126	Coefficient_B[1]	5.68337553091988
Coefficient_B[2]	-0.004387086717351	Coefficient_B[3]	3.0743241502193E-06
TE Cool	No	Slit Size	10
Grating Lines And Blaze Waveleng...	900/550	Filter Type	Hp
Cylindrical Lens	No	Batch Number	
Patch Number		Security Code	
Application Code			
Number Of Calibration Points	8		
Pixel	72	Wavelength	5460.74
Pixel	183	Wavelength	5769.6
Pixel	644	Wavelength	6965.431
Pixel	818	Wavelength	7383.98
Pixel	965	Wavelength	7724.207
Pixel	1211	Wavelength	8264.522
Pixel	1642	Wavelength	9122.967
Pixel	1942	Wavelength	9657.786

- Hardware Setup
  - This menu is active only when the BWSpec software is communicating with an instrument.
  - Opens a **Hardware Setup** window which displays additional settings; the Aux Port control is available.
  - Common Setting
    - Not all features listed will work with specific spectrometers. Check your product's User Manual/Sales Order for details relating to additional controls.



- AuxPort
  - Not all features listed will work with specific spectrometers. Check the product's User Manual/Sales Order for details relating to additional controls.

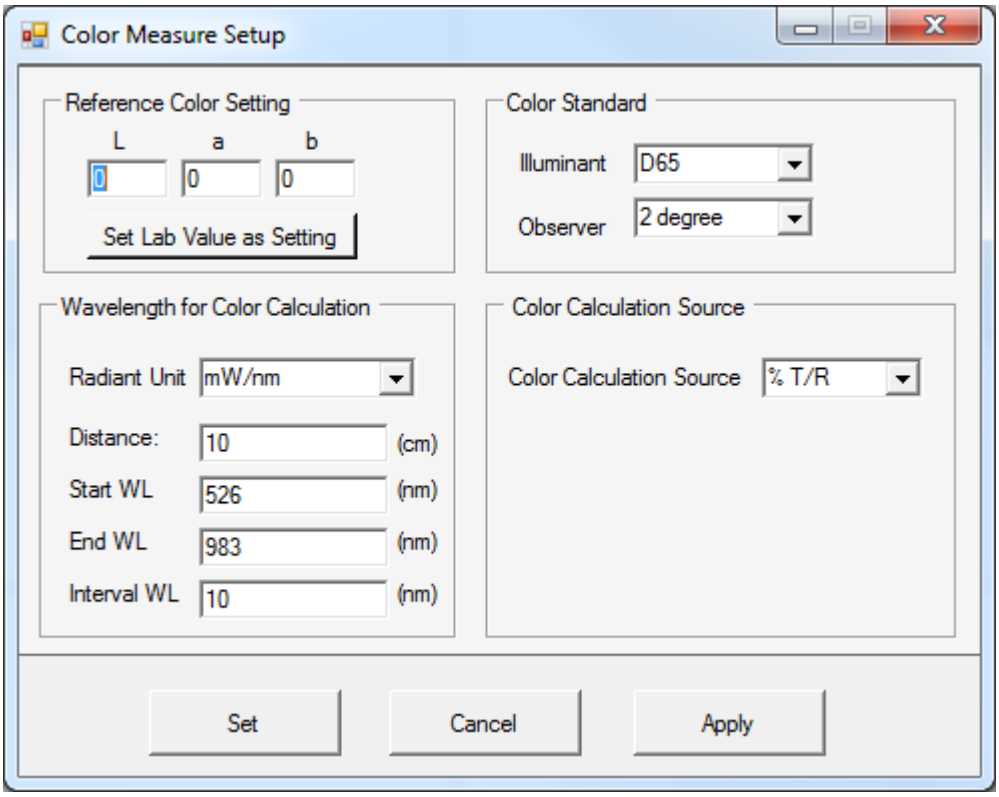


  - This page varies upon different models. See instrument user manual for more information.

- BAC151A Camera
  - Turn on the BAC151A camera

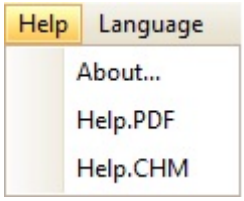
- BAC151B Camera
  - Turn on the BAC151B camera

- Color Setup…
  - Opens a **Color Measure Setup** window.
    - This feature is to be used with color measuring systems.
    - Check the **Color Measurement** section of this User Manual for additional details.
    - Check the User Manual of your color measurement system for additional details.



- Performance Test
  - This feature is designed to be used when the software is communicating with a Raman instrument. The Performance Test provides a procedure for testing the accuracy and repeatability of the instrument readings.
  - See section 11.12 for details.

5.8 Help



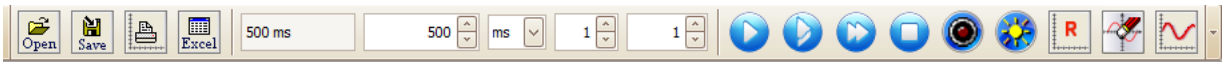
- About…
  - Opens the **About** window providing B&W Tek, Inc. contact information and the version number of the BWSpec software.
- Help.PDF
  - Opens the BWSpec User Manual found in the folder location where BWSpec was installed.

- Help.CHM
    - Opens an XML version of the BWSpec User Manual.

5.9 Language

- English
    - Changes the BWSpec GUI to English.
        - A Restart of BWSpec is required for this change to take place.
- Chinese
    - Changes the BWSpec GUI to Chinese.
        - A Restart of BWSpec is required for this change to take place.
- Japanese
    - Changes the BWSpec GUI to Japanese.
        - This is an option that is sold separately. A password is required to enable this feature.
            - To purchase this feature, contact us at http://bwtek.com/support/
        - A Restart of BWSpec is required for this change to take place.
- Import License File
    - This is needed to change the BWSpec GUI to Japanese.

6 TOOLBAR

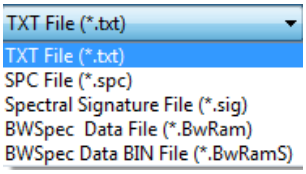


Toolbar

6.1 Open

Open

- For opening files, saved in BWSpec, in the following formats:
  - .txt
  - .spc
  - .sig
  - .BWRam
  - .BWRamS

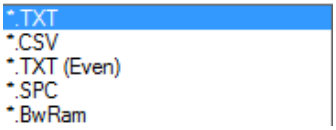


Data from other instruments and software saved in SPC format can also be opened in the BWSpec software.

6.2 Save

Save

- Used to save data of selected spectrum from BWSpec in the following formats:
  - .txt
  - .csv
  - .txt(even)
  - .spc
  - .BwRam



6.3 Print

Print

- Opens a **Print Preview** window with the displayed data and header information from where the user can make changes to the displayed graph and select what printer to use.

6.4 Excel

Excel

- Exports the active/selected single spectrum from the **Spectrum List Panel** to Excel.
  - **Do NOT click on the Excel File during export. This will interrupt the exporting process**

6.5 Integration Time Control

- Total Integration time
  - Integration Time * Multiplier
- Integration Time
  - Exposure time setting for spectrometer (Maximum Value 65,535 ms)
- Unit
  - Time unit for spectrometer acquisition time (µs or ms)
- Multiplier
  - Multiplies the integration time by whole units to give longer exposure. This is used when an exposure time greater than 65,535 ms is needed
- Time Average
  - Range 1 – 65535
  - Average value will take the time average multiplied by the number of scans at the given total integration exposure time and display a single spectrum, which is the average of the x number of scans. This can be used to provide a spectrum with better S/N.

6.6 Acquire Control

- Refer to section 5.3 **Acquire** under **Menu Bar**.

6.7 Reset Graph

- Resets the graph to the default X-axis range for the spectrum and the Y-axis to its set scale.

6.8 Clear Display

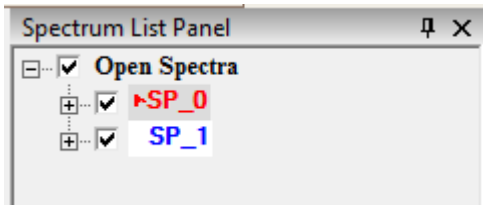
- Removes all spectra on the graph.

6.9 Display Scales

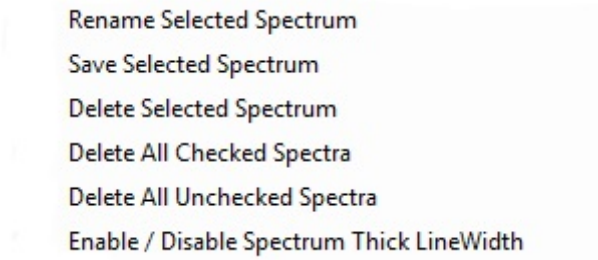
- Opens the **Display Scales** window.
- Refer to section 5.2 **Display Scales**.

7 SPECTRUM LIST PANEL

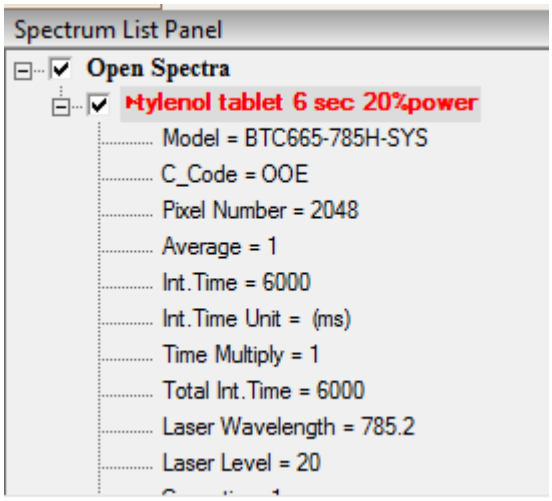
Spectrum List Panel is located on the top-right side of the main screen after being activated.



- Spectra with checkmark signs indicate that the spectra are selected on the current graph display, while spectra without the check marks are hidden from the current graph display. Spectrum highlighted with arrow (color may vary) next to its name indicates the active spectrum currently selected.
- Right Click on individual spectrum from the list will bring up the following menu:

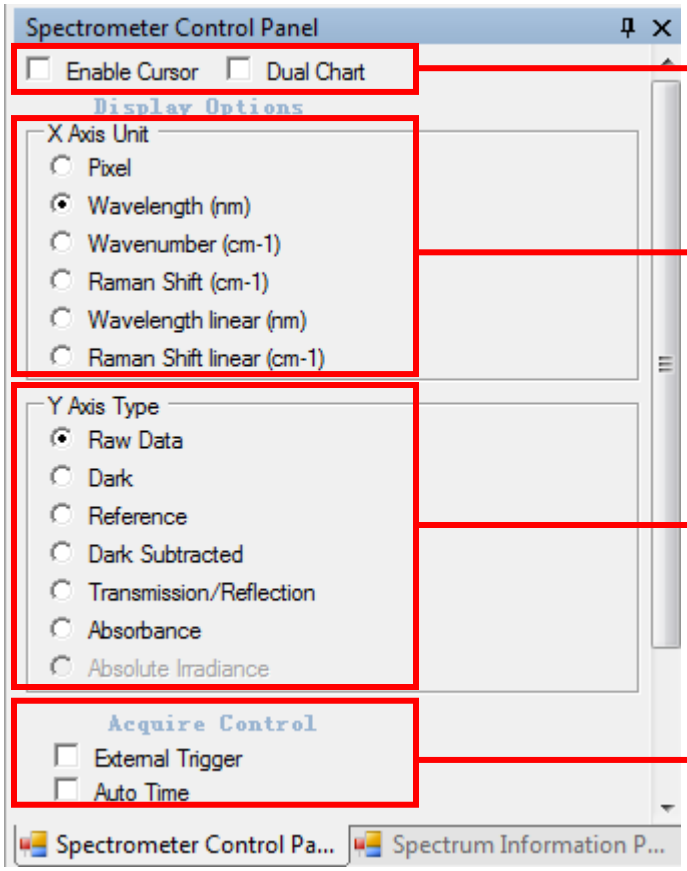


- Toggle the Plus sign to expand the information for a spectrum.



8 SPECTROMETER CONTROL PANEL

The following sections are detailed descriptions of each iem in the BWSpec 4 **Spectrometer Control Panel**.



Additional display options

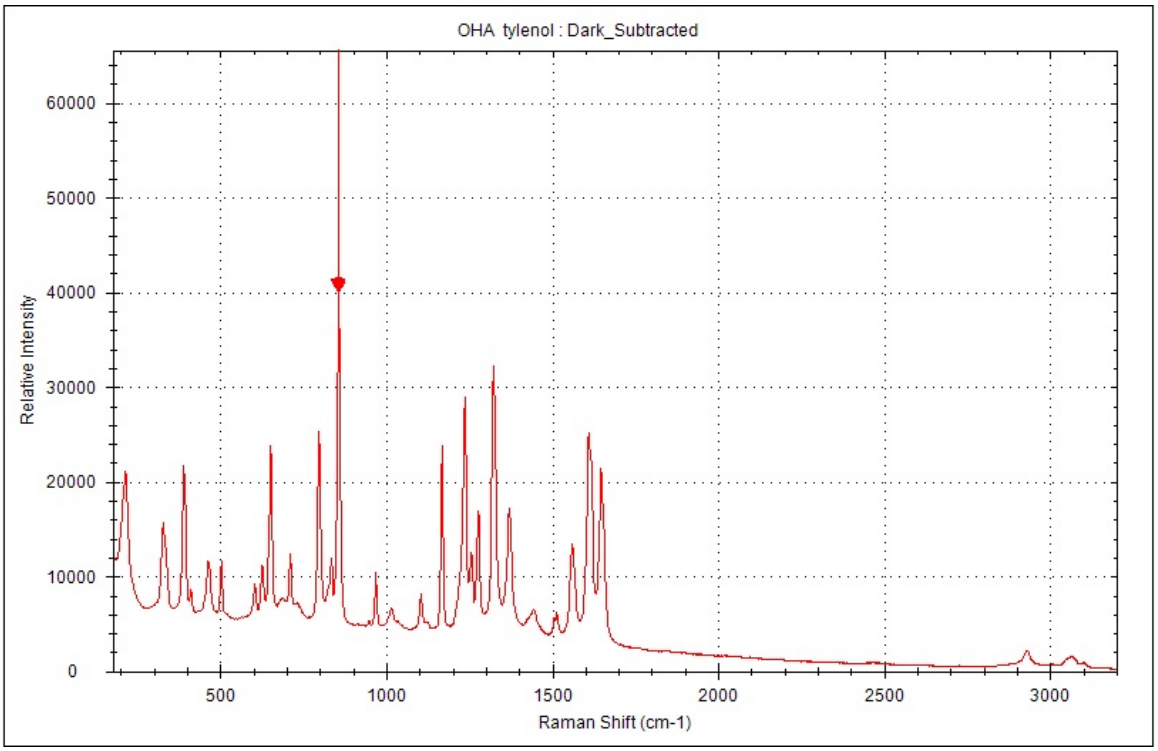
Select desired X-axis spectrum display mode.

Select desired Y-axis spectrum display mode.

Additional control options
Available options may vary depending on your spectrometer or system

8.1 Enable Cursor

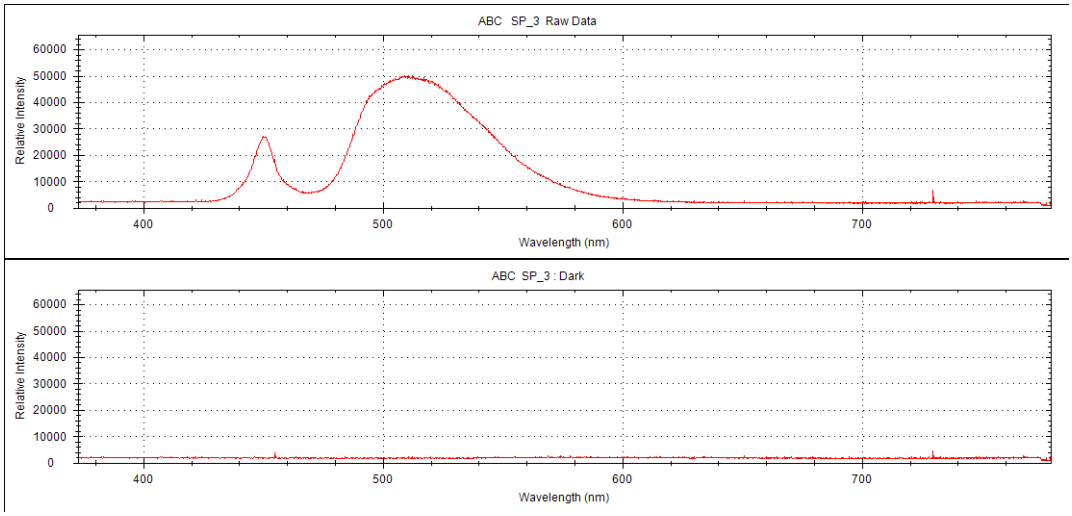
- This provides a vertical line on the graph which follows the mouse cursor. Information relating to the cursor location on the graph will be displayed at the bottom of the main window: *This feature can only be used on a spectrum that is displayed on the graph while the instrument is not acquiring data.*



Pixel = 467 , Wavelength (nm) = 841.26 , Wavenumber (cm-1) = 11886.92 , Raman Shift (cm-1) = 856.0 , Relative Intensity = 36338

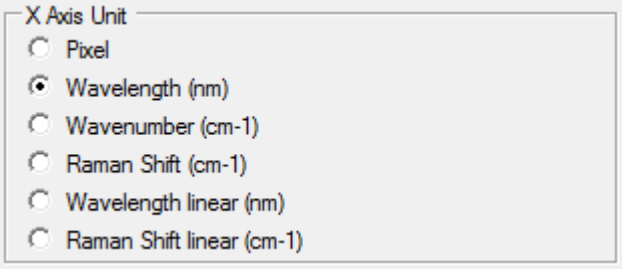
8.2 Dual Chart

- Select to simultaneously display Raw data (top) and a spectrum of your choice (bottom).



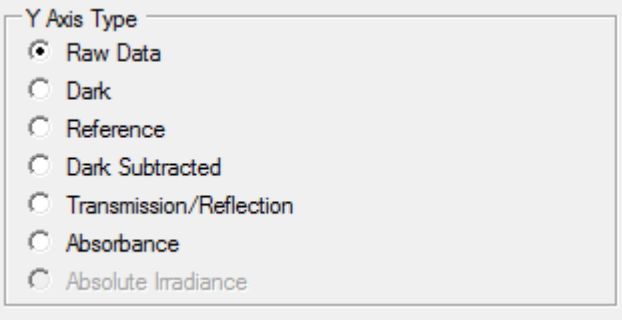
8.3 X Axis Unit

- Changes the X-axis display mode.



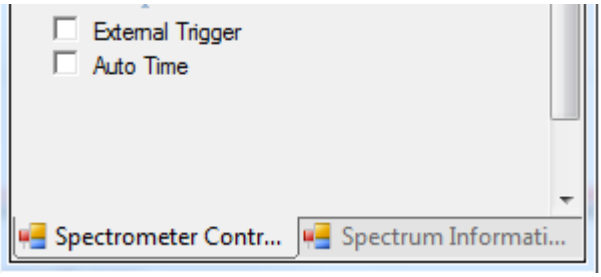
8.4 Y Axis Type

- Changes the Y-axis display mode.



- Raw Data – Shows raw form of the spectrum.
- Dark – Shows spectrum of what is saved into the Dark Array.
- Reference – Shows spectrum of what is saved into the Reference Array.
- Dark Substracted = Raw Array – Dark Array
- Transmission / Reflection (%) = [(Raw Array – Dark Array) / (Reference Array – Dark Array)] * 100
- Absorbance = -log (Transmission (%) / 100)
- Absolute Irradiance – Shows the response of the spectrometer when the **Irradiance Calibration File** is enabled.
    - The spectrometer must have a valid Irradiance Calibration file.
    - See Irradiance Correction Plug-in for additional details.

8.5 Acquire Control



- External Trigger

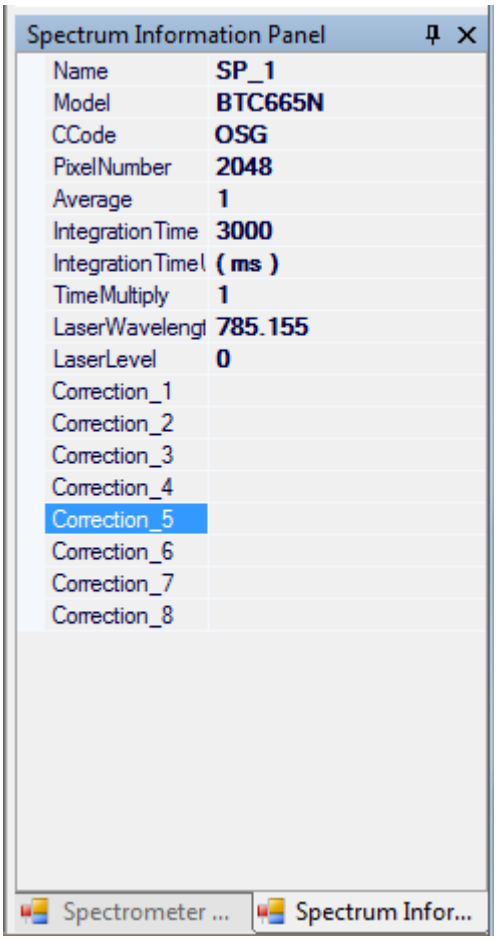
  When enabled, the external trigger will have the following two behaviors depending on hardware setup:
  - External Trigger Mode(default): 1 trigger pulse triggers all averages (a scan with 20 averages will need only 1 trigger pulse);
  - External Pacing Mode: 1 trigger pulse only triggers one average (a scan with 20 averages will need 20 trigger pulses);
  - Refer to section 5.7 and the product user manual for additional details.
- Auto Time
  - When enabled, the software will automatically scan and increase the integration time in increments until the response is close to saturation.

Note:

Additional control options may also appear depending on your spectrometer or system. Eg: illumination LED, laser control, etc.

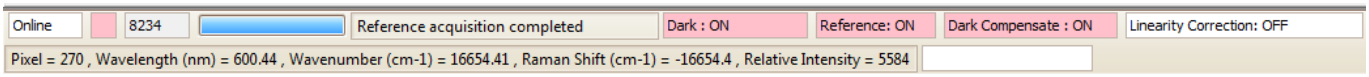
9 SPECTRUM INFORMATION PANEL

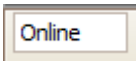
Every spectrum from the list panel will have data displayed in the **Spectrum Information Panel**, including details of the selected spectrum's acquisition parameters.



10 STATUS BAR

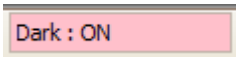
The **Status Bar** is located at the bottom of the main window.

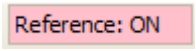


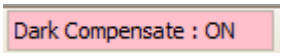
- Shows status of spectrometer.
  - 

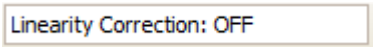
– Spectrometer connected
  - 

- Spectrometer not connected
- 

- Scan count
-  - Acquisition status bar
- 

- Dark Array Status
  - Gives status if a Dark Scan was taken and saved into the Dark Array.
- 

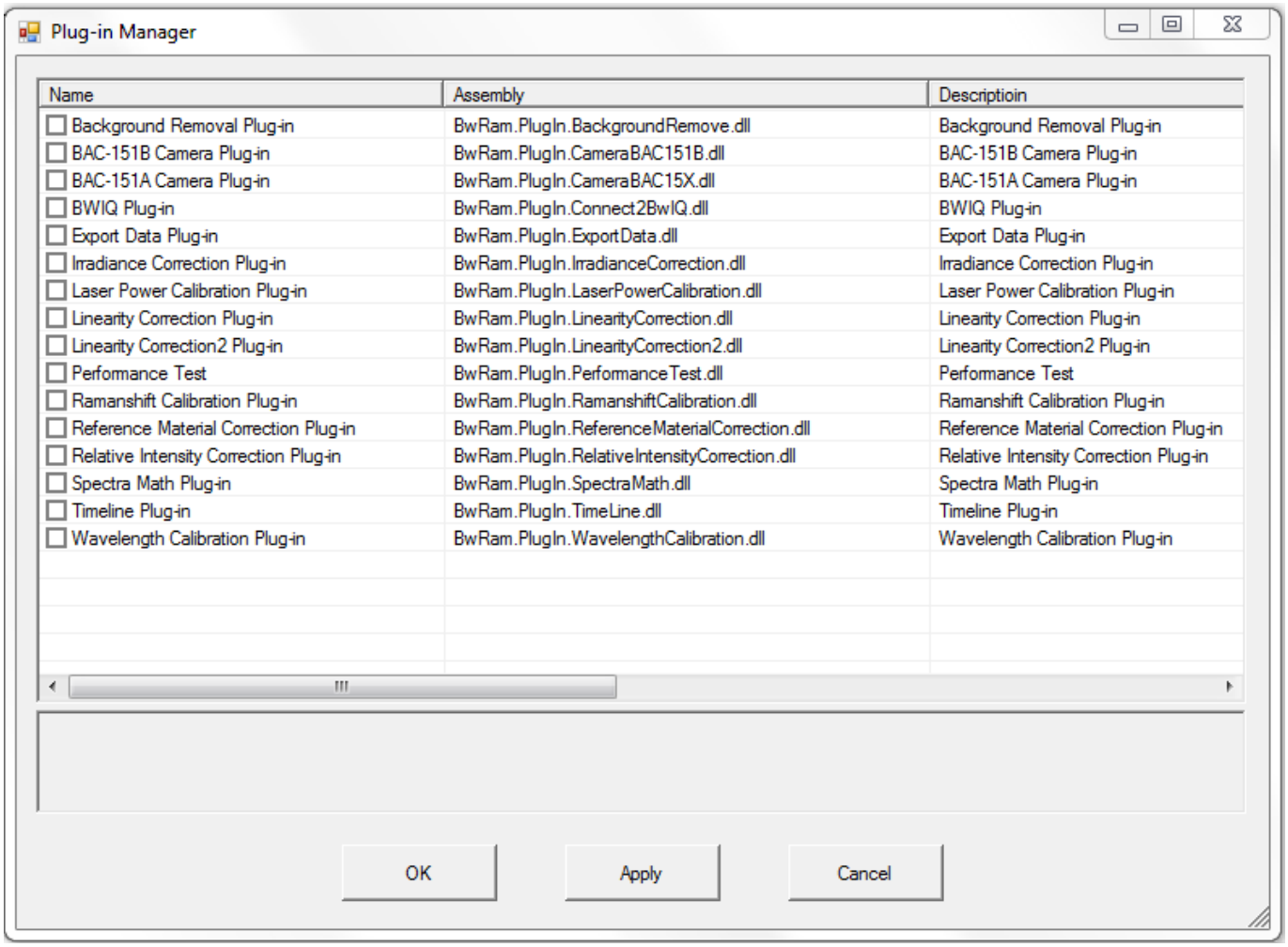
- Reference Array Status
  - Gives status if a Reference Scan was taken and saved into the Reference Array.
- 

- Dark Compensate
  - Gives status of the **Dark Compensate** function
- 

- Linearity Correction
  - Gives status of the **Linear Correction** function

11 PLUG-IN MANAGER

An explanation for each Plug-in function and its location on the Menu Bar once enabled is given below.



11.1 Background Removal Plug-in

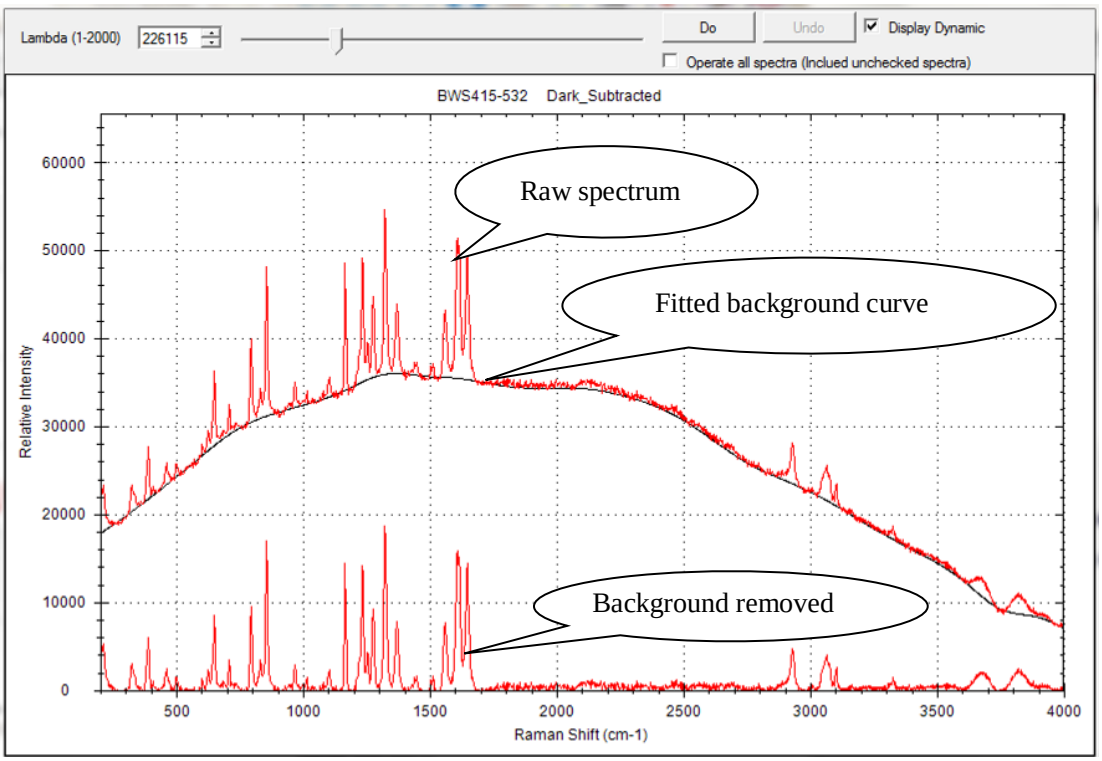
About Background Removal

The **Background Removal** function is used to remove spectrum background (or to perform baseline correction).

Location

Menu Bar → Tools

A display window with three spectra will be displayed: raw spectrum, automatically fitted background curve, and the spectrum after background removal. The lambda factor can be adjusted for manipulating the auto fitted background so as to achieve the desired background removal result. Click **Do** to apply changes.



11.2 BAC-151x Camera Plug-in

About the BAC-151x Camera

This Plug-in is to be used with the accessory BAC151x.

Location

Menu Bar → Tools

Refer to the BAC151x User Manual for details.

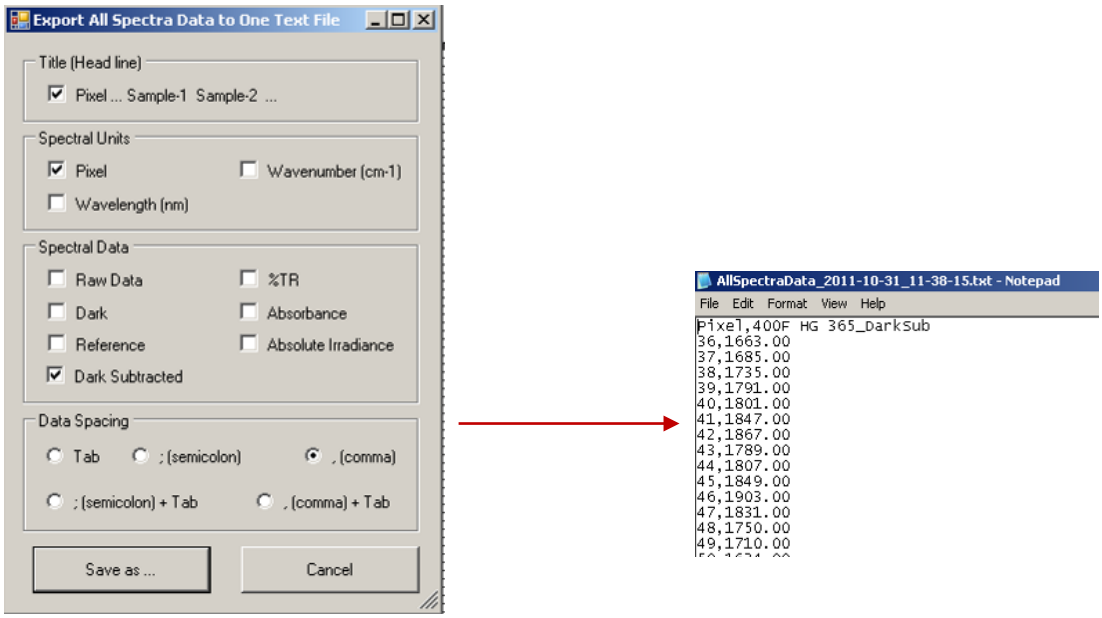
11.3 Export Data Plug-in

About Export Data

Click **Tools** from the menu. Choose **Export Data→ Export All Spectra Data**, and a dialog box will show up. Select the data information to be exported, and click **Save As**. All Spectra will be exported and saved to a text file.

Location

Menu Bar → File



11.4 Irradiance Correction Plug-in

About Irradiance Correction

Irradiance Calibration can be conducted by B&W Tek, Inc. using NIST Traceable Irradiance Standards and calibration setups, if so desired. Irradiance Calibration is an option that can be ordered upon placing a spectrometer order, or through a service request.

Location

Menu Bar → Option

How to Conduct Irradiance Correction

This section is for advanced users only.

In order to conduct an Irradiance Calibration, you must first have a NIST Traceable Lamp Source with Certified Values which cover the spectral range you will be calibrating your spectrometer to and the .DAT file that accompanies your lamp.

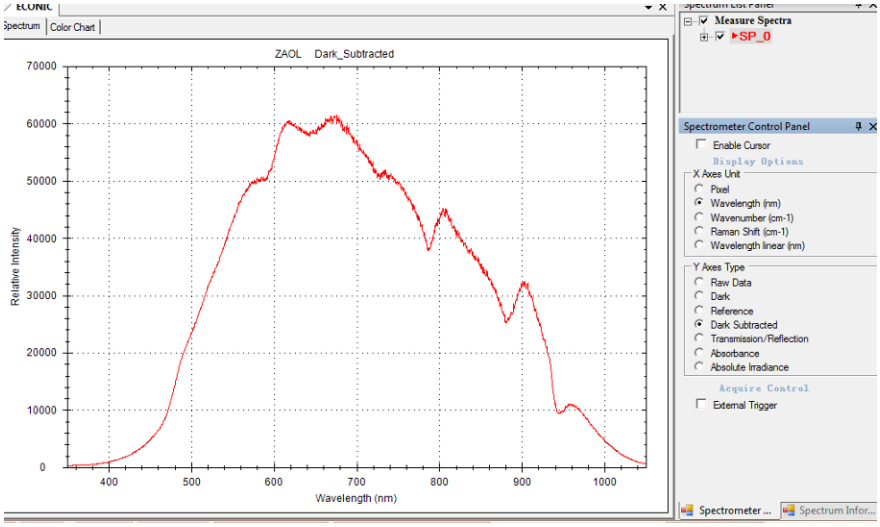
It is also necessary to have the correct input optics for your spectrometer to collect the light, such as a fiber and an integrating sphere.

The spectral irradiance calibration will allow a spectrometer to convert spectral measurements to absolute spectral irradiance measurements in units of light power in W/ [cm^2*nm], mW / [cm^2*nm] or µW / [cm^2*nm]. Alternatively, a spectral irradiance calibration can be used to calibrate the spectrometer for emissive photometric measurements, such as for the color of an emissive source (for example, LED).

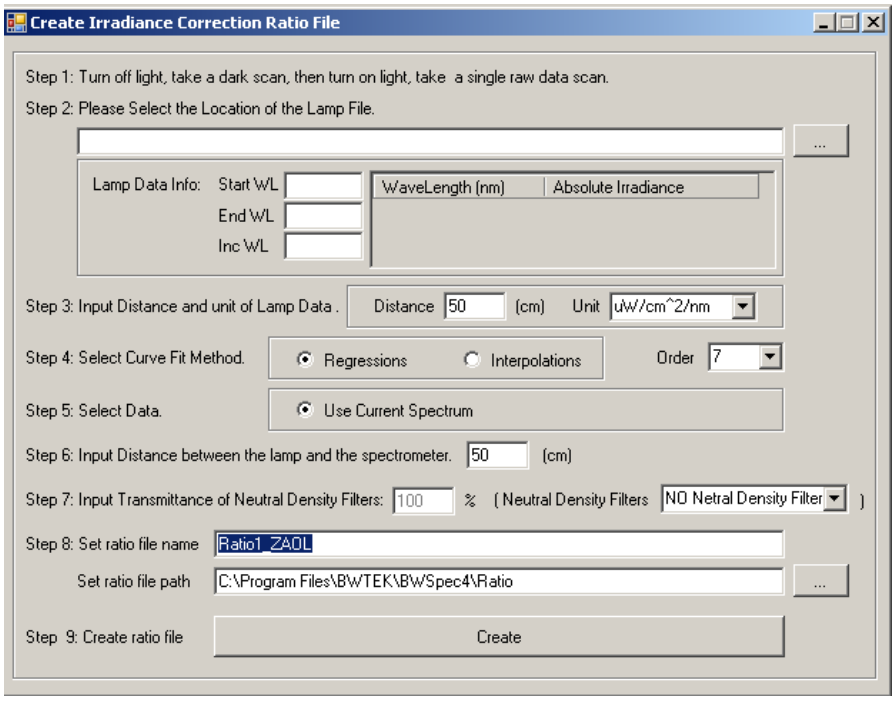
Your setup conditions, distance from source, and lamp current must be as close as possible to what your NIST Certificate states in order to conduct a successful calibration process. Ideally, the light source should not fill the entire spectrometer's angular aperture. The light source should illuminate the spectrometer at a distance specified in the lamp source's calibration data.

Given a correct experimental setup, the spectral irradiance calibration proceeds as followings with the assumption that the spectrometer is equipped with a suitable input optic (linearity correction is highly recommended):

- Adjust the integration time so that the maximum spectral response is just below the spectrometer's saturation level against the certified lamp at a specified distance. Stop the acquisition and freeze all physical setup with minimal disturbance.

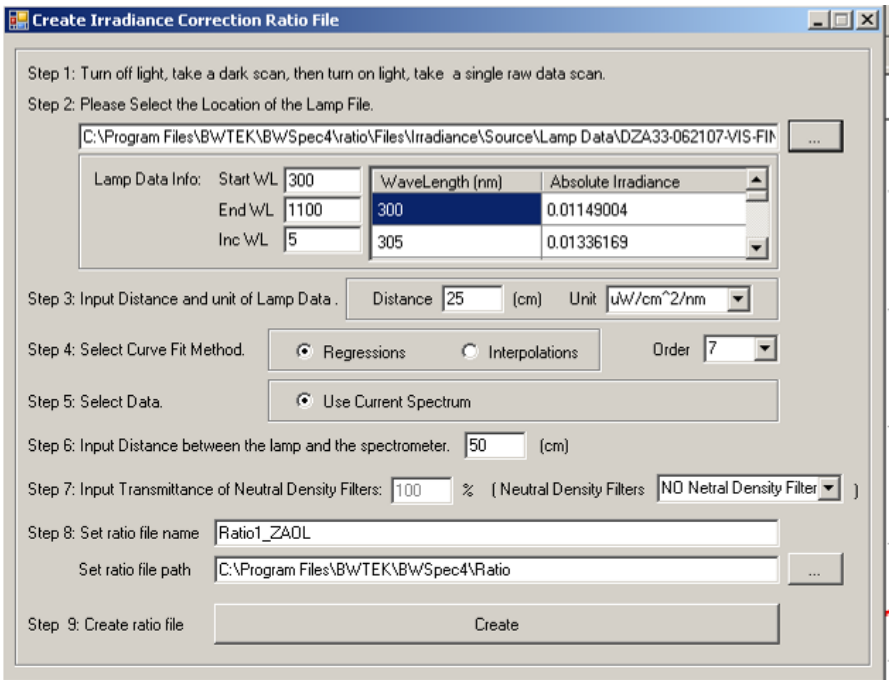


- Step 1: Cover your light input aperture so that no light is gathered by your setup. Take a ***Dark*** scan first. Uncover the aperture, then take a ***Raw*** scan.
- Creation of the Irradiance Ratio File:
  From the Menu Bar, select **Option** → **Irradiance Correction**.



- Step 2: Click the  button and locate the lamp data file for the light source you are using for irradiance calibration. Your lamp data file must be configured in a manner in which BWSpec can read it.

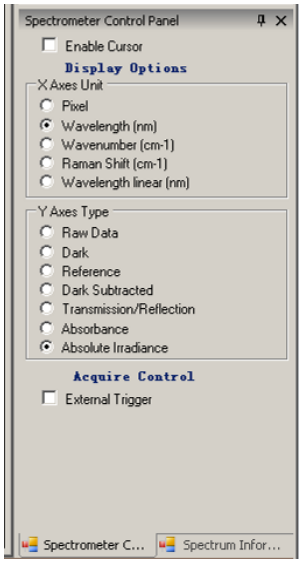
Please refer to the Appendix ***"Definition of Irradiance Data File Format"*** for information on formatting. You can also view the file "S-1169N0.DAT", which can be found in the folder where BWSpec is installed, for an example of format.



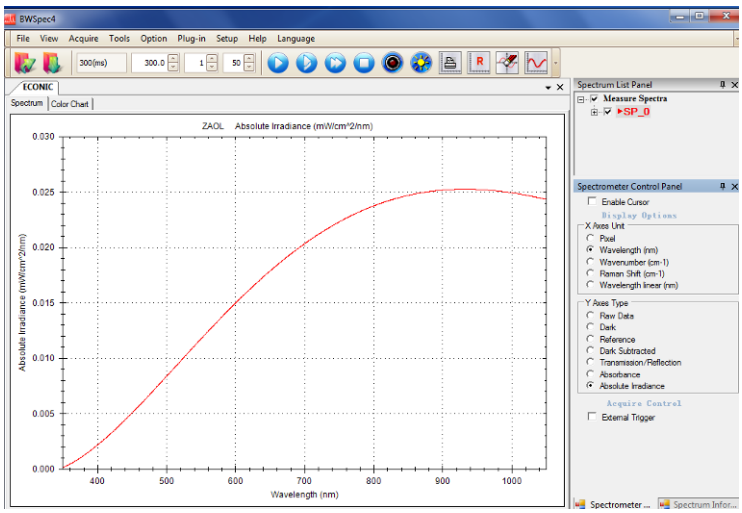
- Step 3: Input the distance at which your Calibrated Light Source was originally calibrated. This information will be contained on your Certificate or the .DAT file. *Be careful to select correct units to match the certified data provided in the reference certified lamp data file.*
- Step 4: Choose either *Regression* or *Interpolation* to calculate Irradiance Ratio file.
- Step 5: Select **Use Current Spectrum** to use ***Dark Subtracted*** data for calculation.
- Step 6: Select the distance between your input optics and your certified light source in your current setup. Also, make sure to enter all calibration related information, such as additional optics used, into the dialog box. Step 7: Input transmittance of neutral density filters.
- Step 8: Indicate the name of the ratio file and where you would like the data to be saved. We suggest that you keep the default naming scheme of the spectrometer (Ratio1_C-code). Set the ratio file path which is the Location where the ratio file will be saved.
- Step 9: Click **Create** to generate the **Irradiance Ratio File**.

Apply the Irradiance Ratio File

- Select **Option→ Enable /Disable Irradiance Correction**.
- Check the box for **Enable Irradiance Correction**.
- Click  to locate the irradiance correction “Ratio1_C-code.txt” file.
- Click **Set**.
- Click “Absolute Irradiance” on the **Spectrometer Control Panel**. The Absolute Irradiance curve will show on the display.



You may need to adjust the X-axis and Y-axis scales in order to get a suitable display scale.



11.5 Linearity Correction Plug-in

About Linearity Correction

Linearity correction will compensate for the detector array's nonlinear response by following a fitted response curve against received detector photons.

Location

Menu Bar → Option

A typical detector array will likely exhibit a nonlinear response with respect to incident photons at low light levels as well as when close to saturation. In these regions, doubling photons or doubling detector exposure time will no longer result in two times the detector's output deviating from a desired linear response range.

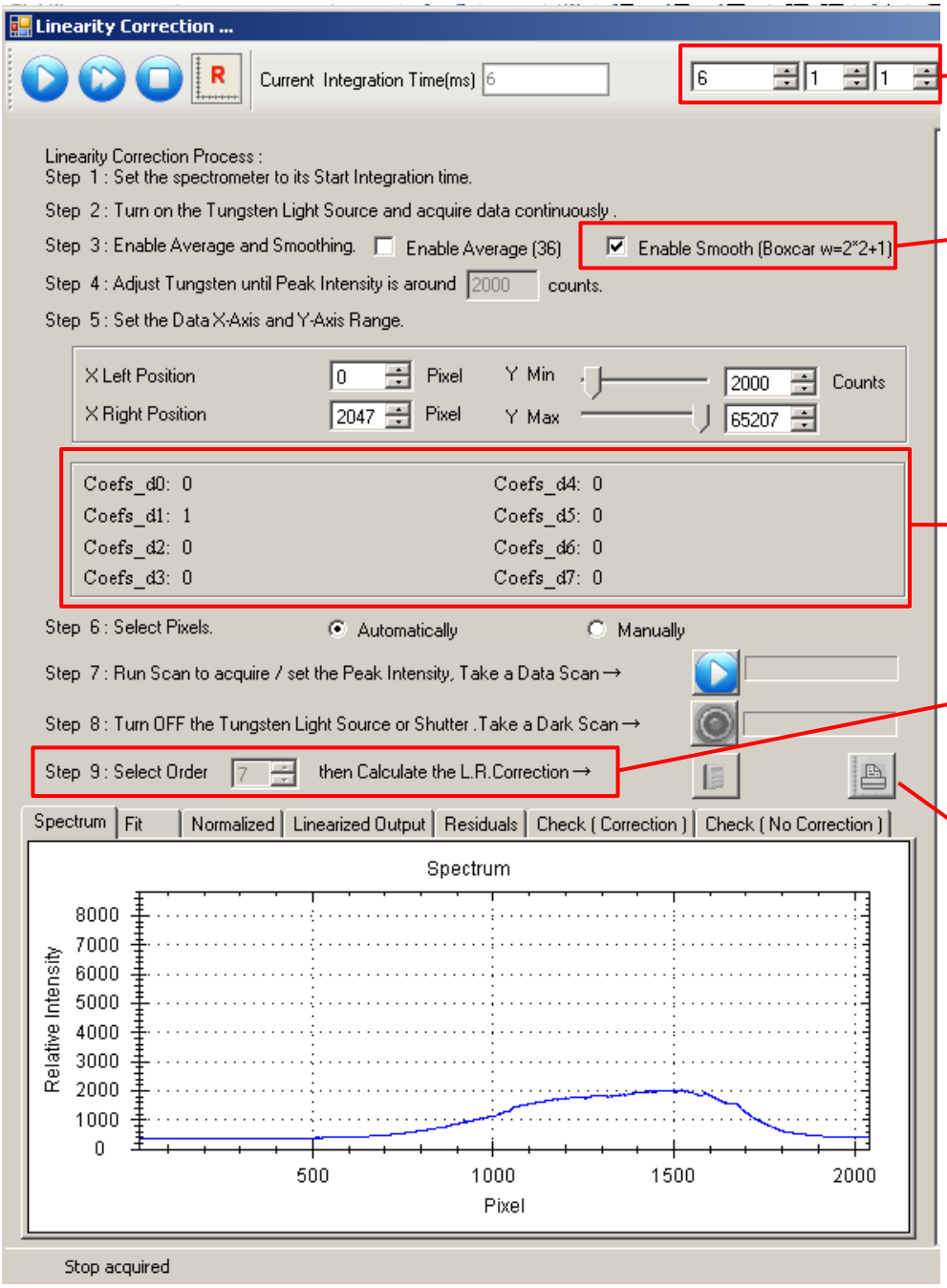
***Note**: "Linearity Correction" must be conducted by the factory in order for the Linearity Correction Coefficients to be saved into device memory. "Linearity Correction" is an upgrade option to be ordered when purchasing the spectrometer or through a service request.*

How to Conduct Linearity Correction

For Advanced users, the linearity correction may be conducted at the customer site.

From the Menu Bar, select **Option→Linearity Correction**. The linearity correction window will appear.

Follow Step 1 through Step 9 instructions in the window to proceed.



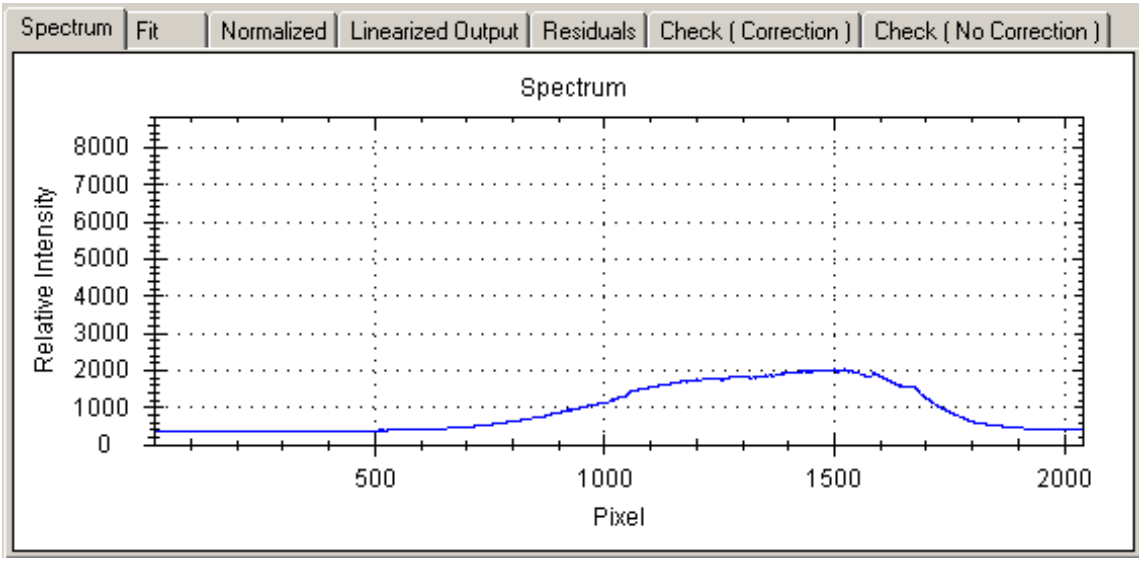
Adjust starting integration time, multiplier, and average

Enable Boxcar smoothing during correction process

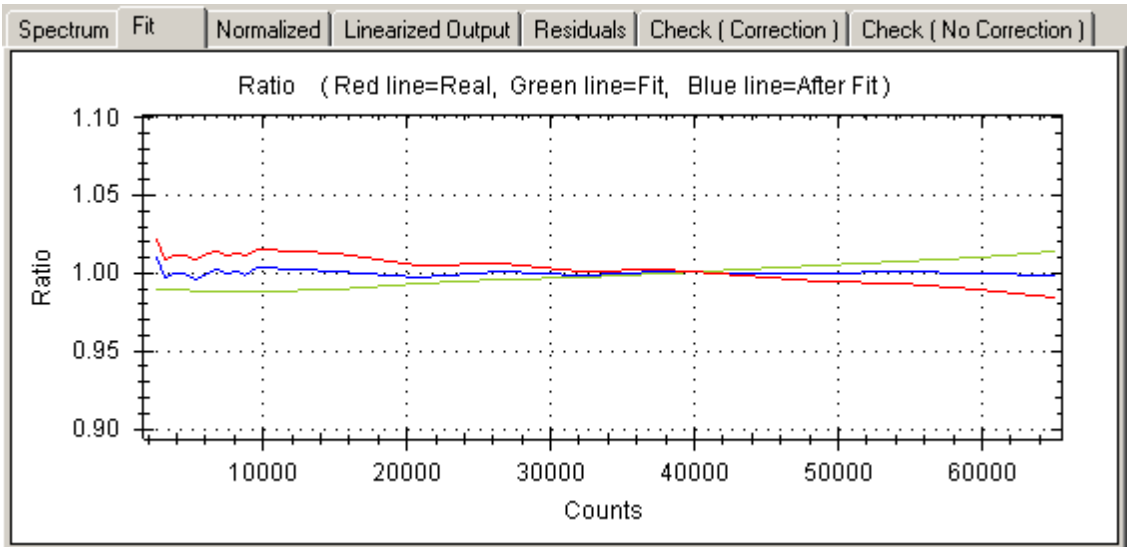
Display current active Linearity Correction Coefficients

Select from 4-7 order fitting curves and calculate Linearity Correction Coefficients

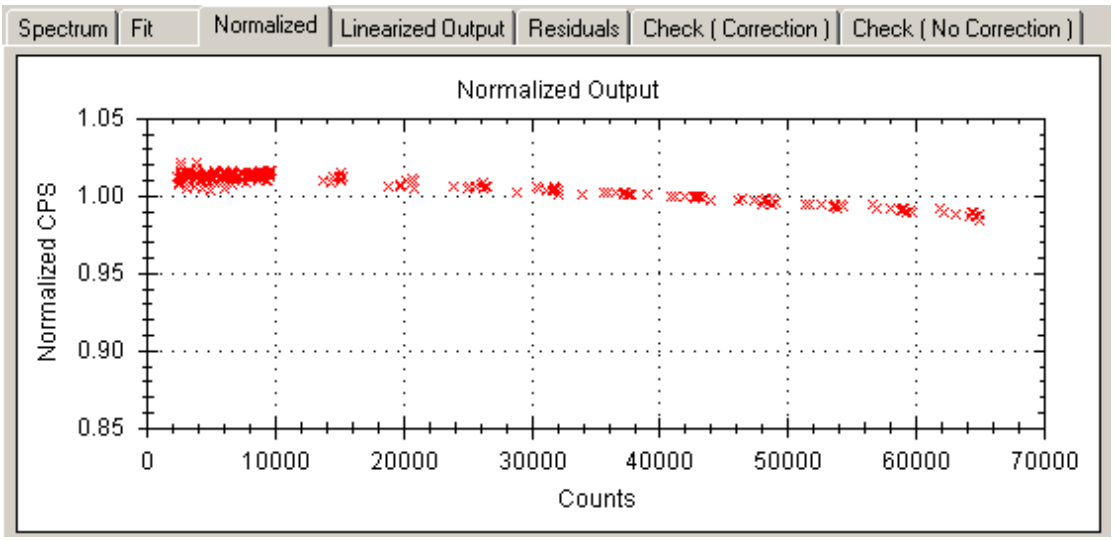
Print Linearity Correction Report



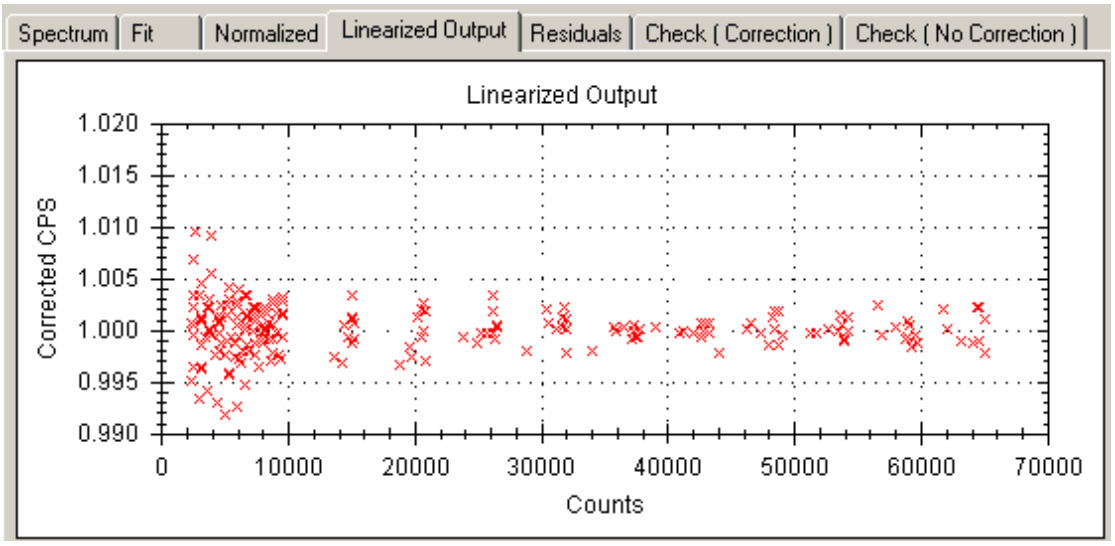
- Spectrum
  - Displays the current spectrum based on the integration time at the top of the window.
  - The graph may be zoomed in or panned just like the main window.
  - Displayed is a Tungsten spectrum that has been attenuated to a Relative Intensity of ~2000 counts.



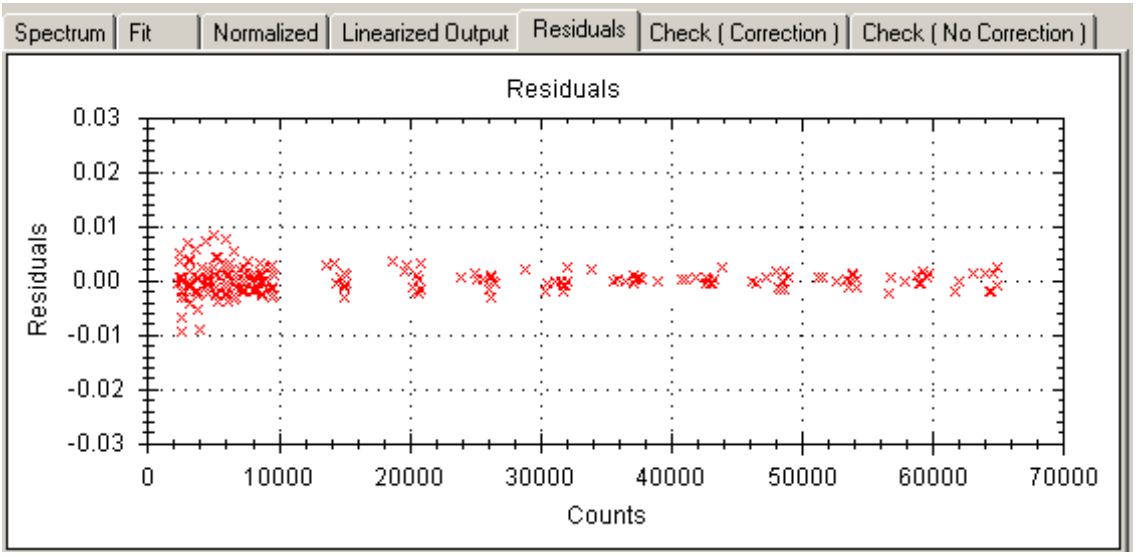
- Fit
  - Displays the fitting curve of the correction based on the Order (Step 9)



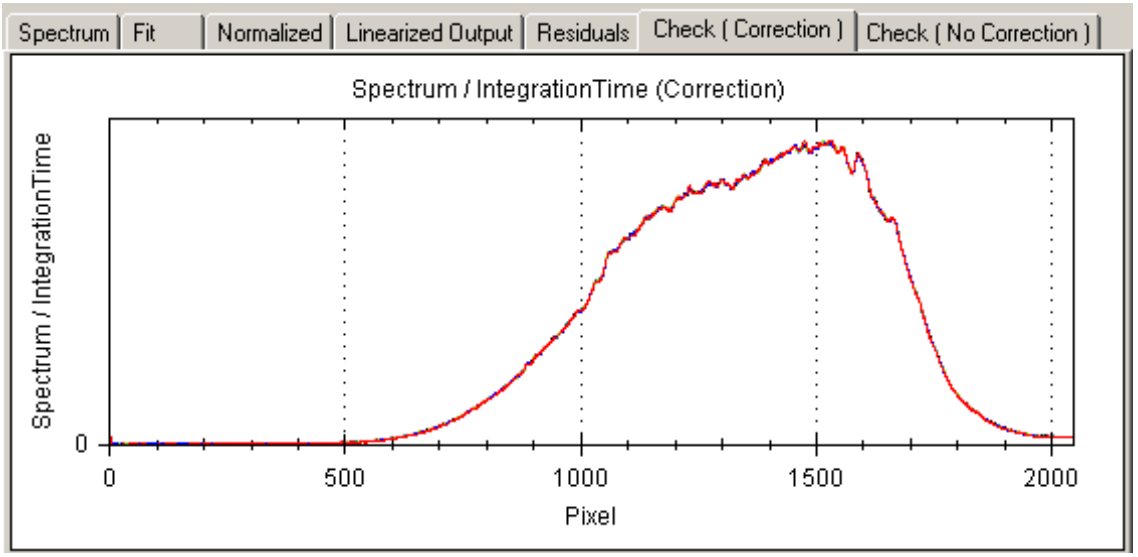
- Normalized
  - Displays the output before correction



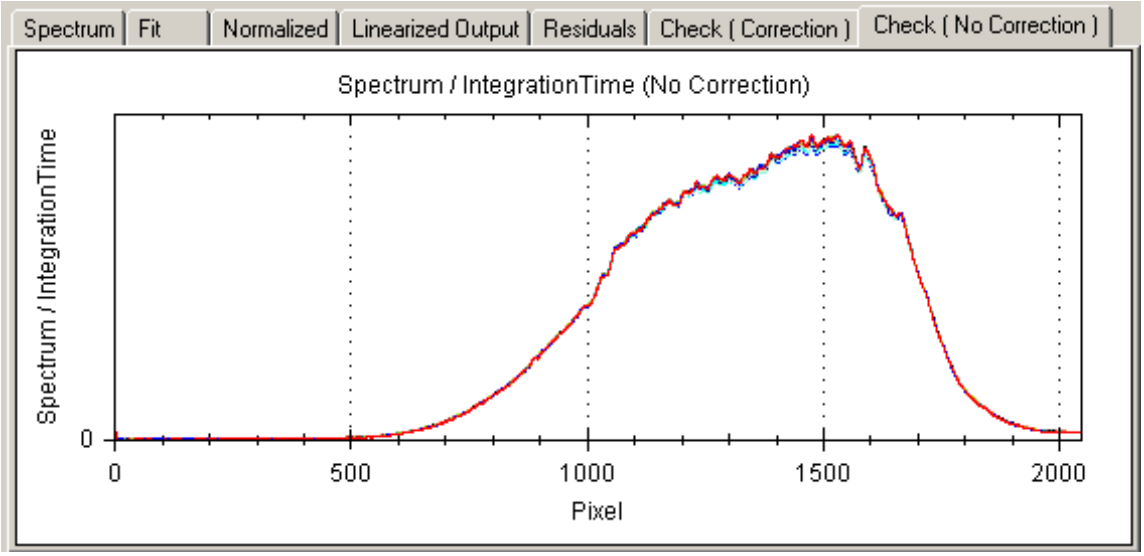
- Linearized
  - Displays the output after correction.



- Residuals
  - Displays the percent difference between the corrected value and the real value of intensity.



- Check (Correction)
  - Displays the corrected Spectrum/Integration vs Time graph



- Check (No Correction)
  - Displays the uncorrected Spectrum/Integration vs Time graph.

Note: *Once the Flash is re-read, the current active Linearity Coefficients will be lost. Linearity Correction conducted by the factory will have the coefficients saved in Flash.*

Note: *The key for a successful linearity correction calibration setup is to provide a light input (Tungsten light source is suggested here) with adjustable intensity for the spectrometer to be calibrated so that the spectrometer shows a light response 500-1000 counts above its dark levels at its shortest integration time. This will provide the calibration with maximum useable dynamic ranges.*

Activate Linearity Correction

To activate linearity correction, go to the Menu Bar and select **Option → Enable /Disable Linearity Correction**.

11.6 Reference Material Correction Plug-in

About Reference Material Correction

In applications such as diffuse reflectance measurements, a certified reflectance standard is often used to serve as a reference. The %R values throughout the measurement range are then calculated by using ratios with respect to the reference in a relative sense. With the available certified %R values, the BWSpec software can calculate the "absolute reflectance" against the reference.

Location

Menu Bar → Option

The following is a table of typical %R values obtained using a certified white PTFE type material spectral reflectance standard (B&W Tek model number SRR-1.25-99 or SRR-2.0-99).

Wavelength (nm)	Certified %R value		Wavelength (nm)	Certified %R value
360	98.5		600	98.9
370	98.7		610	98.9
380	98.7		620	98.9
390	98.7		630	98.9
400	98.8		640	98.9
410	98.8		650	98.9
420	98.8		660	98.9
430	98.8		670	98.9
440	98.8		680	98.9
450	98.8		690	98.9
460	98.8		700	99.0
470	98.8		710	98.9
480	98.9		720	99.0
490	98.9		730	98.9
500	98.9		740	98.9
510	98.9		750	99.0
520	98.9		760	98.8
530	98.9		770	98.9
540	98.9		780	98.9
550	98.9		790	98.9
560	98.9		800	99.0
570	98.9		810	98.9
580	98.9		820	99.0
590	98.9		830	98.9

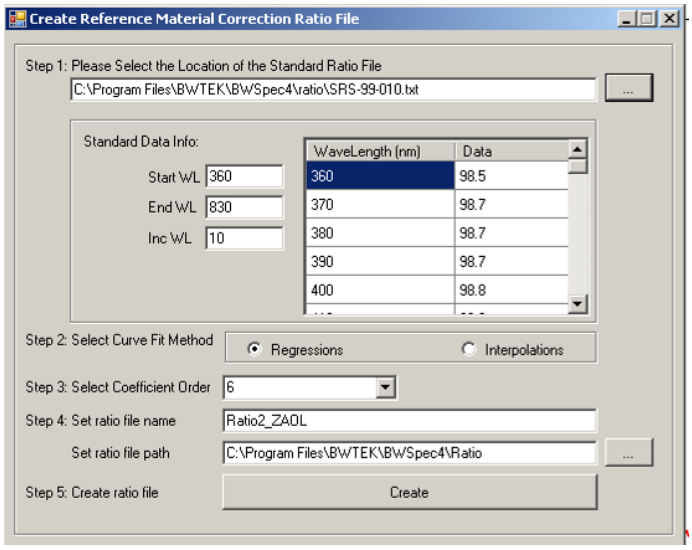
If we define %Rs (non-correction) as the sample percent reflectance at a given wavelength:
%Rs (non-correction) = (Sample intensity/Reference intensity)*100.

After reference material correction:
%Rs (absolute) = %Rs (non-correction) * Certified %R value/100 where all values are calculated at given wavelengths across the calibration wavelength range.

Generate Reference Material Correction Ratio File

This section is for advanced users only.

- Collect a spectrum using reference materials.
- Select **Option→ Reference Material Collection**.
- Click [...] and browse to locate the "Reference Material ratio.txt" file. You will be directed to the default path where this file is stored: C:\Program Files\BWTEK\BWSpec4\ratio\. This file contains the certified values of spectral reflectance over the wavelength range of interest. After the file is loaded, the standard data will be populated.



- Follow the steps stated to fill out the parameters for the correction. The default ratio file name is Ratio2_C-code.
- Click **Create** to generate a Ratio2 file.

Enable Reference Material Correction Files.

- Select **Option→ Enable Reference Material Correction**.
- Check the box for **Enable Reference Material Correction**.

- Click  and locate the “Reference Material correction ratio2.txt” file.
- Click **Set**.

11.7 Relative Intensity Correction Plug-in

About Relative Intensity Correction

Relative intensity correction is specific for Raman spectrometer users. Its purpose is to correct unique relative spectral responses against a traceable standard for individual spectrometers. The corrected spectral response of a Raman spectrometer makes meaningful comparisons between data obtained from different instruments possible. The calibrated spectral response also reveals quantitative vibrational intensity information between different Raman features within a given Raman spectrum.

The relative intensity correction involves the use of Standard Reference Material 2241 (SRM 2241) for Raman spectrometers when a 785nm excitation laser source is used, SRM2242 when a 532nm excitation laser source is used and SRM2244 when a 1064nm excitation laser source is used.

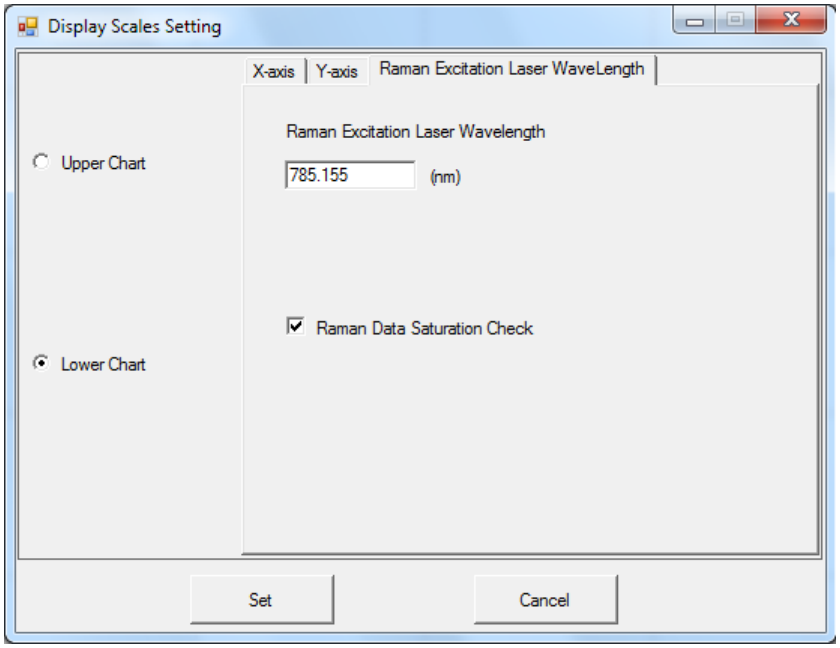
Location

Menu Bar → Option

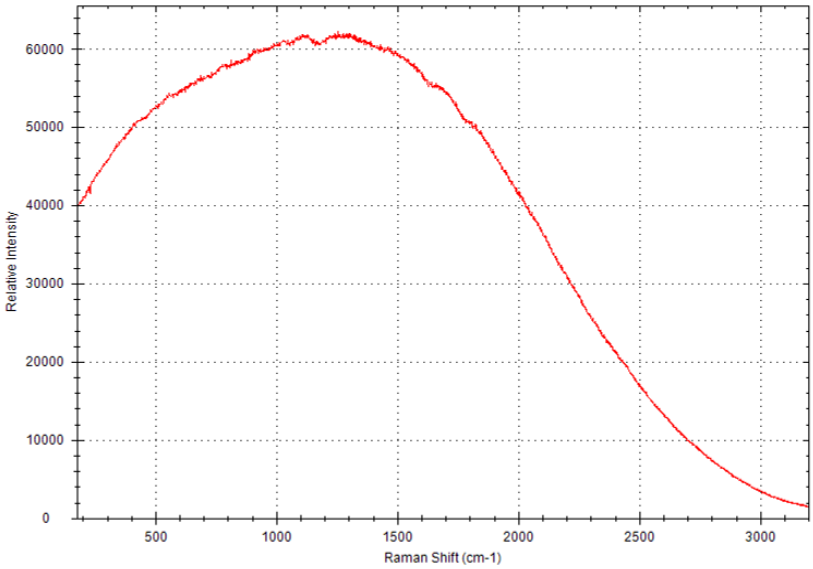
How to conduct a relative intensity correction

This calibration comes standard with B&W Tek’s applicable portable Raman systems. For advanced users, this may be conducted at a customer site with appropriate equipment. A probe must be connected to a Raman system or a laser and a spectrometer in order to get proper results.

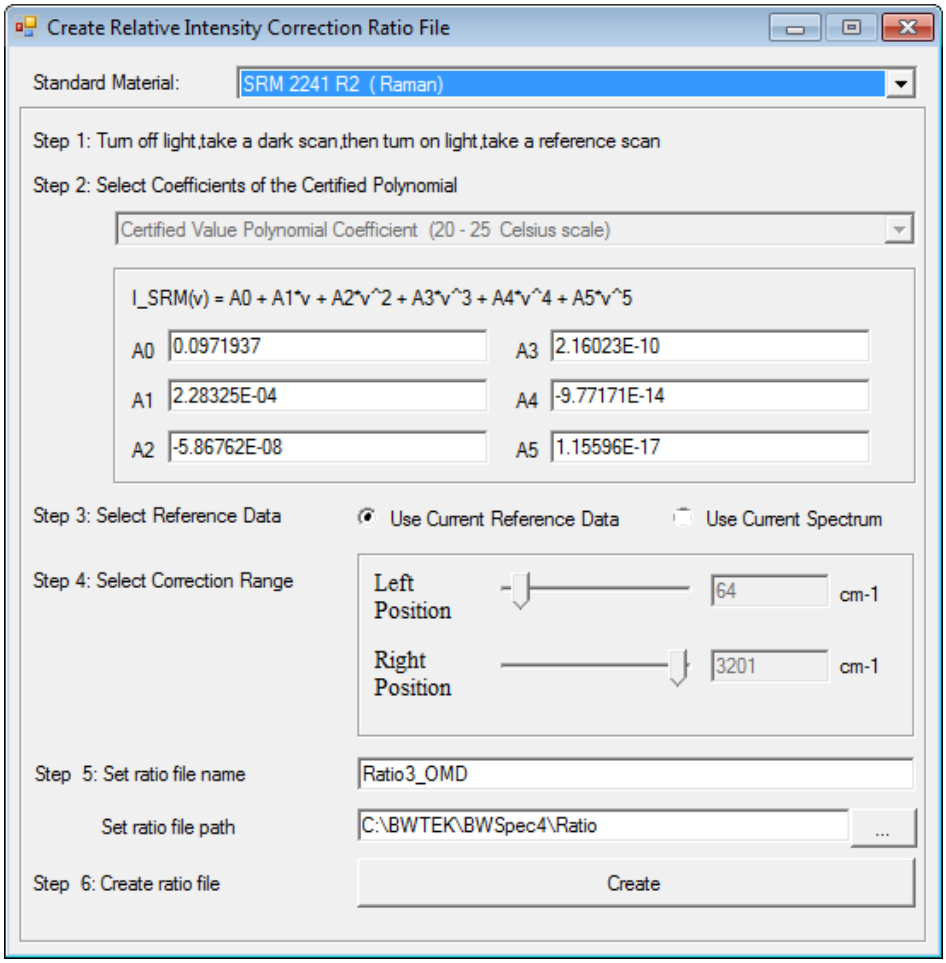
- Ensure that the wavelength of the excitation laser you are using is entered into the **Raman Excitation Laser Wavelength** page on the **Display Scales** (for example, 785nm). You will need to determine the laser wavelength and put in the appropriate measured value.



- Determine the appropriate integration time: use the standard reference material SRM2241 (for 785nm), SRM2242 (for 532nm) or SRM 2244(for 1064nm) to run a scan. The integration time of the scan should be adjusted to a value such that the highest intensity level is just below saturation level (65000 counts).
- Run a dark scan with the same integration time. For B&W Tek, Inc. Raman systems, the laser turns off automatically when the dark scan is being collected. For modular Raman spectrometers, make sure the laser is off when a dark scan is being collected.
- Run a reference scan using the same standard reference material with the same integration time with laser turned on.



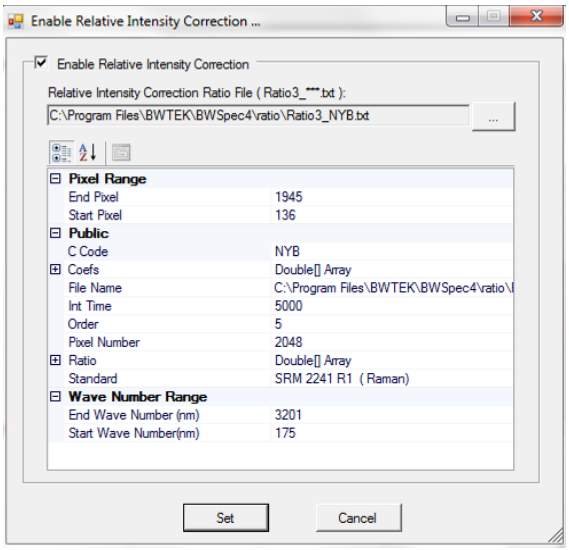
- From the Menu Bar, select **Option** → **Relative Intensity Correction**. The **Relative Intensity Correction** window will appear.

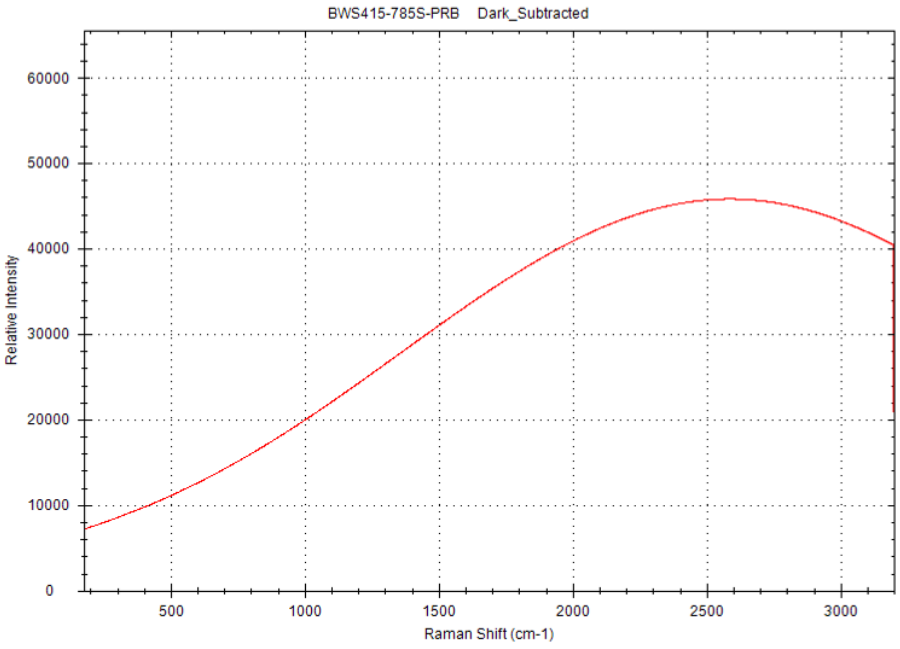


- Select the appropriate standard material (for example, SRM2241).
- Select **Use Current Reference Data**.
- Set the ratio file name and the path where the ratio file will be stored.
- Click the **Create** button. The **Relative Intensity Correction** file is created and the Ratio3 file is saved in the designated path.

Apply Relative Intensity Correction

To activate the relative intensity correction feature, go to the Menu Bar and select **Option** → **Enable /Disable Relative Intensity Correction**. Check the box for **Enable Relative Intensity Correction**, and click on ... to locate the Ratio3 file specific to the system that was calibrated. Click **Set** to apply.





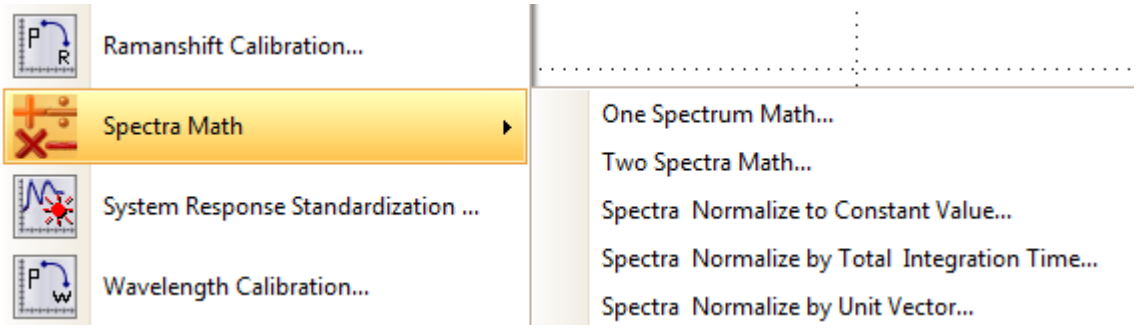
11.8 Spectra Math Plug-in

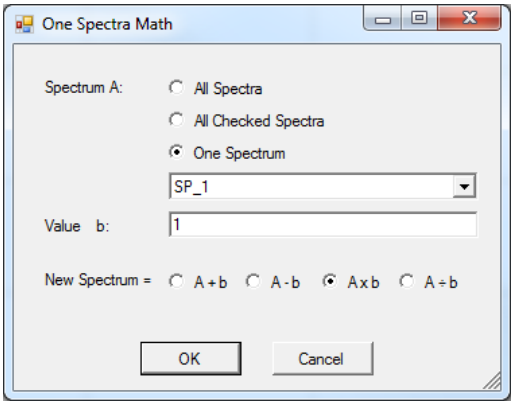
About Spectra Math

This function provides the ability to perform math functions on a single or multiple spectra.

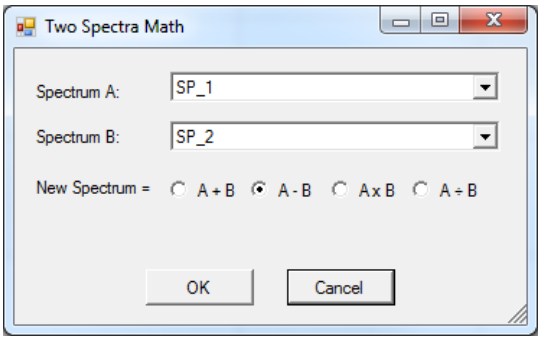
Location

Menu Bar → Tools

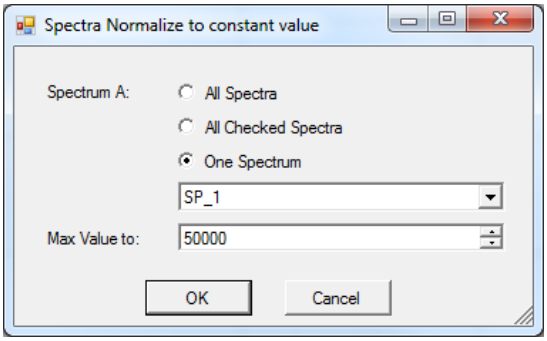


- One Spectrum Math…
  - 

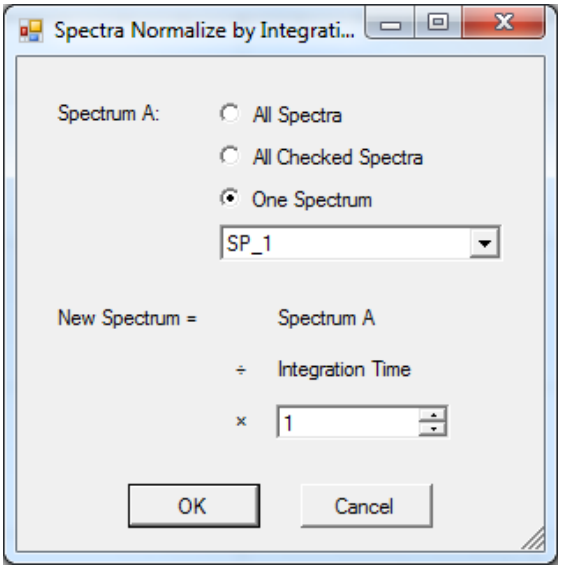
- Two Spectra Math…
  - Perform a math function on two spectra.



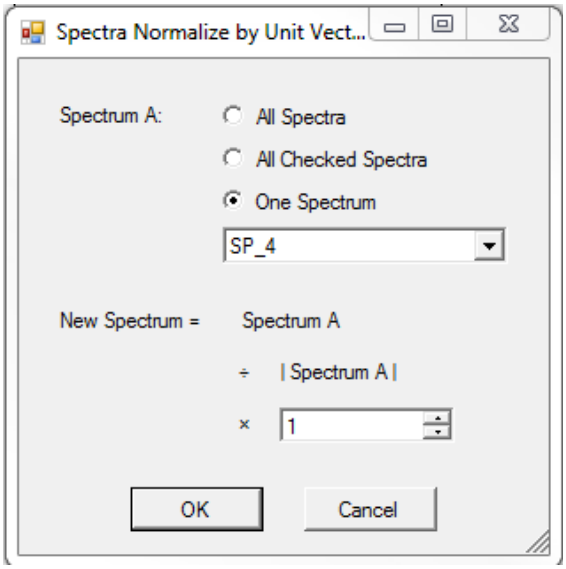
- Spectra Normalize to Constant Value…
  - Normalize spectra to a constant.



- Spectra Normalize by Total Integration Time…
  - Normalize spectra by integration time.



- Spectra Normalize by Unit Vector
  - Normalize spectra by Unit vector



11.9 Timeline Plug-in

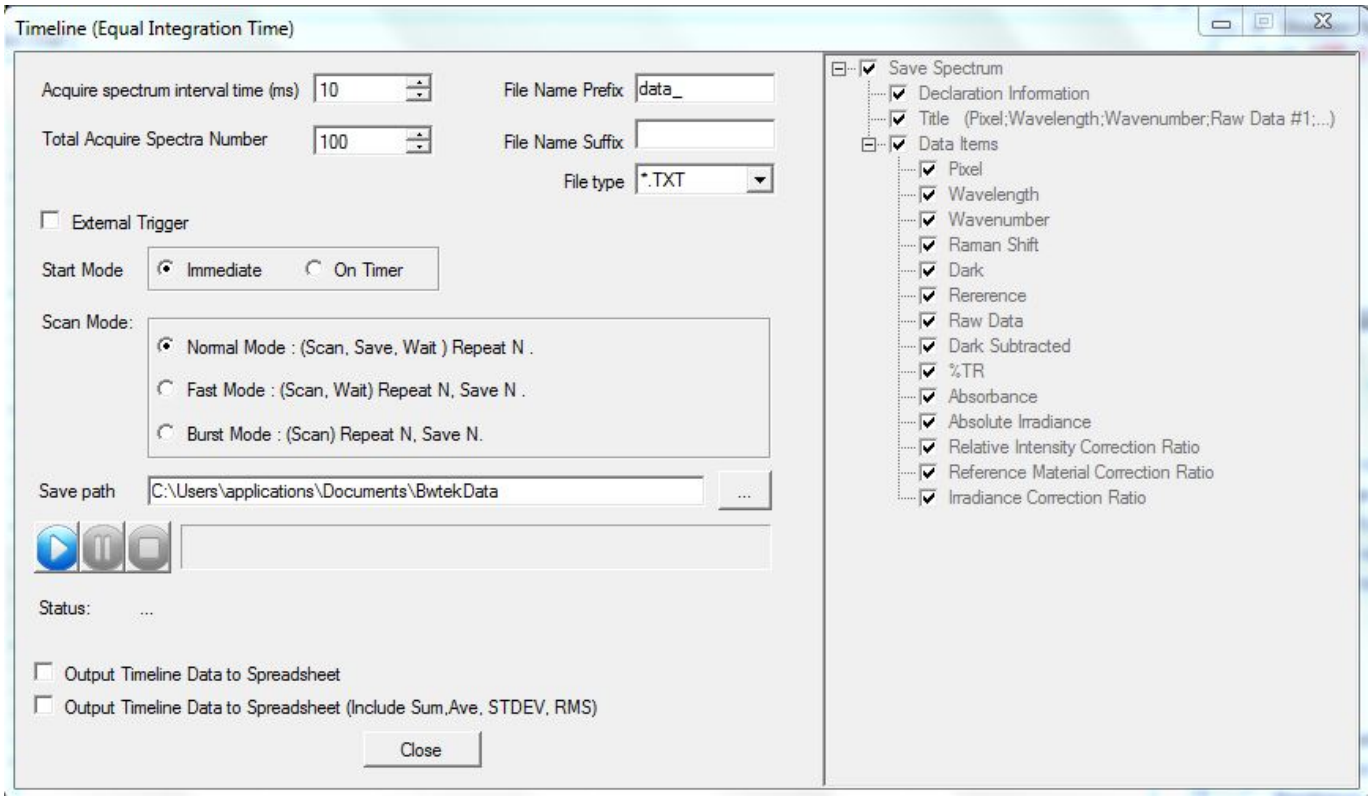
About Timeline

The **Timeline** function provides automated, timed recording of acquired spectra within the scheduled time interval parameters set by the user. These spectra are then saved into individual files. The data acquisition parameters such as laser power and integration time must be set before entering the timeline dialog.

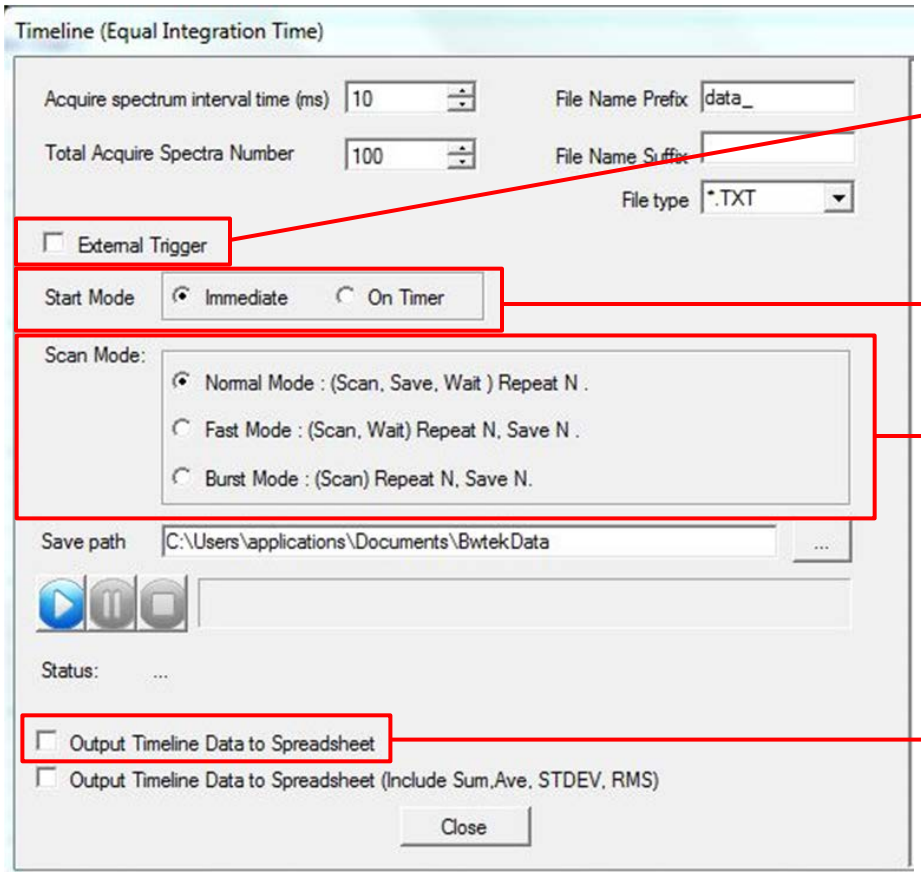
Location

Menu Bar → Acquire

Timeline (Equal Integration Time)



Click **Acquire→Timeline→Timeline (Equal Integration Time**), and a dialogue box will appear. Before starting a timeline scan, you need to enter settings, including interval time, number of scans, file name suffix and file name prefix, select save data format and save path. Click the  button to start timeline scan. The spectra collected will be saved in the designated path. If no specific suffix is assigned, a default of _1, _2, _3 and so on will be assigned to each spectrum.



Enable External Trigger function in Timeline mode

Start Timeline acquisition with immediate effect, or on a timer countdown

Spectra acquisition modes available depending on your spectrometer or system

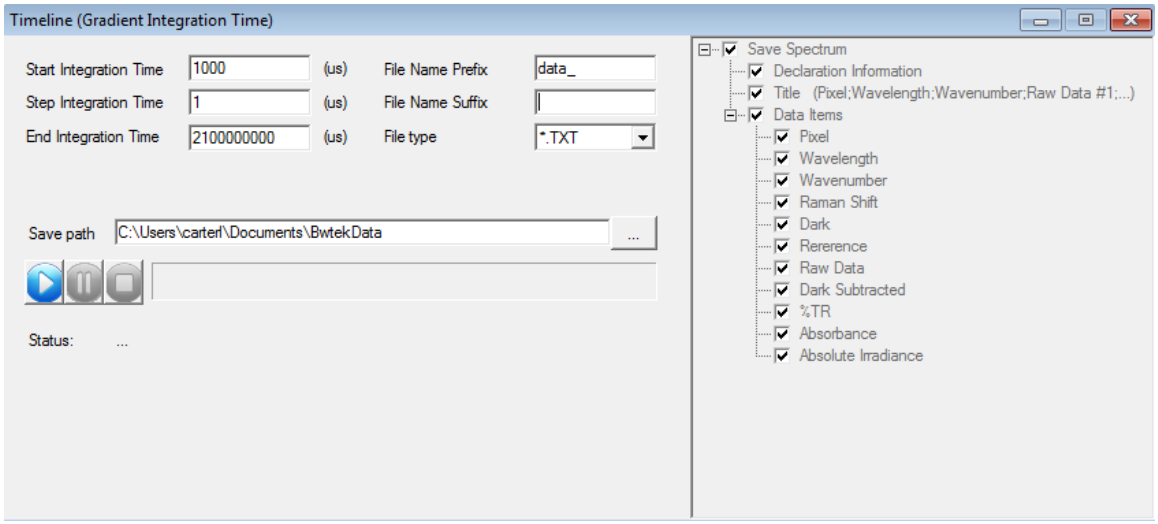
Output all spectra data into a spreadsheet after acquisition is completed

Note:

Burst Mode is currently available on Exemplar series spectrometer models with USB3 connectivity. USB2 connections can still be used for operation in Burst Mode but may result in a loss of performance such as limited Frames of spectra.

Timeline (Gradient Integration Time)

Click **Acquire** and select **Timeline**. Next click **Timeline (Gradient Integration Time)**, and a dialogue box will appear.

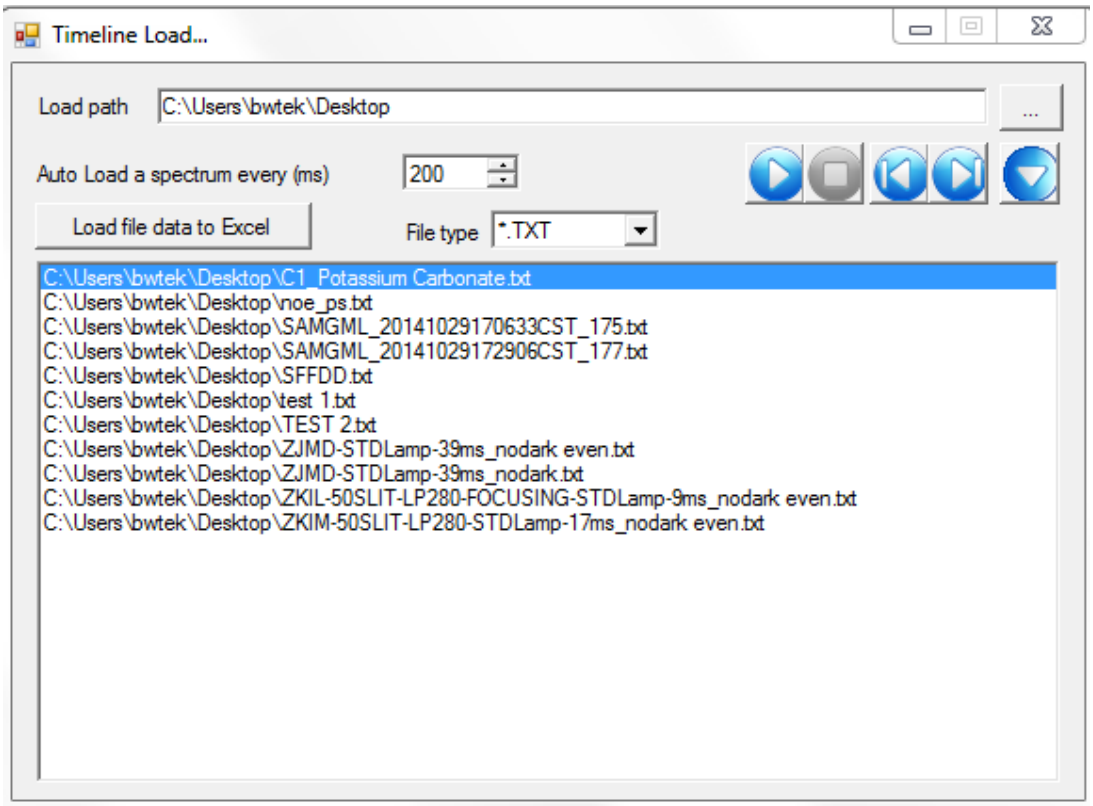


With gradient integration time, the integration time will change automatically according to the setting. When you finish one time acquisition, the integration time will automatically add a step time to your last integration time, which will then be your next acquisition integration time. You can input step time in the dialogue box labeled **Step Integration Time**. After each scan, the integration time will add this step time as the next acquisition integration time to be used.

Timeline Load

To automatically load the files that were saved previously, click **Acquire** and select **Timeline → Timeline Load**. Click **Load path** to select the folder location for the timeline data when the corresponding files are displayed on the Spectrum display panel.

- Click the  button to automatically load each data file individually.
- Click the  button to manually load the spectrum file forward, one at a time.
- Click the  button to manually load the spectrum file backwards, one at a time.
- Click the  button to resize the Timeline Load window.
- Click **File type** to select a saved file format and **Load file data to Excel** button to load all the data in the selected folder location into a Microsoft Excel spread sheet. Please do not try to access the Excel sheet until the data finished loading.



11.10 Wavelength Calibration Plug-in

This Plug-in is not intended to be used by end users. If your spectrometer is in need of calibration, please contact B&W Tek, Inc. at http://bwtek.com/support/. Wavelength Calibration must be conducted by B&W Tek, Inc. or OEM customers equipped with certified and traceable Light Standards and specialized calibration setups.

11.11 Raman Shift Calibration Plug-in

This Plug-in is not intended to be used by end users. Raman Shift Calibration must be conducted by B&W Tek, Inc., certified Service Center, or Distributor equipped with specialized calibration setups. B&W Tek, Inc. will not be responsible for any loss of your work and for any consequence if factory configuration is accidentally changed or corrupted.

11.12 Performance Test Plug-in

About Performance Test

The **Performance Test** is a procedure that evaluates a Raman instrument's performance with regards to accuracy and repeatability of instrument readings. This feature designed to be used when the software is communicating with a Raman instrument.

The performance test will validate a single peak of a reference standard spectrum. It will check if the peak is within acceptable limits: the peak's signal must be within 30% of the factory settings and the peak's shift must be no more than one pixel off of the factory settings, where the factory setting is a predefined reference standard spectrum.

It is recommended that a reference file be created as soon as possible with the new unit. Reference files are user created and do not come pre-loaded with the software. The performance test should be performed on a regular basis to ensure consistency in the performance and operation of the instrument.

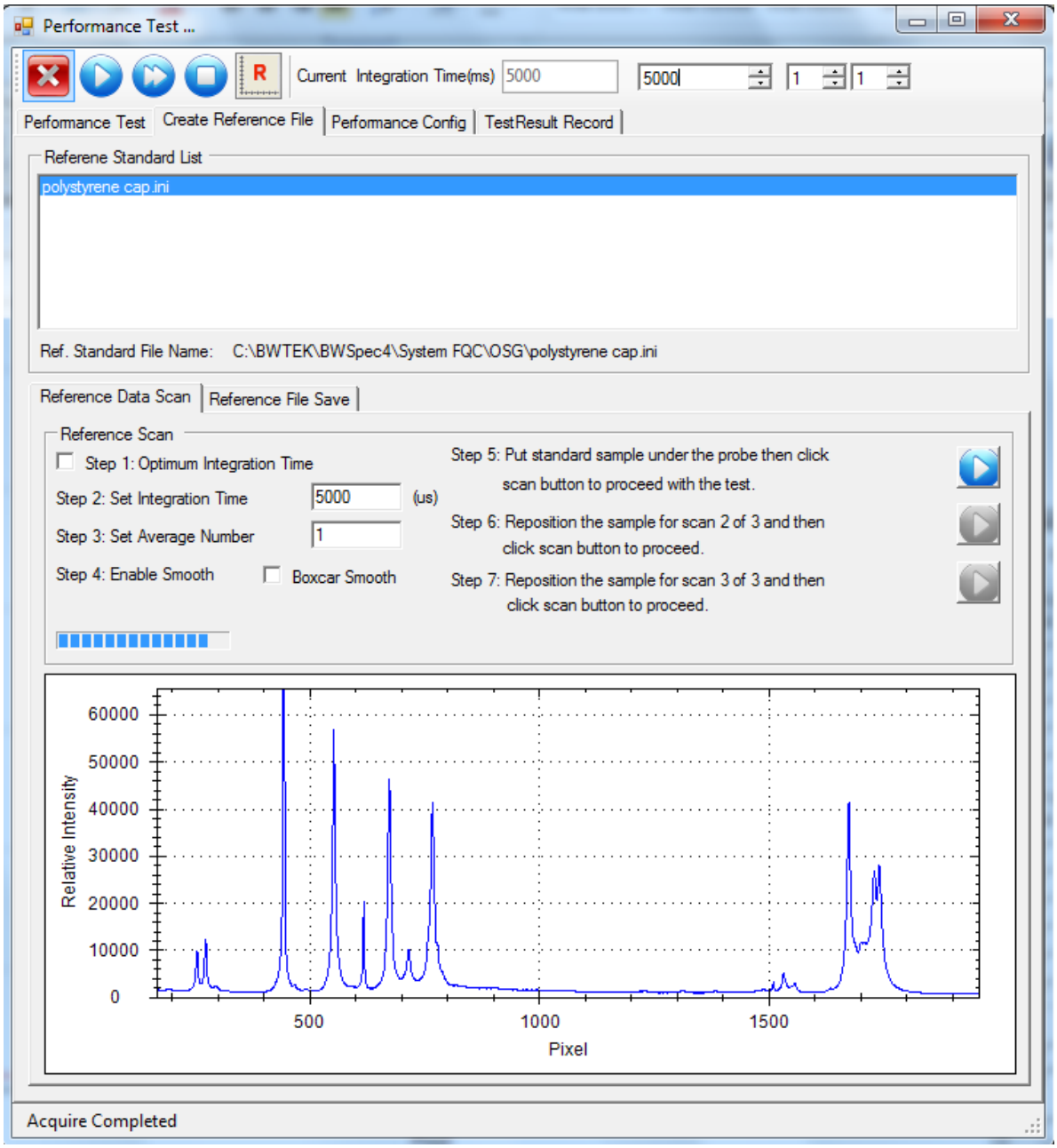
Location

Menu Bar → Setup

Create Reference File

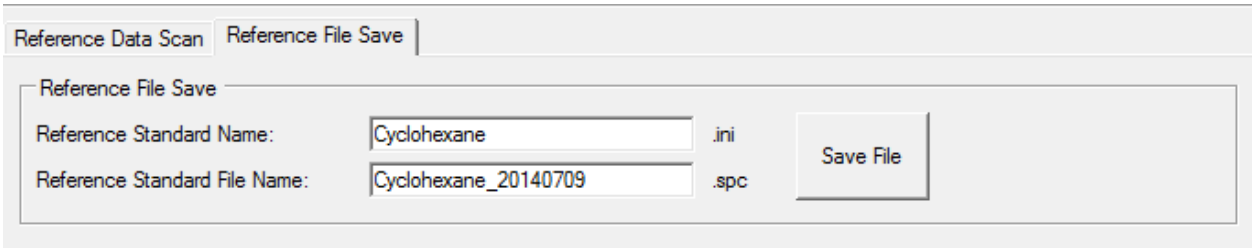
A new reference file may be created in this tab. The user is responsible for providing a Raman-active

sample with distinguished peaks. Use the Acquire Spectrum buttons and the Integration Time at the top of the window to determine the correct values for the Reference Data Scan. Make sure the peaks are visible and distinguishable. By selecting Optimum Integration Time, the system will determine the best integration time to use.



- Reference Data Scan

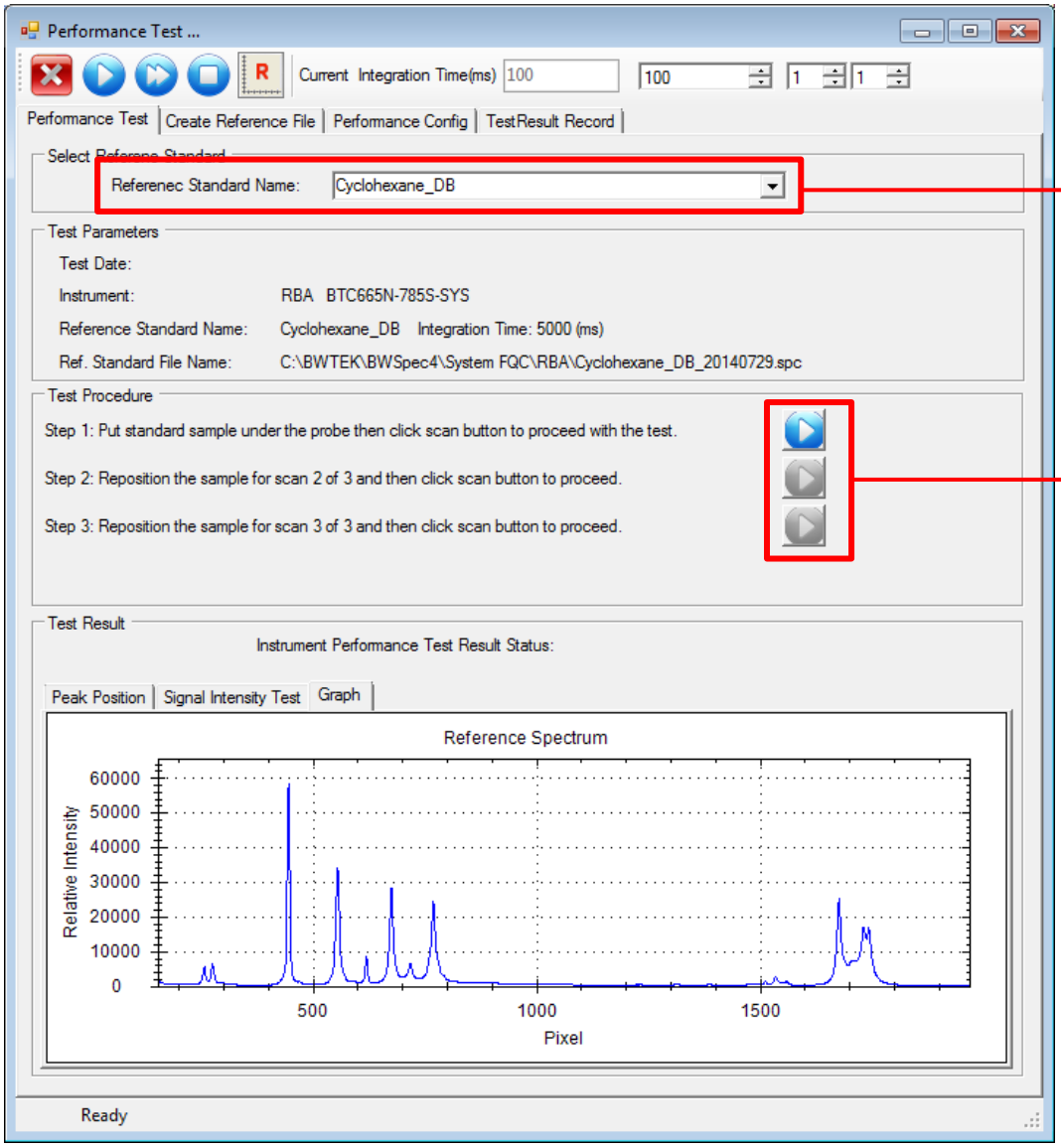
- Follow the steps and select the appropriate integration time (ms), average number, and the option of smoothing for the scan
- Take three scans of the Reference Sample in different positions.
- There is no overlay of each scan



- Reference File Save
  - After all three scans are taken, go to the Reference File Save to create a standard File Name
  - The file will automatically be stored in C:\BWTEK\BWSpec4

Performance Test

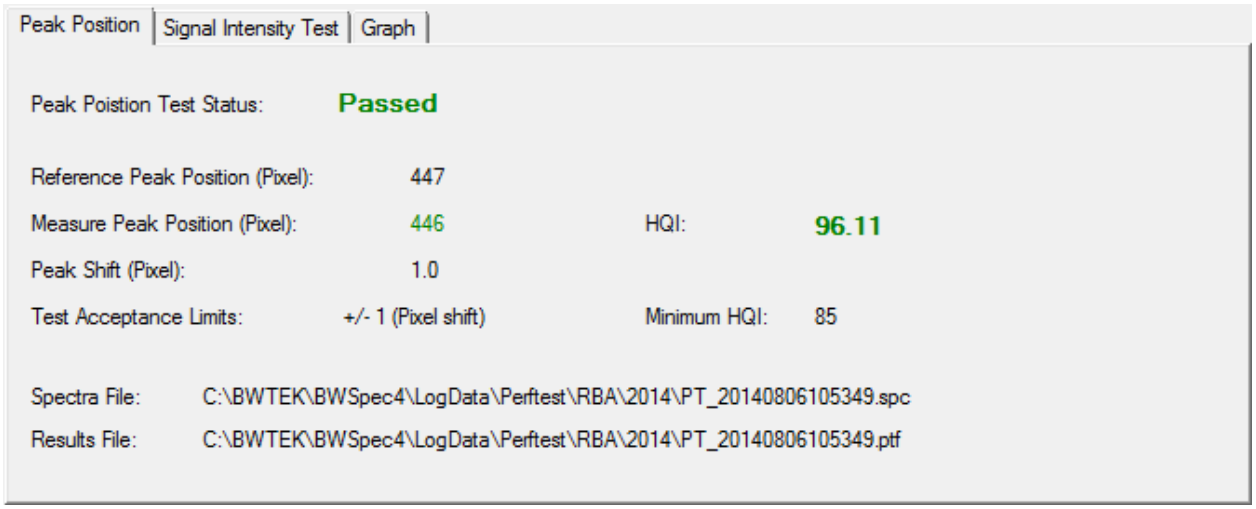
Click **Setup** then **Performance Test** and a dialogue box will appear. The **Performance Test** tab allows the user to select a pre-configured reference standard. A reference standard may be created in the **Create Reference File** tab.



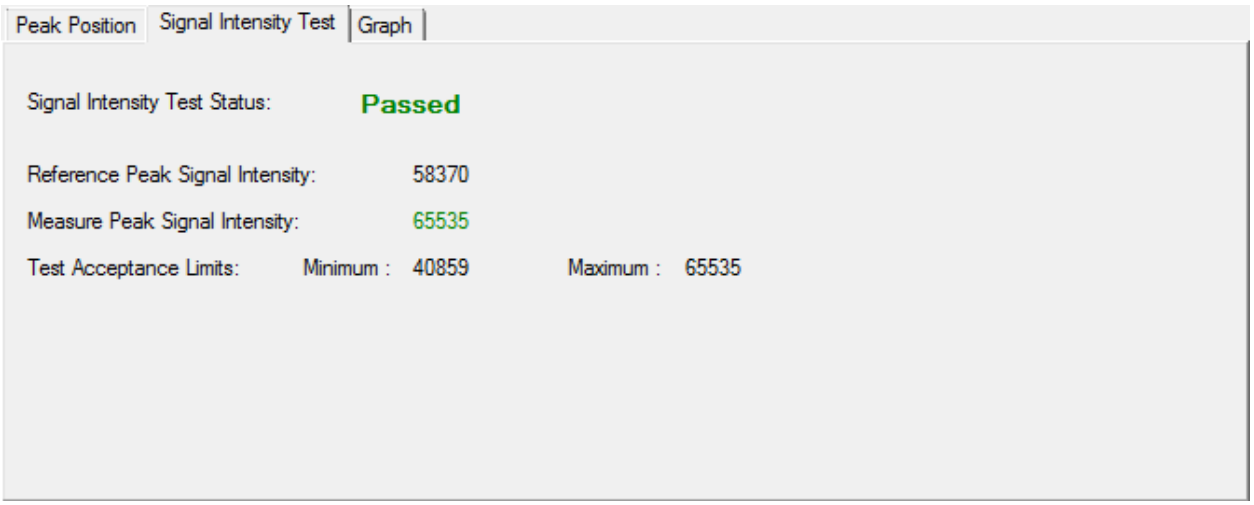
Select a pre-configured reference standard

Scan the reference sample with the probe three different times at different positions on the sample

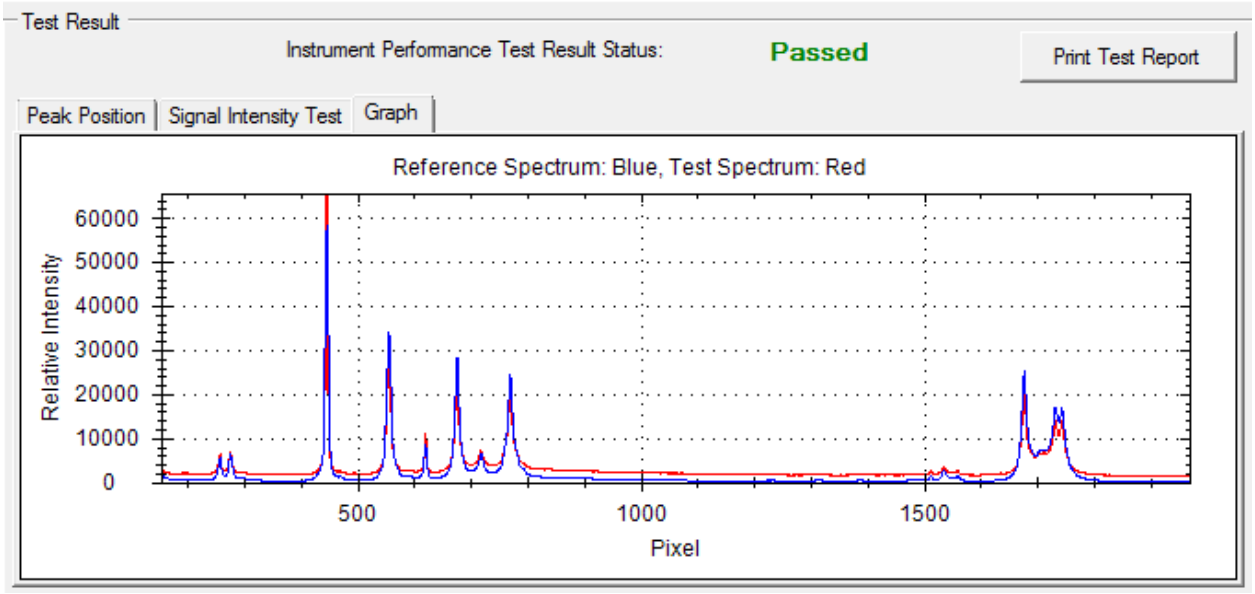
- Select Reference Standard
  - Use the same reference standard that is going to be used as a sample in the performance test. The default is polystyrene.
- Test Parameters
  - Test Date: will be filled in at the conclusion of the test.
  - Instrument: Is the Raman unit that is currently being used for testing and is automatically filled.
  - Reference Standard name: Is the name of the reference standard selected; this will also show the integration time when the Reference Standard was made.
  - Ref. Standard File Name: The file name and location of the reference file.
- Test Procedure
  - Follow each of the steps to take three scans of the Reference Standard at different positions.
  - The integration time is pre-selected based on the Reference Standard.
- Test Result
  - After the three sample scans are taken the software will compare the scans to the reference sample.
  - The shift between the measured peak and predefined reference peak is no more than one pixel and the measured peak's signal is within 30% of the predefined reference peak's intensity (factory settings).
  - The performance test will fail if the peak position, signal intensity test or HQI fails. In such cases, the instrument should not be used for measurements since it cannot provide consistent readings.
  - Once the test is completed, the collected spectrum and test results are saved in the files. The spectrum is stored in a Grams SPC data file format (*.spc), while the test results are saved in a BWTek proprietary binary file format (*.ptf). These can be viewed in the **Test Result Record** tab.



- Peak Position
  - Displays the peak position of the Reference Sample and the Measured Sample and the acceptable limits of the test including pixel shift and HQI.



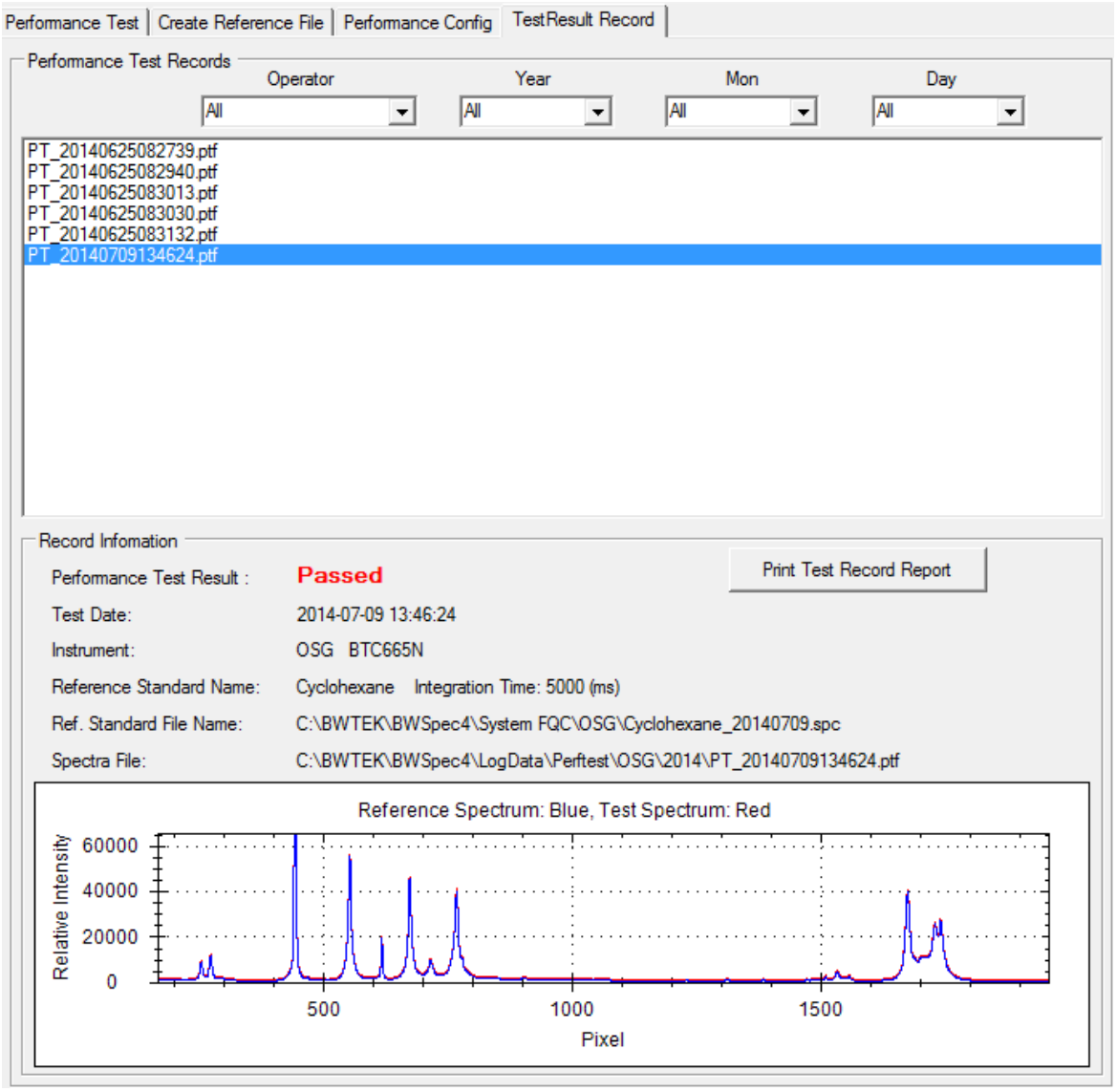
- Signal Intensity Test
  - Displays the peak signal intensity of the Reference Sample and the Measured Sample and the acceptable limits of the test.



- Graph
  - Displays the Spectrum of the Reference Sample and the Measured Sample as a graph of relative intensity vs pixels.

Test Result Record

The spectrum is stored in a Grams SPC data file format (*.spc), while the test results are saved in a BWTek proprietary binary file format (*.ptf).

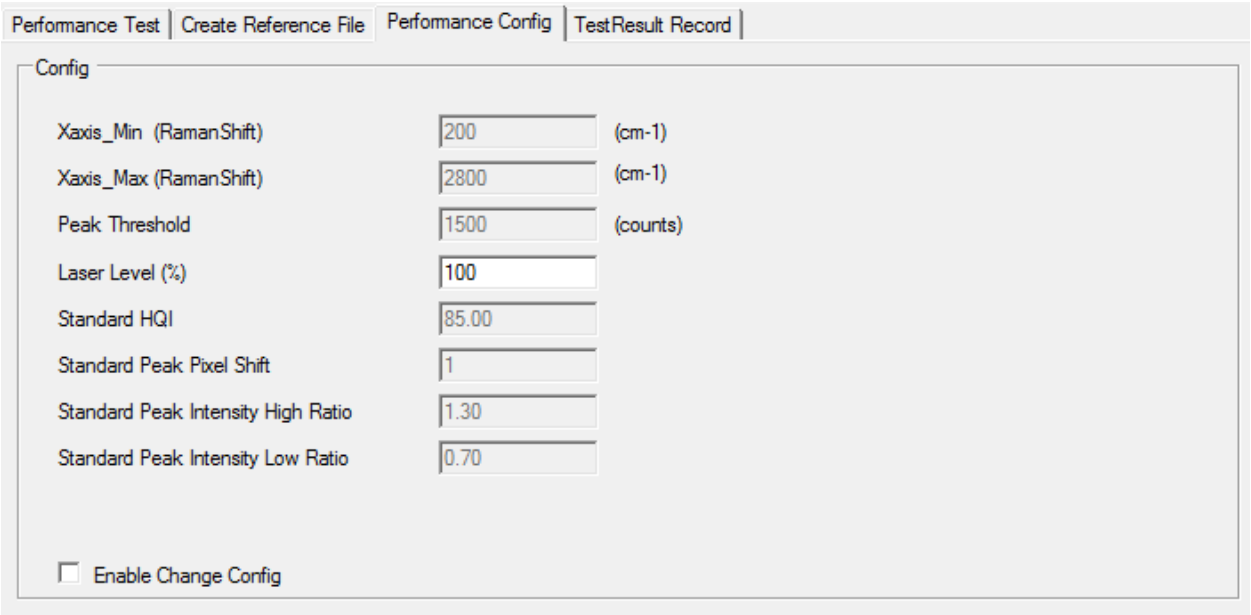


- Performance Test Records
  - The test records may be searched by Operator or by Date
  - Select the file to view its information
- Record Information
  - The results of the Performance test are displayed
  - Click the **Print Test Record Report** to view and print the record.

Performance Config

- Config (Configuration)

- This displays the configuration of the Raman instrument in the performance test.
- When the Enable Change Config box is checked the top four values can be changed.
- We recommend that only our Advanced users attempt to change the values.



11.13 System Response Standardization

About System Response Standardization

Previously named as "Laser Power Calibration" in BWSpec4.03. This Plug-in is not intended to be used by end users. System Response Standardization must be conducted by B&W Tek, Inc., certified Service Center, or Distributor equipped with specialized calibration setups. B&W Tek, Inc. will not be responsible for any loss of your work and for any consequence if factory configuration is accidentally changed or corrupted.

12 COLOR MEASUREMENT

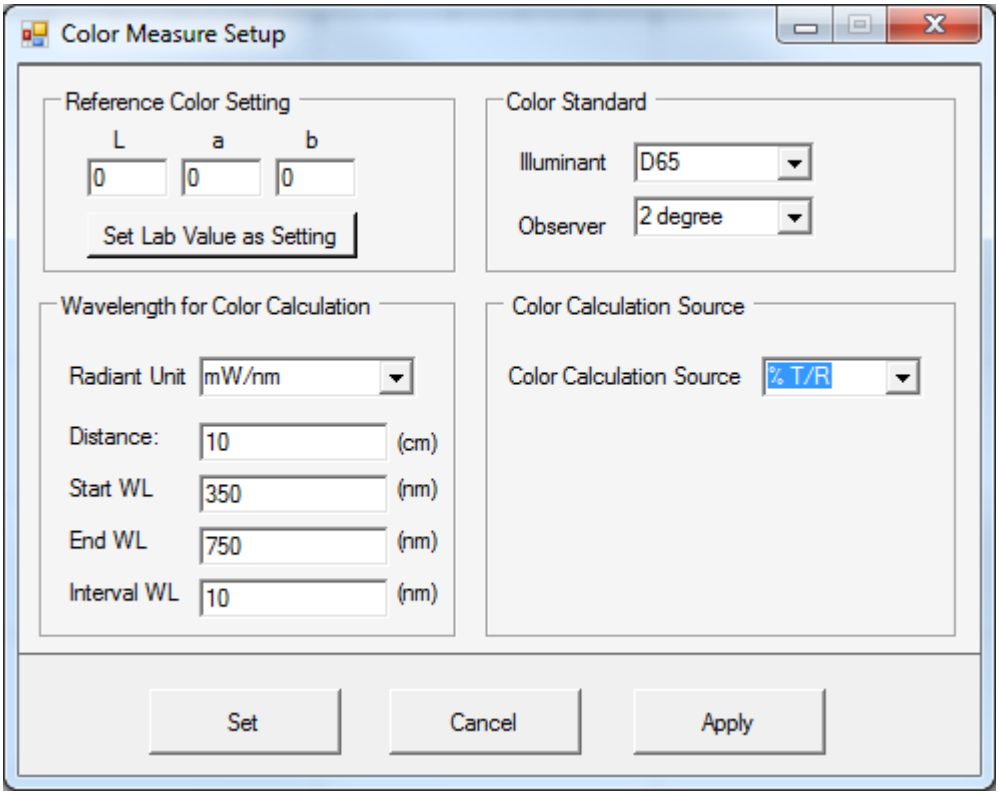
About Color Measurement

The color measurement characterizes an object (for example, illumination source) in terms of its chromaticity and radiometry. Chromaticity refers to the quality of the object regardless of its luminance, while radiometry measures the radiant energy or electromagnetic energy of the object.

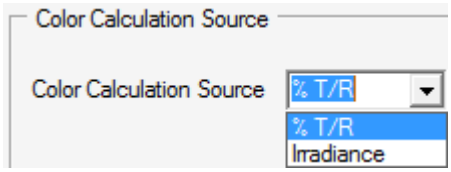
Note: *The color measurement result shown in the* ***Color Chart*** *tab is only available when the spectrometer in use has a spectral range that incorporates spectral values between 400 nm and 700 nm.*

Before performing a color measurement, the system should be normalized by taking a Reference scan or irradiance calibrated.

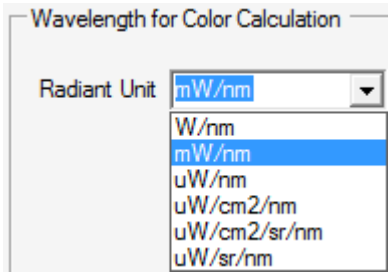
From the Menu Bar, select Setup → Color Setup. A dialog box will display, where the settings for color measurement can be adjusted.



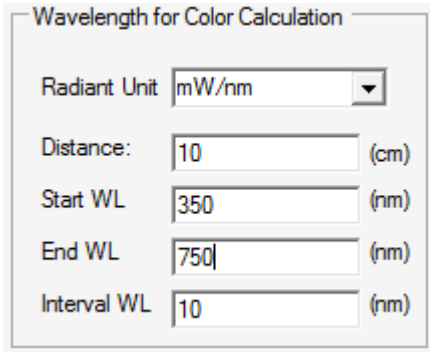
- Inside the box for **Color Calculation Source**, a dropdown menu will allow users to choose between **%T/R** or **Irradiance** for the measurement.



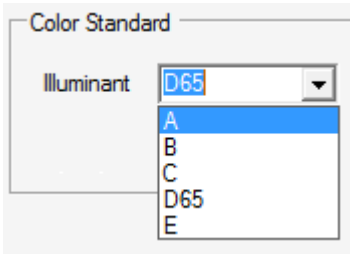
- **Radiant Unit** can be selected from the **Wavelength for Color Calculation** box:

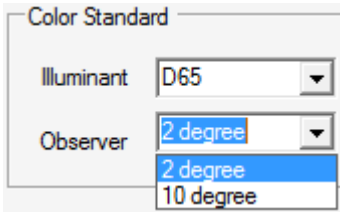


- Choose **Distance**, **Start WL**, **End WL**, and **Interval WL** for the measurement.



- Select your color measurement standard from the **Color Standard** box, including **Illuminant** and **Observer**.

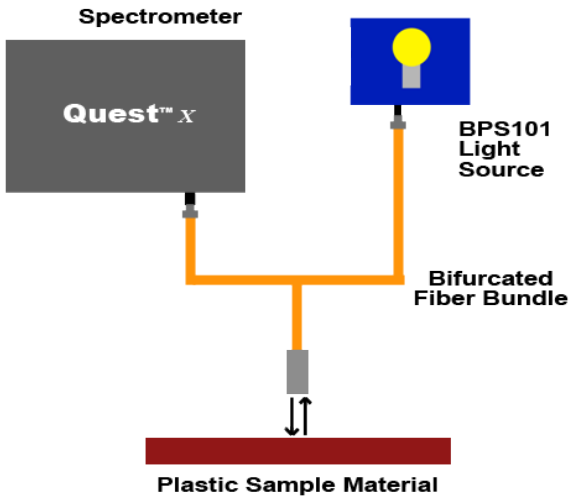




Reference and Dark Scan for %T/R Measurement

To perform a %T/R based color measurement, a white reflectance standard in reflectance setup and a stable light source covering the color range should be used. Light sources such as the BPS101 and BPS120 from B&W Tek, Inc. are suitable candidates.

As the apparent color of reflective objects depends upon both the spectral response of the spectrometer and the spectral output of the illumination source, a reflectance reference scan should be performed often so that the error due to the lamp drift is minimized.



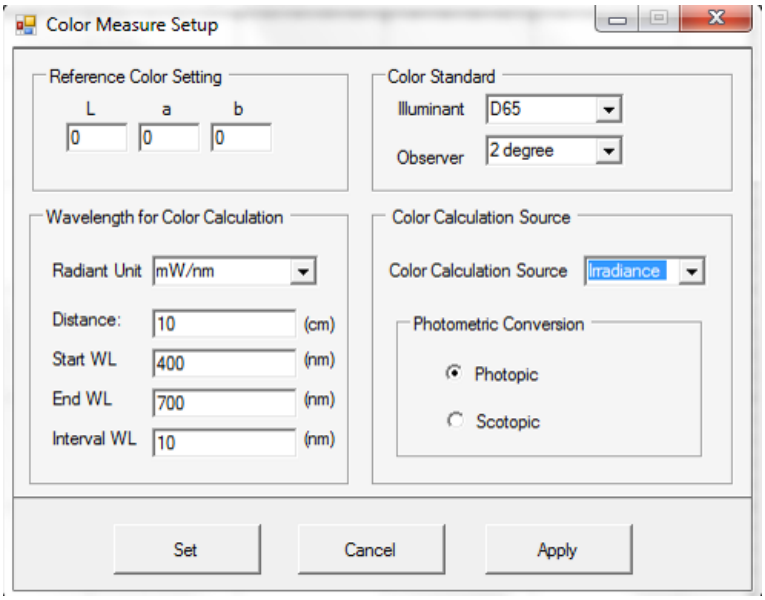
Connect the light source and the spectrometer via a fiber reflectance probe.
Turn on the light source and allow it to warm up.

- Perform a reference scan.
- Perform a dark scan using the same integration time as the reference scan. Make sure to place the probe onto an absorbing black material or physically block the light from entering into the probe for the dark scan.

Irradiance for Color Measurement

To perform an irradiance calibration based color measurement:

- From the Menu Bar, select **Setup** → **Color Setup**. A dialog box will display, where the settings for color measurement can be adjusted. Inside the box for **Color Calculation Source**, select **Irradiance** for the measurement.

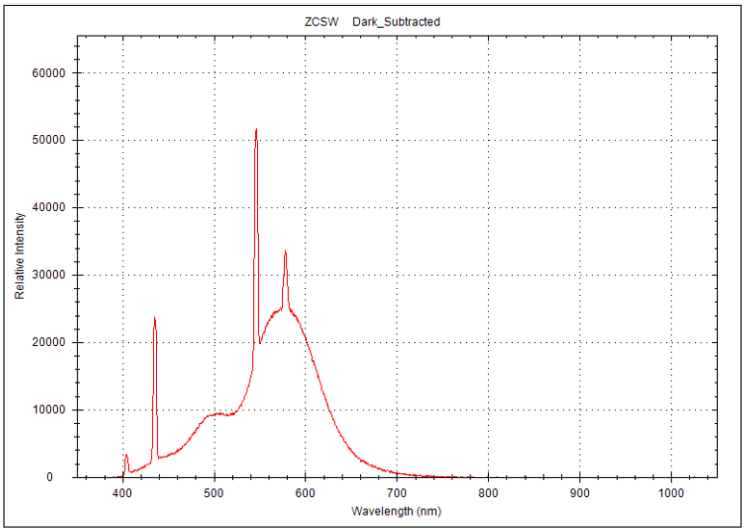


- Enable irradiance calibration from **Option** → **Enable /Disable Irradiance Correction**, and select the corresponding irradiance correction ratio file (Ratio1_ccode.txt).
- Select **Photopic** or **Scotopic** Photometric Conversion option to calculate perceived color.
- Click Apply.

Color Analysis

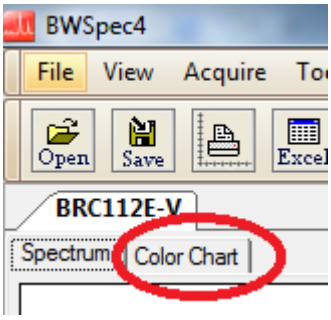
To acquire sample color data:

- Place the probe onto the desired sample to be measured.
- Acquire data scan on the sample material intended for color analysis.

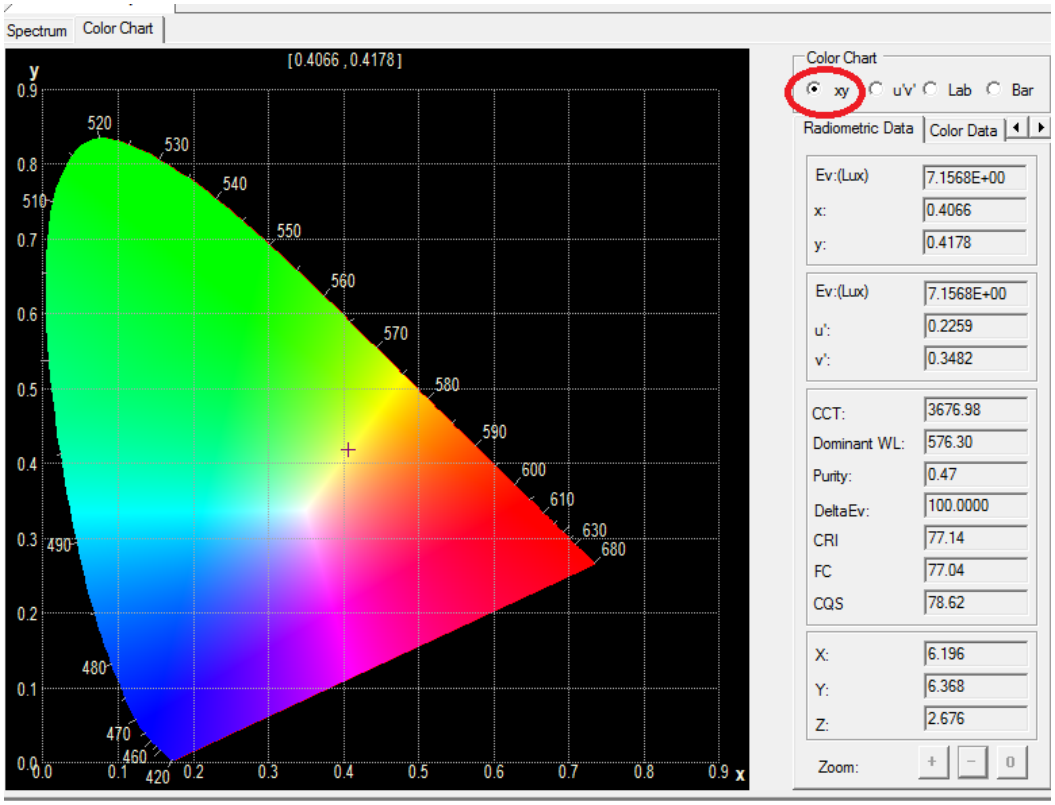


Data Display

Click the **Color Chart** tab for the chromaticity diagram and data display.
Options for four different CIE color spaces are available:

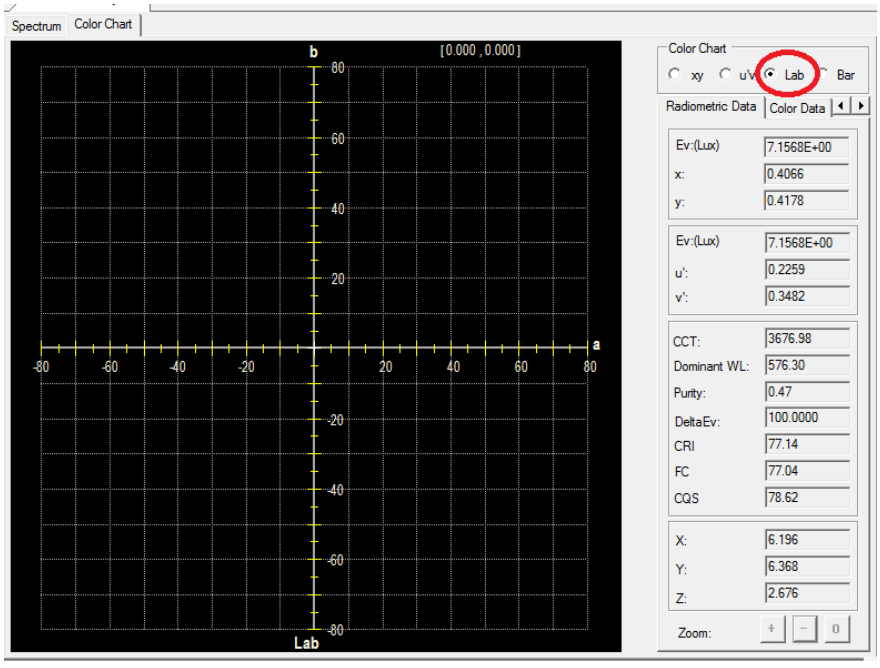


- CIEXYZ color space

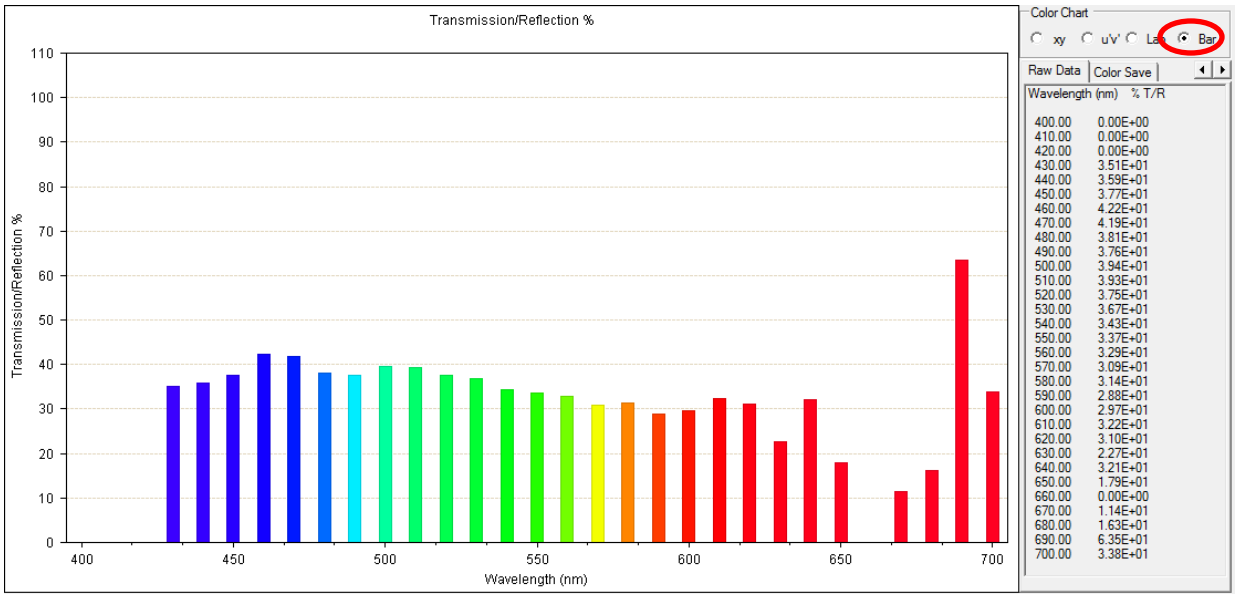


- CIELUV color space

- CIELAB color space

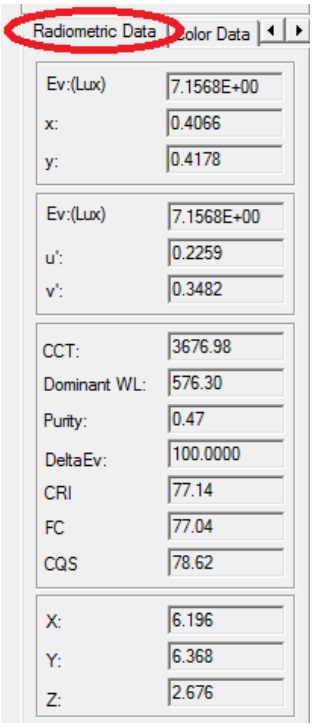


- Color Bar

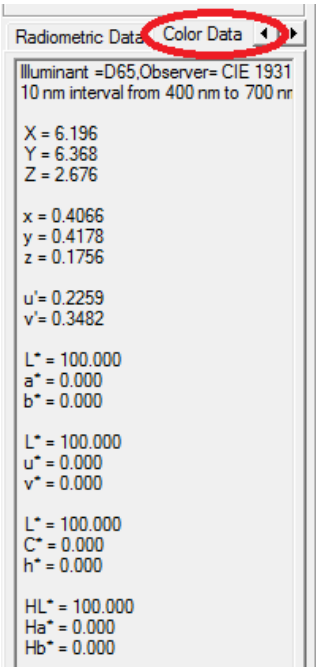


The radiometry and chromaticity data is displayed in five categories.

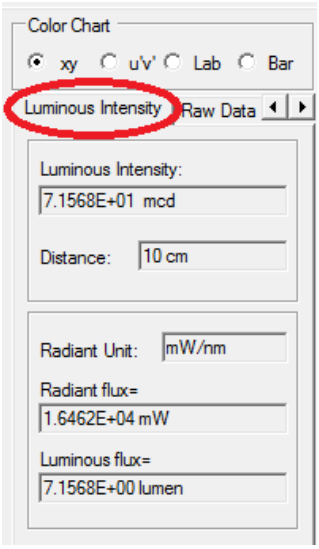
- Radiometric Data



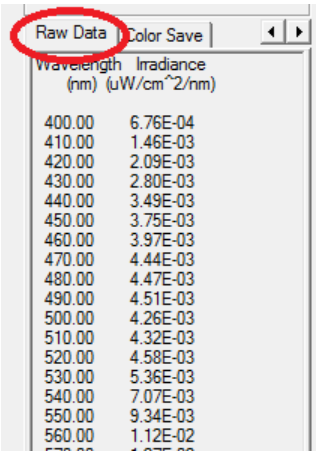
- Color Data



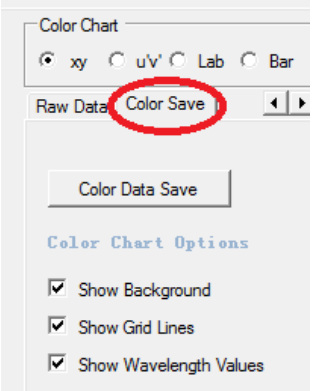
- Luminous Intensity



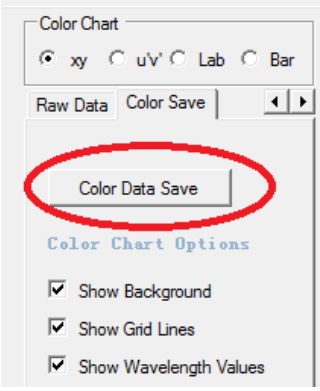
- Raw Data



- Color Save

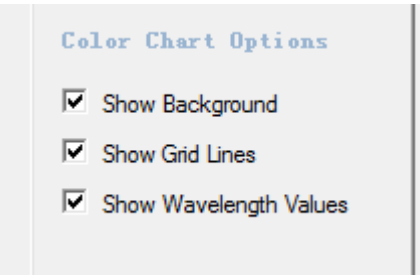


Click **Color Data Save** to save the color data as a BWSpec Color TXT file (.*txt).



There are three **Color Chart Options** available for color diagram settings:

- Show Background
- Show Grid Lines
- Show Wavelength Values



13 IRRADIANCE RATIO FILE DATA DEFINITION

Ratio1_ccode.txt File details and explanation of data:

RATIO1_ccode.TXT INFORMATION	EXPLANATION
BWSpec Version=BWSpec 4.02	Software Version used when the ratio file is created
Irradiance Ratio File Version=1.0	Ratio File Version
CCode=XXX or XXXX	C-code of Unit
Int.Time=1100	Integration Time used when the ratio file was created
Distance=75	Distance used for the ratio file creation from the calibration light source to the light input optics aperture
Lamp Name=350-780.DAT	Name of Lamp Data File Used
Lamp StartWL=350	Starting WL of Lamp Data File Used
Lamp EndWL=780	Ending WL of Lamp Data File Used
Lamp IncWL=10	Increments of WL interval from Start WL to End WL
Lamp Measure Distance=75	Distance for which Lamp Data file was created
Lamp Unit Index=2	Index 0 =W/cm^2/nm; Index 1 = mW/cm^2/nm; Index 2 = uW/cm^2/nm; Units will match the Lamp Data file and the units of the irradiance data
Lamp Coefs Order=7	Order of curve fit for Regression when creating the ratio file
Coefs_C0=-102.802359649056	Curve Fit Values
Coefs_C1=1.38796702045458	Curve Fit Values
Coefs_C2=-0.00789398471358277	Curve Fit Values
Coefs_C3=2.45424259313939E-5	Curve Fit Values
Coefs_C4=-4.51571710685247E-8	Curve Fit Values
Coefs_C5=4.93405335866037E-11	Curve Fit Values
Coefs_C6=-2.9685358194907E-14	Curve Fit Values
Coefs_C7=7.588143959E-18	Curve Fit Values
irrands_yaxis_min=0	Y-axis minimum Display Scales Settings value
irrands_yaxis_max=4.38087481104945	Y-axis maximum Display Scales Settings value
irrands_DispWLMin=350	X-axis minimum wavelength Display Scales Settings
irrands_DispWLMax=780	X-axis maximum wavelength Display Scales Settings
start_wv_irrands=350	Start WL for Irradiance Calibration (should match Lamp StartWL)
end_wv_irrands=780	End WL for Irradiance Calibration (should match Lamp EndWL)
interval_wv_irrands=10	Increments of WL interval from Start WL to End WL (should match Lamp IncWL)
Pixel ; Ratio ; Ratio	Pixel number ; Ratio (Linearity Correction disabled) ; Ratio (Linearity Correction enabled)
272;5.88055754188743E5;4.87368884634631E-5	
273;6.81553361643328E-5;5.60679388523222E-5	
274;7.19969136787624E-5;5.9194063207757E-5	

14 DEFINITION OF IRRADIANCE DATA FILE FORMAT

Certified Standard Lamp data file example:

Start WL=250 ---------- **starting wavelength (nm)**
End WL=2500 ---------- **ending wavelength (nm)**
Distance=50 ---------- **distance at which lamp data is generated**
units=mW/cm^2/nm ---------- **lamp data unit, choice of: W/cm^2/nm; mW/cm^2/nm; uW/cm^2/nm**
S-1169 ---------- **designation of the standard lamp (name, serial number …etc.)**
5 ---------- **starting flag**
250 ---------- **flag for starting wavelength (nm)**
2500 ---------- **flag for ending wavelength (nm)**
10 ---------- **increment of wavelength per data point**
0.760E-05 ---------- **standard lamp irradiance data at wavelength = 250 nm (250+0*10)**
1.788E-05 ---------- **standard lamp irradiance data at wavelength = 260nm (250+1*10)**
3.156E-05 ---------- **standard lamp irradiance data at wavelength = 270nm (250+2*10)**
…..
…..

3.795E-03 ---------- **standard lamp irradiance data at wavelength = 2500nm (250+225*10)**
5 ---------- **ending flag**

Appendix A: Declaration of Text File

The text file has two block areas: flag block and data block. The flag block contains acquisition parameters and settings. The data block contains the acquired spectra data. The flag block length may vary and an example of text file (flag block highlighted by yellow) is shown below.

To read all data, user should

1. Find line “Pixel; Wavelength; Wavenumber; Raman Shift; Dark; Reference; Raw data #1;Dark Subtracted #1;%TR #1;Absorbance #1;Irradiance (lumen) #1”;
2. Read from next line , it is the data of pixel 0
3. Continue to read the next [pixelnumber-1] line

File Version;BWSpec4.03_20_C //BWSpec4 version that saved file
Date;2015-07-16 19:56:56 //saved file date
title;BRC112 //spectrometer title name that saved data
model;BRC112 //spectrometer model
c code;ABC //spectrometer c code
operator; //operator that saved file
port1;0 //port number if spectrometer is RS232 interface (obsolete)
baud1;3 //baudrate index if spectrometer is RS232 interface (obsolete)
pixel_start;0 //start pixel
pixel_end;2047 //end pixel
step;1 //the data index step
units;0 // Spectrometer x-axis unit (0=Pixel, 1=wavelength, 2=wavenumber, 3=Raman shift)
bkcolor;16777215 //Display Chart background color RGB value
show_mode;0 //Spectrometer display option 0=RawData,1=Dark,2=Reference,3=Dark Subtracted, 4=%TR, 5=Absorbance,6=Absolute Irradiance)
data_mode;0 // Transmit data mode, 0=Binary data mode, 1=ASCII data mode (obsolete)
pixel_mode;0 // Display Chart Mode .0=normal, 1=Pixel Monitoring (obsolete)
intigration times(ms);1 //Spectrometer integration time of saved data
average number;1 //Spectrometer average number of saved data
time_multiply;1 // Integration time multiplier
spectrometer_type ;17 // Spectrometer model id number
yaxis;1 // Display Chart Y-axis Setting (0=Auto, 1=Manual)
yaxis_min;0 // Display Chart Y-axis Minimum, if Y-axis setting is Manual
yaxis_max;65535 // Display Chart Y-axis Maximum, if Y-axis setting is Manual
xaxis;1 // Display Chart X-axis Setting (0=Auto, 1=Manual)
xaxis_min;71 //Display Chart X-axis Minimum, if X-axis setting is Manual
xaxis_max;1949 // Display Chart X-axis Maximum, if X-axis setting is Manual

irrands_DispWLMin;100 // Display Chart X-axis Minimum, if X-axis setting is Manual and show_mode=6
irrands_DispWLMax;1000 // Display Chart X-axis Maximum, if X-axis setting is Manual and show_mode=6
yaxis_min_6;0 // Display Chart Y-axis Minimum, if Y-axis setting is Manual and show_mode=6
yaxis_max_6;0 // Display Chart Y-axis Maximum, if Y-axis setting is Manual and show_mode=6
irradiance_unit;0 //absolute irradiance data unit (0=W/cm^2/nm , 1=mW/cm^2/nm, 2=uW/cm^2/nm)
Color_Data_Flag;0 // data source for color calculation (0=%TR, 1=irradiance)
Color_StartWL;400 // Start wavelength of color calculation
Color_EndWL;700 // End wavelength of color calculation
Color_IncWL;10 // Step wavelength of color calculation in nm
power_unit_index;1 // Photometry Power Unit [0=(W/nm), 1=(mW/nm), 2=(Uw/nm), //3=(uW/cm2/nm), 4=(uW/cm2/sr/nm), 5=(uW/sr/nm)]
photometric_index;0 // Photometric Conversion (0=Photopic, 1=Scotopic)
Illuminant_index;3 // Illuminant of color, (0=A, 1=B, 2=C, 3=D65, 4=E)
observer_index;0 //Observer of color, (0=2 degree, 1=10 degree)
lab_l;0 // Reference Color setting , l of Lab
lab_a;0 // Reference Color setting, a of Lab
lab_b;0 // Reference Color setting, b of Lab
radiometric_flag;0 // Photometric or Photopic or Scotopic flag (0= Photometric, 1= Photopic, 2= Scotopic)
coefs_a0;732.046000000089 // The coefficients (A0) of Pixel convert to Wavelength
coefs_a1;0.256049999999959 // The coefficients (A1) of Pixel convert to Wavelength
coefs_a2;-4.90450000000253E-05 // The coefficients (A2) of Pixel convert to Wavelength
coefs_a3;8.18407999999919E-10 // The coefficients (A3) of Pixel convert to Wavelength
coefs_b0;-29079.7965557277 // The coefficients (B0) of Wavelength convert to Pixel
coefs_b1;97.1304303120123 // The coefficients (B1) of Wavelength convert to Pixel
coefs_b2;-0.111241614377263 // The coefficients (B2) of Wavelength convert to Pixel
coefs_b3;4.46263025785099E-05 // The coefficients (B3) of Wavelength convert to Pixel
coefs_r0;325.634643285781 // The coefficients (R0) of Pixel convert to Raman shift
coefs_r1;-0.371893845826952 // The coefficients (R1) of Pixel convert to Raman shift
coefs_r2;0.000853220967122155 // The coefficients (R2) of Pixel convert to Raman shift
coefs_r3;3.37498265875635E-08 // The coefficients (R3) of Pixel convert to Raman shift
coefs_j0;-112.640169933252 // The coefficients (J0) of Raman shift convert to Pixel
coefs_j1;1.91244080985067 // The coefficients (J1) of Raman shift convert to Pixel
coefs_j2;-0.000774766051834558 // The coefficients (J2) of Raman shift convert to Pixel
coefs_j3;1.20204126521674E-07 // The coefficients (J3) of Raman shift convert to Pixel
enable_coefs_r;0 //Use coefficient R0..R3 Enable. (0=Disable, 1=Enable)
all_data_save;1 //all pixel data saved (0=No, 1=Yes)
select_option;-1 //(obsolete)
interval_time;1 //(obsolete)

pixel_num;2048 //total pixel number
sel_pixel_start;31 //start pixel for calculate RMS (obsolete)
sel_pixel_end;2047 //end pixel for calculate RMS (obsolete)
sel_pixel_delta;1 //interval pixel for calculate RMS (obsolete)
dark_compensate;0 //Dark compensate Enable. (0=Disable, 1=Enable)
dark_compensate_value_1;0 // (obsolete)
dark_compensate_value_2;0 // (obsolete)
dark_compensate_value_3;0 // (obsolete)
monitor pixel_0;0 // (obsolete)
monitor pixel_1;0 // (obsolete)
monitor pixel_2;0 // (obsolete)
monitor pixel_3;0 // (obsolete)
monitor pixel_4;0 // (obsolete)
monitor pixel_5;0 // (obsolete)
vertical_select_flag;0 // (obsolete)
vertical_line3;0 // (obsolete)
vertical_line4;0 // (obsolete)
vertical_line3_wv;349.605625506025 // (obsolete)
vertical_line4_wv;349.605625506025 // (obsolete)
vertical_line_flag;0 // (obsolete)
vertical_line_ratio;0 // (obsolete)
laser_wavelength;784.5 // Raman excitation wavelength (nm), not used if enable_coefs_r=1
laser_powerlevel;0 //laser power
overlay_js;0 //(obsolete)
Relative Intensity Correction Flag;0 //1=use relative intensity correction, 0=not use relative intensity correction

Pixel;Wavelength;Wavenumber;Raman Shift;Dark;Reference;Raw data #1;Dark Subtracted #1;%TR #1;Absorbance #1;Irradiance (lumen) #1;

0; ; ; ;1439.0000;65535.0000;1793.0000;354.0000;0.0000;0.0000;0.0000; //pixel 0 ‘s data

1; ; ; ;1439.0000;65535.0000;1793.0000;354.0000;0.0000;0.0000;0.0000; //pixel 1 ‘s data

2; ; ; ;1234.0000;65535.0000;1307.0000;73.0000;0.0000;0.0000;0.0000; //pixel 2 ‘s data

3; ….

